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MODELING THE EFFECTS OF INHOMOGENEOUS PRESSURE DISTRIBUTION IN THE EVOLUTION OF METAMORPHIC ROCKS

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ABSTRACT

Recent studies of in metamorphic petrology provide the evidence of pressure deviations from the lithostatic values as well as spatially inhomogeneous distributions. Such discrepancies arise from the complex chemo-mechanical interactions between the minerals which take place deep in the Earth. Conventionally, we assume the pressure takes the value given by Archimedes's formula which is directly proportional to the depth. Nevertheless, when considering deforming rocks together with mineral reactions, stresses emerge from both volume changes due to reactions and the overburden which lead to inhomogeneous pressure distributions. Thus, in general, the Archimedes's formula is not valid. Previous studies of metamorphic rocks separated the chemical and the mechanical actions on the mineral assemblages. This separation results in inappropriate models since the volume changes, caused by the chemical interactions between the minerals, strongly influence the inhomogeneous pressure distribution, and thus, its description requires a comprehensive treatment of the coupled chemo-mechanical interactions. Herein, we address the mechanical effects acting upon a chemically active metamorphic rock which results in inhomogeneous pressure distributions. We present a fully coupled thermodynamically-consistent model for chemo-mechanical interactions in multicomponent solids. We describe the Helmholtz free energy of a multicomponent elastic solid undergoing both diffusion and chemical reaction. Our formulation of the constitutive equations, which describe the evolution of the system towards equilibrium, satisfies the second law of thermodynamics. Furthermore, we present simulation results which give an insight into the phenomenon and verify the interleaving between the chemical and mechanical responses.

PHASE-FIELD METHODS ON DEFORMING SURFACES

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ABSTRACT

Phase-field models for phase transitions and brittle fracture on deforming surface structures are presented. For the modeling of phase transitions, the partial differential equation (PDE) is the Cahn-Hilliard equation for curved surfaces, which can be derived from surface mass balance in the framework of irreversible thermodynamics [3]. For the modeling of fracture, the formulation is based on Griffith's theory. For the surface deformation, the PDE is the (vector-valued) Kirchhoff-Love thin shell equation. The mathematical problems are governed by two coupled fourth-order nonlinear PDEs that live on an evolving two-dimensional manifold.

The PDEs can be efficiently discretized using C1-continuous interpolations without derivative degrees-of-freedom. Structured NURBS, locally refinable (LR) NURBS [2] and unstructured spline spaces [1] with pointwise C1-continuity are utilized for these interpolations. The resulting finite element formulations are discretized in time by the generalized-alpha scheme with adaptive time-stepping, and they are fully linearized within a monolithic Newton-Raphson approach.

A curvilinear surface parameterization is used throughout the formulations to admit general surface shapes and deformations. The behavior of the coupled systems are illustrated by several numerical examples exhibiting phase transitions and dynamic brittle fracture on deforming surfaces.

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ON FINITE ELEMENT FORMULATIONS FOR PHASE FIELD MODELS OF TWO-PHASE FLUID FLOWS

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ABSTRACT

In this work a finite element method is considered for the numerical simulation of the Navier-Stokes-Korteweg (NSK) and Navier-Stokes-Cahn-Hilliard (NSCH) equations; which are both widely used phase-field models. The former approach considers liquid-vapour flows of a single component (i.e. water/water vapour) and the latter models (specifically [1]) consider the mixture of two incompressible components with different densities and viscosities. Significantly both phase-field models mentioned have been shown in some cases to converge to the sharp interface models as the interface thickness tends to zero [2, 3]. Ultimately, the purpose of implementing these models is to tackle physically relevant multi-phase flow problems, for instance, demonstrating the cavitation phenomenon when oil/water flow through a restricted orifice. Initially, the NSK model is formulated using a quadratic b-spline grid with Nitsche's method to impose boundary conditions. Previous contributions [4, 5] demonstrate the successful implementation of the Navier-Stokes-Korteweg equations using isogeometric methods for both isothermal and non-isothermal applications. The requirement for quadratic b-splines comes about as a result of third-order partial-differential terms appearing in the governing equations, which require $\mathcal{C}^1$ continuous basis functions globally. It is observed in [6], that it is possible to reformulate the NSK equations with the Laplacian of the density as a new auxiliary variable, which permits the use of linear finite elements in computation. The NSK model is demonstrated for various benchmark problems in 2D and 3D using both b-splines and standard finite elements. The formulation of the NSCH model is quite different. The model adopted from [1] consists of the incompressible Navier-Stokes equations coupled with the Cahn-Hilliard equations. Due to the incompressibility, the pressure and velocity are inherently unstable. This is usually overcome by using LBB stable mixed elements [7], or by adding stabilisation in the formulation. In the present work, the former approach is considered when solving the coupled system. Throughout this work a priority is placed on increasing computational efficiency (i.e. through segregation and parallelisation), as well as to affirm a relation between results of the NSK and NSCH models and their adherence to actual physical behaviour.

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TRIANGULATION-BASED ISOGEOMETRIC ANALYSIS OF THE CAHN–HILLIARD PHASE-FIELD MODEL

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ABSTRACT

This paper presents the triangulation-based isogeometric analysis of the Cahn–Hilliard phase-field model. The Cahn–Hilliard phase-field model is governed by a time-dependent fourth-order partial differential equation. The corresponding primal variational form involves second-order operators, making it challenging in C^0-continuous finite element analysis. Isogeometric analysis[1] however, provides C^1 and higher-order continuity. NURBS-based isogeometric analysis has been shown applicable to the Cahn–Hilliard phase-field model[2]. Recently, the triangulation-based isogeometric analysis emerges with its unique benefits[3,4]. In this work, we extend the triangulation-based isogeometric analysis to solving the primal variational form of the Cahn–Hilliard equation in C^1-continuous domains. We validate our method by convergence analysis, then demonstrate detailed system evolution from randomly perturbed initial conditions in periodic two-dimensional squares and three-dimensional cubes. We incorporate our adaptive time-stepping scheme in these numerical experiments. The advantages of our method over NURBS-based isogeometric analysis are highlighted with examples featuring complex geometry and local refinement. The triangulation-based isogeometric analysis offers optimal convergence, time step stability, complex geometry compatibility and local refinement capability in our work.

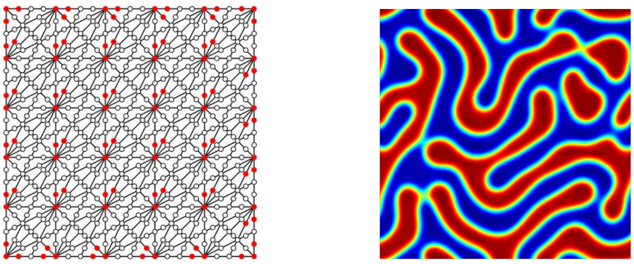

Figure 1: Mesh of the triangulation-based isogeometric analysis(left) and two-phase coarsening(right)

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