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# Fast optimization-based conservative remap of scalar fields through aggregate mass transfer

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ABSTRACT

We develop a fast, efficient and accurate optimization-based algorithm for the high-order conservative and local-bound preserving remap (constrained interpolation) of a scalar conserved quantity between two close meshes with the same connectivity. The new formulation is as robust and accurate as the flux-variable flux-target optimization-based remap (FVFT-OBR) [1,2] yet has the computational efficiency of an explicit remapper. The coupled system of linear inequality constraints, resulting from the flux form of remap, is the main efficiency bottleneck in FVFT-OBR. While advection-based remappers use the flux form to directly enforce mass conservation, the optimization setting allows us to treat mass conservation as one of the constraints. To take advantage of this fact, we consider an alternative mass-variable mass-target (MVMT-OBR) formulation in which the optimization variables are the net mass updates per cell and a single linear constraint enforces the conservation of mass. In so doing we change the structure of the OBR problem from a global linear-inequality constrained QP to a singly linearly constrained QP with simple bounds. Using the structure of the MVMT-OBR problem, and the fact that in remap the old and new grids are close, we are able to develop a simple, efficient and easily parallelizable optimization algorithm for the primal MVMT-OBR QP. Numerical studies on a variety of affine and non-affine grids confirm that MVMT-OBR is as accurate and robust as FVFT-OBR, but has the same computational cost as the explicit, state-of-the-art FCR.



## 1. Introduction

We develop a fast, efficient and accurate optimization-based algorithm for the high-order conservative and local-bound preserving remap (constrained interpolation) of a scalar conserved quantity between two close meshes with the same connectivity. This task originates in Arbitrary Lagrangian–Eulerian (ALE) methods [3], which are the main motivation for our work. In the ALE context we are given the mean value of the primitive variable (an unknown positive scalar function, such as density) on each cell of the old (Lagrangian) mesh. The conserved variable, such as mass, is the product of this mean value and the cell volume. The objective is to find an accurate approximation of the mass on the new (rezoned) mesh. The

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remapped cell mass divided by the volume of the new cell approximates the density, which must satisfy physically motivated bounds.

The paper continues the development and study of the optimization-based remap (OBR) approach initiated in [1,2]. There we rephrase remap as a global inequality-constrained quadratic program (QP) for the mass fluxes exchanged between neighboring cells. The objective is to minimize the distance between these fluxes and some given *target* fluxes subject to constraints that enforce physically motivated local bounds on the primitive variable (density). The resulting flux-variable flux-target (FVFT) OBR has valuable theoretical and computational properties, which set it apart from advection-based [4–6], mass "repair" [7,8], or flux-correction motivated [9] algorithms.

In a nutshell, these methods invoke local "worst-case" scenarios to preserve the local bounds through monotone reconstruction, mass redistribution, or convex combinations of low and high-order fluxes. This entangles accuracy considerations with the enforcement of the bounds, which tends to obscure the sources of discretization errors and complicates the analysis of the algorithms.

In contrast, the OBR strategy completely separates accuracy from the enforcement of the physically motivated local bounds. The latter define a feasible set for the QP, whereas the minimization of the objective function enforces the former. As a result, FVFT-OBR always finds a globally optimal, i.e., *the best possible*, with respect to the target fluxes, remapped mass that also satisfies these bounds. The linear constraints that express the local bounds are completely impervious to cell shape and so, OBR is applicable to arbitrary grids, including polygonal and polyhedral grids.

Thorough convergence studies in [1] confirm that the FVFT-OBR formulation is as accurate as the state-of-the-art Flux-Corrected Remap (FCR) [9] for a collection of classical remap test cases. However, a series of "torture" tests in one and two dimensions demonstrate that FVFT-OBR is significantly more robust than FCR and the representative advection-based remappers. The dual QP provides a convenient structure-exploiting setting for the effective solution of FVFT-OBR by the reflective Newton method [10]. Numerical studies in [1] indicate that the computational cost of FVFT-OBR is proportional, up to a constant, to the cost of an explicit remapper such as FCR. The proportionality constant observed in [1] varies between 1.8 and 3.2.

These figures do not count potential gains from the increased robustness of FVFT-OBR, which enables larger displacements between the old and new mesh. Nonetheless, further efficiency gains in OBR are desirable to enhance its standing as a viable competitor to explicit remappers. Accordingly, the main focus of this paper is on improving the computational efficiency of OBR. Our principal goal is to develop an OBR formulation that fully retains the robustness and accuracy of FVFT-OBR, yet has the computational efficiency of the *explicit*, state-of-the-art FCR.

The main efficiency bottleneck in FVFT-OBR is the coupled system of linear inequality constraints. The coupling of the variables stems from writing the new cell masses in flux form, which automatically conserves the total mass. While the flux form is needed for conventional remappers, it is arguably less critical in an optimization setting where conservation of mass can be treated as an explicit constraint. To take advantage of this fact, we consider an alternative *mass-variable mass-target* OBR (MVMT-OBR) formulation in which the optimization variables are the net mass updates per cell. While this formulation introduces a single global equality constraint to conserve mass, it completely decouples the inequality constraints because there is only one variable per cell. As a result, by switching to these new variables we change the structure of the OBR problem from a global linear-inequality constrained QP to a singly linearly constrained QP with simple bounds.

Of course, trading automatic mass conservation for an explicit constraint only makes sense if the resulting QP can be solved more efficiently. Using the structure of the MVMT-OBR problem, and the fact that in remap the old and the new grids are close, we are able to develop a simple, efficient and easily parallelizable algorithm for the primal MVMT-OBR QP. Preliminary studies of the computational cost suggest that this algorithm is as efficient as the explicit FCR. This makes the new formulation fully competitive in terms of speed with any conventional remapper. At the same time, thorough computational studies confirm that the MVMT-OBR formulation retains the accuracy and robustness of FVFT-OBR.

The use of the fully decoupled net mass update variables instead of the coupled flux variables opens up an additional possibility to simplify and improve MVMT-OBR by discarding the variables associated with static cells, i.e., the cells that do not move during the rezone step. Since the net mass update on a static cell equals zero, we can increase the efficiency of MVMT-OBR by not computing the variables whose values are known to be zero. This modification could bring about significant additional performance gains in applications such as propagation of waves, in which there are large numbers of static cells. We show that skipping the static cels in the MVMT-OBR formulation does not lead to a loss of key theoretical properties such as existence of optimal solutions and preservation of linearity.

The remainder of this section introduces the relevant notation. Section 2 presents the MVMT-OBR formulation. There we also prove that MVMT-OBR is well-posed and preserves linear functions. The section closes with a discussion of the swept region implementation of MVMT-OBR. Section 3 develops the optimization algorithm for the solution of the MVMT-OBR QP. Numerical studies in Section 4 focus on the accuracy, robustness and efficiency of MVMT-OBR. We summarize our conclusions and map directions for future work in Section 5.

### 1.1. Notation

The computational domain $\Omega$ is a bounded subset of $\mathbf{R}^d$, $d = 1, 2, 3$. The old (Lagrangian) grid $K_h(\Omega)$ is a conforming partition of $\Omega$ into cells $\kappa_i,\ i = 1, \ldots, K$. The total numbers of vertices, edges and sides in the mesh are $V$, $E$ and $S$, respectively.