Computational Phase-field Modeling: Applications in Fluids, Solids and Biomechanics

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Phase-field modeling is emerging as a promising tool for the treatment of problems with interfaces. The classical description of interface problems requires the numerical solution of partial differential equations on moving domains in which the domain motions are also unknowns. The computational treatment of these problems requires moving meshes and is very difficult when the moving domains undergo topological changes. Phase-field modeling may be understood as a methodology to reformulate interface problems as equations posed on fixed domains. In some cases, the phase-field model may be shown to converge to the moving-boundary problem as a regularization parameter tends to zero, which shows the mathematical soundness of the approach. However, this is only part of the story because phase-field models do not need to have a moving-boundary problem associated and can be rigorously derived from classical thermomechanics. In this context, the distinguishing feature is that constitutive models depend on the variational derivative of the free energy. In all, phase-field models open the opportunity for the efficient treatment of outstanding problems in computational mechanics, such as, the interaction of a large number of cracks in three dimensions, cavitation, film and nucleate boiling, tumor growth or fully three-dimensional air-water flows with surface tension.

In addition, phase-field models bring a new set of challenges for numerical discretization that will excite the computational mechanics and computational mathematics communities. These include, for example, higher-order partial-differential spatial operators, stiff semi-discretizations, stable time-stepping algorithms and the treatment of sharp internal layers in the solution. In this course, I will show how Isogeometric Analysis (a generalization of finite elements that uses functions from computational geometry) presents a unique combination of attributes that can be exploited on phase-field modeling, namely, higher-order accuracy, robustness, two- and three-dimensional geometric flexibility, compact support, and, most importantly, higher-order continuity.

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