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Optimization-based remap and transport: A divide and conquer strategy for feature-preserving discretizations

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ABSTRACT

This paper examines the application of optimization and control ideas to the formulation of *feature-preserving* numerical methods, with particular emphasis on the conservative and bound-preserving remap (constrained interpolation) and transport (advection) of a single scalar quantity. We present a general optimization framework for the preservation of physical properties and specialize it to a generic optimization-based remap (OBR) of mass density. The latter casts remap as a quadratic program whose optimal solution minimizes the distance to a suitable *target* quantity, subject to a system of linear inequality constraints. The approximation of an exact mass update operator defines the target quantity, which provides the best possible accuracy of the new masses without regard to any physical constraints such as conservation of mass or local bounds. The latter are enforced by the system of linear inequalities. In so doing, the generic OBR formulation separates accuracy considerations from the enforcement of physical properties.

We proceed to show how the generic OBR formulation yields the recently introduced flux-variable flux-target (FVFT) [1] and mass-variable mass-target (MVMT) [2] formulations of remap and then follow with a formal examination of their relationship. Using an intermediate flux-variable mass-target (FVMT) formulation we show the equivalence of FVFT and MVMT optimal solutions.

To underscore the scope and the versatility of the generic OBR formulation we introduce the notion of adaptable targets, i.e., target quantities that reflect local solution properties, extend FVFT and MVMT to remap on the sphere, and use OBR to formulate adaptable, conservative and bound-preserving optimization-based transport algorithms for Cartesian and latitude/longitude coordinate systems. A selection of representative numerical examples on two-dimensional grids demonstrates the computational properties of our approach.

1. Introduction

Fundamental physical properties of natural phenomena give rise to the salient analytical properties of their mathematical models. However, the discretization of these models can cause the loss of key mathematical relationships, potentially leading to ill-posed discrete equations, the emergence of spurious modes, or physically impossible solutions. Coupled multiphysics

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simulations, where the output from one constituent component provides the input to another component, can further exacerbate the loss of structural and qualitative information in the discrete model. There, an unphysical solution from one component can cause a cascading breakdown of the subsequent components and compromise the whole simulation.

Thanks to extensive research efforts over the past 20 years it is now well understood that a discrete "vector calculus" setting, i.e., discrete spaces and operators that mimic basic vector calculus properties such as the Poincare lemma, the Gauss divergence theorem and the Stokes circulation theorem, enables *structure-preserving* discretizations of a large class of Partial Differential Equations (PDEs); see [3–7] and the references therein.

However, advances in structure-preserving numerical methods stand in sharp contrast with the limited mathematical and algorithmic understanding of *feature-preserving* discretizations, i.e., discretizations that reproduce qualitative properties of the exact solutions, such as local bounds, maximum principles, and symmetries, to name a few. The root cause for this imbalance is that such properties emerge from the interplay of function space structures with differential and boundary operators, i.e., they are model specific, whereas the given functional space structures can be shared by multiple mathematical models. For instance, the same discrete vector calculus setting can support the structure-preserving discretization of models ranging from pure diffusion to conservation laws, yet the unique qualitative properties of the models at each extreme, such as the maximum principle and local bounds are not guaranteed to emerge automatically from that setting.

The fluid nature of the qualitative properties makes it difficult to enforce them directly in the discretization process, that is by relying solely on the mesh structure and the discrete variables. As a rule, this strategy ties together the preservation of the desired features with geometric conditions on the mesh and/or restrictions on the accuracy. A typical example is the discrete maximum principle (DMP) for the Poisson equation, which requires a monotone, or M-stiffness matrix. To ensure this property on triangular elements the sum of the two angles opposing each interior edge should be less than π, and the polynomial degree should be 1 [8–10]. An extension of DMP to more general triangular or quadrilateral meshes requires nonlinear modifications of the governing equations such as the nonlinear stabilized finite element method for the Poisson equation [11,12], the nonlinear extension of the diamond scheme [13], and the nonlinear finite volume scheme in [14].

High-order maximum-principle satisfying and positivity preserving schemes for conservation laws exist in one dimension [15], or on rectangular meshes [16,17]. An extension of these schemes even to triangular elements is highly nontrivial [18]. A similar interdependence between mesh, accuracy and preservation of a physical property exists in many of the slope and flux limiters in use today. As a result, many of them do not preserve linear functions on irregular meshes [19], which impacts accuracy and robustness. This interdependence is propagated to any algorithm that employs limiters such as advection-based remappers in Arbitrary Lagrangian Eulerian (ALE) methods [20].

This paper draws upon and continues our previous efforts to develop an alternative, optimization-based *divide-and-conquer* strategy [21–24] for the formulation of stable, accurate and physically consistent discretizations. Specifically, here we focus on the application of optimization and control ideas to separate stability and accuracy considerations from the enforcement of the desired physical properties. In a nutshell, given a mathematical model and a list of desirable physical properties, our approach seeks the corresponding discrete model in the form of a constrained optimization problem in which

- the objective is to minimize the distance, measured in some suitable norm, between the discrete solution and a given *target* solution;
- a discrete model that is *stable and accurate* but is not expected to possess all desired physical properties defines the target solution;
- the optimization constraints *enforce* any desired physical properties that are not already present in the target solution.

This strategy offers a number of important theoretical and computational advantages in the formulation of feature-preserving numerical methods:

- the numerical solution is a global optimal solution from a feasible set defined by the desired physical properties, i.e., it is always the best possible, with respect to the target, approximate solution that also possesses these physical properties;
- the decoupling of the target definition from the preservation of the physical properties allows one to adapt the numerical solution to different problems by choosing the most appropriate target definition and objective function for these problems;
- the enforcement of the desired properties as optimization constraints is impervious to the mesh structure and/or field representations, thereby enabling feature-preserving methods on arbitrary unstructured meshes, including polygonal and polyhedral meshes.

The present work applies the optimization-based strategy to the high-order accurate and feature-preserving remap (constrained interpolation) and transport (advection) of a single scalar conserved quantity ("mass"). The features that we aim to preserve through the use of optimization are (a) the conservation of total mass and (b) physically motivated local bounds on the primitive variable (the density). The remap task arises in Arbitrary Lagrangian–Eulerian (ALE) methods, where high-order remapping between meshes is critical for the accuracy of the simulation, especially in conjunction with a *continuous rezone* approach, which requires remapping at every time step [25,26]. The second task, i.e., the stable, accurate and