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Comparison of high order finite element and discontinuous Galerkin methods for phase field equations: Application to structural damage

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ABSTRACT

Phase field equations are used to model a wide range of multiphase problems such as separation of fluids, solidification, viscous fingering, fracture and fatigue. A wide variety of methods to numerically solve phase field equations can be found in the literature. In particular, high order methods are an effective option when accuracy improvement is desired. In the first part of this work, we analyze the accuracy and computational efficiency of the high order finite element method (FEM) and discontinuous Galerkin (DG) method applied to the second-order Allen–Cahn (AC) and fourth-order Cahn–Hilliard (CH) equations. Several schemes for time integration are used for these equations. The explicit schemes are the forward Euler, classical fourth-order Runge–Kutta (RK4) and the strong stability preserving ten stages fourth-order Runge–Kutta (RKSSP-10,4) described in Gottlieb et al. (2011). The backward Euler and trapezoidal implicit methods are adopted in the full and semi implicit schemes, as proposed in Eyre (unpublished). Manufactured solutions for one dimensional problems are used in order to evaluate the errors and to compare the different numerical methods. By choosing an adequate discretization for AC equations resulting from the previous analysis of the first part of the work, in the second part, we propose a numerical semi implicit scheme to solve the damage and fracture model described in Boldrini et al. (2016). This procedure employs the FEM for spatial discretization, the Newmark method for time integration of the kinematics equation and the backward Euler for the damage phase field evolution. Finally, results for 2D benchmark tests are presented for the fracture phase field model and the convergence to a sharp crack for a small width of the damage phase field layer γ is verified.

1. Introduction

Phase fields are the key ingredients of a successful modeling strategy for situations involving appearance and evolution of several kinds of interfaces. In this methodology such interfaces are considered transition layers instead of sharp fronts, and their localization is given by specific level sets of the considered phase field. This approach has several advantages when compared to the sharp interface approach. From the physical point of view, it is possible to derive thermodynamically

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consistent models for complex situations, while it is much more difficult to do so with sharp interfaces. In general, it is not easy to obtain consistent governing equations for the kinematics of the sharp interfaces. From the point of view of numerical simulations, phase field models are more adequate since evolution of complex interface geometry can be obtained, while the corresponding numerical simulations for sharp interfaces are much more difficult, sometimes impossible.

The first phase field model was originally developed in 1958 by John W. Cahn and John E. Hilliard [1], in order to describe the process of phase separation of two fluids. They developed the fourth-order nonlinear Cahn–Hilliard (CH) equation for a phase field variable $\varphi(x, t)$ related to the continuous concentration function of the fluids in the mixture. The range of the variable is $-1 \leq \varphi(x, t) \leq 1$, where $\varphi = 1$ indicates the region occupied by fluid A and $\varphi = -1$ indicates the region occupied by fluid B. The fluids are separated by a transition region defined by a diffuse interface thickness parameter γ such that $-1 < \varphi < 1$. An alternative proposal was presented by Kim [2], with a phase field $\varphi(x, t)$ in the range $0 \leq \varphi(x, t) \leq 1$. In 1972, Sam Allen and John Cahn [3] developed a second-order nonlinear partial differential equation, called the classical Allen–Cahn (AC) equation, describing the phase separation in iron alloys. We remark that both equations, AC and CH, are based on the Ginzburg–Landau free energy functional [2,4]. However, while the CH equation is conservative, the classical AC equation is non-conservative (there is, however, a modified version of the AC equation using Lagrange multipliers which is conservative; see [2]).

The concepts of the original CH and AC equations were extended to a great variety of applications along the time such as, biology and medicine, with the study of tumor growth [5] and vesicle-fluid iteration [6], and in engineering with the study of fluid–structure interaction problems [7], crack propagation [8–10], damage and fatigue models [11,12] and others.

