Optimization-based computational modeling, or how to let someone else do the hard work

Mathematical and algorithmic foundations for optimization-based modeling: A new strategy for the compatible discretization and scalable solution of multiphysics problems

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Abstract

We present a new, optimization-based strategy for modeling and simulation of complex multiphysics problems whose constituent components are governed by physical laws with disparate mathematical structures. Our approach relies on optimization and control ideas to (i) assemble and decompose multiphysics operators in a way that enables parallelism, and (ii) preserve their fundamental physical properties in the discretization process. In so doing we are able to synthesize

- compatible, feature-preserving discretizations of multiphysics problems, from high-resolution compatible discretizations of their constituent physics components, and
- efficient, scalable multiphysics solvers from fast solvers for their constituent physics components.

The optimization-based modeling and simulation framework departs substantially from the dominant computational strategies for multiphysics problems. Established approaches treat discretization and solution as separate tasks, and the former is burdened with the preservation of physical properties such as maximum principles, positivity, or monotonicity. Because our framework assembles discrete multiphysics models from high-resolution discretizations of their constituent physics components, the operator decomposition required for fast, scalable solvers is embedded in the problem formulation from the onset. Our approach also relieves discretization from tasks that impose severe geometric constraints on the mesh, or tangle accuracy and resolution with the preservation of physical properties. Two examples will illustrate the scope of our approach approach: an optimization-based framework for multi-physics coupling, and an optimization-based algorithm for constrained interpolation and transport.