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Isogeometric Analysis of Phase-field Models: Application to the Cahn-Hilliard and Navier-Stokes-Korteweg Equations

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ABSTRACT

Phase-field methodology has emerged as a powerful tool for modeling the evolution of microstructures and the interactions of defects in a wide range of materials and physical processes. Examples where phase-field models have been applied include solidification, solid-solid phase transitions, domain structure evolution in shape memory alloys, ferroelectrics, and ferromagnetic materials, grain growth, dislocation mechanics, and fracture.

Phase-field methodology typically leads to partial-differential equations of higher order.
For example, the Cahn-Hilliard equation, a phase-field representation of spinodal decomposition involves fourth-order spatial partial-differential operators. Traditional numerical methodologies for dealing with higher-order operators on very simple geometries include finite differences and spectral approximations. In real-world engineering applications simple geometries are not very relevant, and therefore more geometrically flexible technologies need to be utilized. It is primarily this reason that has led to the finite element method being the most widely used methodology in engineering analysis. The primary strength of finite element methods has been in the realm of second-order spatial operators. The reason for this is variational formulations of second-order operators involve integration of products of first-derivatives. These are well defined and integrable if the finite element basis functions are piecewise smooth and globally *C*0-continuous, which is precisely the case for standard finite element functions. On the other hand, fourth-order operators necessitate basis functions that are piecewise smooth and globally *C*1-continuous. There are a very limited number of two-dimensional finite elements possessing *C*1-continuity applicable to complex geometries, but none in three-dimensions. As a result, a number of different devices have been employed over the years to deal with higher-order operators. All represent theoretical and computational complexities of one degree or another. It may be said that after 50 years of finite element research, no general, elegant and efficient solution of the higher-order operator problem exists.

Recently, a new methodology, isogeometric analysis, has been introduced into computational mechanics that is based on recent developments in computational geometry, computer aided design (CAD), and animation. Isogeometric analysis is a generalization of finite element analysis possessing several advantages: 1) It enables precise geometric

definition of complex engineering designs thus reducing errors caused by low-order, faceted geometric approximation of finite elements. 2) It simplifies mesh refinement because even the coarsest model is a precise geometric model. Thus no link is necessary to the CAD geometry in order to refine the mesh, in contrast with the finite element method, in which each mesh represents a different approximation of the geometry. 3) It also holds promise to vastly simplify the mesh generation process, currently the most significant component of analysis model generation, and a major bottleneck in the overall engineering process. 4) The *k*-refinement process has been shown to possess significant accuracy and robustness properties, compared with the usual *p*-refinement procedure utilized in finite element methods.

k-refinement is a procedure in which the order of approximation is increased, as in the *p*-method, but continuity (i.e., smoothness) is likewise increased, in contrast to the *p*-method. Isogeometric analysis thus presents a unique combination of attributes that can be exploited on problems involving higher-order differential operators, namely, higher-order accuracy, robustness, two- and three-dimensional geometric flexibility, compact support, and, most importantly, $C1$ and higher-order continuity. These properties open the way to application to phase-field models, and potentially very new ways to solve vexing problems of engineering importance. In addition, there are other areas of engineering interest that involve higher-order operators that isogeometric technology may be successfully applied to, such as, for example, rotation-free thin shell theory, strain-gradient elastic and inelastic material models, etc. Consequently, there is considerable additional potential to the further development of this technology.

In this paper, we present our initial efforts at applying isogeometric analysis to phase-field models. Most of our work has focused on the Cahn-Hilliard equation, but preliminary results for the Navier-Stokes-Korteweg system for liquid-vapor flows are also presented.