Due to the diversity of applications and their importance, different methods have been used to numerically solve the AC and CH equations. For spatial discretization, there are low order approximations based on the finite difference method (FDM) [13] and the finite volume method (FVM) [14]. For high order methods, there are the finite element method (FEM) [15], the discontinuous Galerkin method (DG-FEM) [16], the local discontinuous Galerkin method (LDG-FEM) [17,18] and the least square spectral element method [19]. There are also many procedures for time discretization including low and high order methods such as forward Euler and the fourth-order Runge–Kutta (RK4), respectively [20]. Some of the spatial discretization methods may lead to great instability for the explicit time marching schemes. To solve this difficulty, Gottlieb, Ketcheson and Shu in [21] proposed the strong stability preserving fourth-order Runge–Kutta procedure with ten stages (RKSSP(10,4)). Although using more stages, this procedure allows larger time steps still preserving stability. On the other hand, Eyre treated the diffusive terms implicitly in [22] and called the procedure as the semi implicit Euler method.

Initially, this work intends to evaluate the efficiency of spatial and time discretization methods by numerically solving the AC and CH phase field equations. For this purpose, the computational time and approximation errors are evaluated for a manufactured solution by application of the FEM and DG method. The time integration methods considered are the forward Euler, RK4, RKSSP (10,4), backward Euler and trapezoidal. The combination of the above methods provides the explicit, semi implicit and fully implicit schemes. The last one considers a tangent matrix numerically evaluated using the second order complex derivative approximation [23].

In the second part of this work, a thermodynamically consistent fracture phase field model (including damage and fatigue of materials) developed in Boldrini et al. [11] is considered. Since the understanding of evolution of damage, fatigue and fracture in materials is an important issue in many engineering applications, many researchers have contributed to several aspects of such phenomena (see for instance Lemaitre and Desmorat [24], Kanninen and Popelar [25] and Anderson [26]). However, some of these aspects, crack initiation for instance, are rather difficult to include in a phenomenological model in a thermodynamically consistent way. The development of this kind of models, properly describing initiation and evolution of fatigue, damage and ultimately the fracture for different types of materials, is nowadays a very important and challenging task. In recent years, the phase field methodology has appeared as a promising way to accomplish these requirements. The present situation is exemplified by briefly mentioning some representative works that use this kind of methodology. In Aranson et al. [27], a continuum field model that captures crack initiation, propagation, dynamic fracture instability, sound emission, crack branching and fragmentation was presented. In Karma et al. [28], another continuum model for mode III dynamic fracture based on phase field was used to simulate a two dimensional crack motion in a strip geometry above the Griffith threshold. In Borden et al. [29], a quasi-static model was numerically solved by means of the Galerkin method using NURBS and T-spline bases as the finite dimensional approximation spaces, obtaining numerical results with good agreement with experimental results. Quasi-static and dynamic fractures in brittle materials have been extensively studied by using phase field models. A review of finite element approximations for such models can be found in Ambati et al. [30]. The phase field formulation of the interactions between interfacial damage and bulk brittle cracking in complex microstructures was presented in Nguyen et al. [31]. By using incremental minimization of a suitable free-energy functional, a phase field theory for fracture of nonlinear elastic materials was developed by Clayton and Knap [32]. Some engineering brittle materials present ductile behavior after reaching the strength limit which creates a small-scale zone ahead the crack tip that exhibits growth and coalescence. A phase field model for this kind of situation was presented in Vignollet et al. [33].

However, there are some mathematical deficiencies with the models developed in the above works. For instance, the thermodynamic consistency of some of the presented models is unclear. Others works consider just isothermal situations. Crack initiation is not usually considered, and so most of the known fracture models introduce some damage where the crack starts and then propagates through it. The phase field fracture model developed in Boldrini et al. [11] addressed these deficiencies, by presenting a general thermodynamically consistent non-isothermal continuum thermo-mechanic framework for the evolution of damage, fatigue and fracture in materials under the hypothesis of small deformation. The

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