OPTIMIZATION-BASED PROPERTY PRESERVING METHODS, OR GOING BOLDLY BEYOND COMPATIBLE DISCRETIZATIONS

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Abstract. Homological approaches such as finite element exterior calculus, mimetic finite differences and Discrete Exterior Calculus [1, 2] have been a game changer in the quest for structure-preserving discretization of PDEs. However, these techniques face serious difficulties in at least two contexts. First, many practically important models don't fit neatly in an exterior calculus structure. Examples include multiphysics problems in which different constituent model components may place conflicting requirements on the representation of the variables and heterogeneous problems which combine fundamentally different mathematical models. Preservation of relevant physical properties such as maximum principles, local solution bounds, symmetries, and Geometric Conservation laws provide another context in which homological techniques don't fare well. Indeed, while they ensure stability and accuracy of the discretization, stable and accurate does not imply property preserving.

In this talk we examine the application of optimization and control ideas to the formulation of *feature-preserving* heterogeneous numerical methods (HNM). An HNM is a collection of dissimilar numerical models from multiple disciplines functioning together as a unified simulation tool. We develop a general optimization framework, which couches the assembly of numerical parts into an HNM, and the preservation of the relevant physical properties into a constrained optimization problem. The mismatch between the states of the different components and suitable target solutions define the optimization objective, while the relevant physical properties provide the optimization constraints. Two complementary case studies illustrate the scope of the optimization approach. In the first study we apply the framework to formulate an optimization-based heterogeneous numerical method, which couples local and nonlocal material models [3]. The second study develops an optimization-based conservative and local bounds preserving semi-Lagrangian scheme for passive tracer transport [4, 5].

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Keywords: compatible discretization, optimization, property preservation

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