SAND2011-1584C

Optimization–based modeling with applications to transport. Part 1. Abstract formulation

Pavel Bochev[1], Denis Ridzal[2], and Joseph Young[1]

[1] Numerical Analysis and Applications,
[2] Optimization and Uncertainty Quantification,
Sandia National Laboratories[3], Albuquerque, NM 87185-1320, USA,
{pbboche,dridzal,josyoun}@sandia.gov

Abstract. This paper is the first of three related articles, which develop and demonstrate a new, optimization–based framework for computational modeling. The framework uses optimization and control ideas to assemble and decompose multiphysics operators and to preserve their fundamental physical properties in the discretization process. An optimization–based monotone, linearity preserving algorithm for transport (OBT) demonstrates the scope of the framework. The second and the third parts of this work focus on the formulation of efficient optimization algorithms for the solution of the OBT problem, and computational studies of its accuracy and efficacy.

1 Introduction

In this, and two companion papers [1, 2], we formulate, apply and study computationally a new optimization-based framework for computational modeling. The framework uses optimization and control ideas to (i) assemble and decompose multiphysics operators and (ii) preserve their fundamental physical properties in the discretization process. It develops further the approach in [3, 4], which demonstrates an optimization-based synthesis of fast solvers. Here we focus on application of the framework for the preservation of physical properties. We develop an optimization-based algorithm for transport (OBT) of a positive scalar function (density), which is monotone and preserves local bounds and linear functions on arbitrary unstructured grids.

The OBT algorithm combines the incremental remap (constrained interpolation) strategy for transport in [5] with the reformulation of the remap step as an inequality constrained quadratic program (QP) [6]. The objective in this QP is to minimize the discrepancy between target high-order mass fluxes and the approximate mass fluxes subject to inequality constraints derived from physically motivated bounds on the primitive variable (density). The merger of these ideas yields a new type of transport algorithms that can be applied to arbitrary

[3] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

unstructured grids and extended to higher than second-order accuracy by using suitably defined target fluxes.

Our approach differs substantially from the dominant methods for transport, which preserve the physical properties directly in the discretization process through monotonic reconstruction of the fields. The slope and flux limiters used for this purpose tie together preservation of physical properties with restrictions on the mesh geometry and/or the accuracy. As a result, many of them do not preserve linear functions on irregular grids [7], which impacts accuracy and robustness. An alternative is to use sophisticated "repair" procedures [8] or error compensation algorithms [9], which fix the out-of-bound values and maintain positivity on arbitrary unstructured grids. However, limiters and "repair" procedures obscure the sources of discretization errors, which complicates the analysis of the transport schemes, and their higher-order extensions on unstructured grids are very complex.

2 An abstract framework for optimization–based modeling

The abstract framework for optimization–based modeling in this section merges at an abstract level many of the ideas explored in [3, 4, 6]. To explain the basic concepts it suffices to consider a coupled problem with two "physics" components $\mathcal{L}_1 : X_1 \times X_2 \times D_1 \mapsto Y$ and $\mathcal{L}_2 : X_2 \times X_1 \times D_2 \mapsto Y$ respectively, where X_i, $i = 1, 2$, and Y are Banach spaces for the solution and the data, respectively. The spaces D_i, $i = 1, 2$, supply the model parameters. Given a set of parameters $d_i \in D_i$ the multiphysics problem is to seek $\{u_1, u_2\} \in X_1 \times X_2$ such that

$$\mathcal{L}_1(u_1, u_2; d_1) + \mathcal{L}_2(u_2, u_1; d_2) = 0\,. \tag{1}$$

Regarding (1) we make the following assumptions

A.1 There exist subsets $\mathcal{U}_i \subseteq X_i$ such that $u_i \in \mathcal{U}_i$ for any solution of (1).

A.2 $\mathcal{L}_i$ are well-posed: given $\widetilde{u}_2 \in \mathcal{U}_2$ the equation $\mathcal{L}_1(u_1, \widetilde{u}_2; d_1) = 0$ has a unique solution $u_1 \in \mathcal{U}_1$. Conversely, if $\widetilde{u}_1 \in \mathcal{U}_1$, then $\mathcal{L}_2(u_2, \widetilde{u}_1; d_2) = 0$ has a unique solution $u_2 \in \mathcal{U}_2$.

A.3 There are discrete spaces X^h_{ij}, $i, j = 1, 2$; Y^h, and discrete operators $\mathcal{L}^h_1 : X^h_{11} \times X^h_{12} \times D_1 \mapsto Y^h$ and $\mathcal{L}^h_2 : X^h_{22} \times X^h_{21} \times D_2 \mapsto Y^h$, such that for $\widetilde{u}^h_2 \in X^h_{12}$, $\widetilde{u}^h_1 \in X^h_{21}$ the problems $\mathcal{L}^h_1(u^h_1, \widetilde{u}^h_2; d_1) = 0$ and $\mathcal{L}^h_2(u^h_2, \widetilde{u}^h_1; d_2) = 0$, have unique solutions, and $\lim_{h\to 0} \|u_i - u^h_i\|_{X^h_{ii}} = 0$; $i = 1, 2$.

A.4 Robust and efficient solvers $(\mathcal{L}^h_i)^{-1}$ exist for each discrete constituent component operator $\mathcal{L}^h_i$.

Remark 1. A.1 is a formal statement of intrinsic physical properties (maximum principle, positivity, monotonicity, and etc.) of the exact solution of (1). A.2 states that the component physics operators $\mathcal{L}_i$ are well-posed and preserve these properties so long as the inputs are admissible. A.3–A.4 imply that each $\mathcal{L}_i$ can be discretized and solved in a stable, accurate and efficient manner, however, in A.3–A.4 it is not assumed that $\mathcal{L}^h_i$ preserve the physical properties in A.1.

Assumptions A.1–A.4 can be satisfied for most problems of interest by breaking down the multiphysics model into sufficiently small constituent components. However, in general, $X_{11}^h \neq X_{21}^h$ and $X_{22}^h \neq X_{12}^h$, which is a formal way of saying that stable discretizations of $\mathcal{L}_1$ and $\mathcal{L}_2$ may require *mutually exclusive* field representations. Consequently, $\mathcal{L}_1^h + \mathcal{L}_2^h$ is not guaranteed to be a meaningful, let alone a well-posed discrete operator. This means that even with A.1–A.4 holding, we are not assured that (i) a stable and accurate *monolithic* discretization of the multiphysics problem (1) is readily available, and (ii) if such a discretization exists, the resulting problem can be solved in a robust and efficient manner.

Our strategy for dealing with these two fundamental issues arising in the discretization of complex multiphysics problems is based on non-standard application of optimization and control ideas. Specifically, we reformulate (1) into an equivalent *multi-objective constrained optimization problem*. The cost functional in this problem minimizes discrepancies between multiple versions of the exact solution subject to constraints derived from the component physics operators and the condition that physical properties are preserved in the optimal solution. In so doing our approach exposes the component physics operators and separates the preservation of physical properties from mesh geometry and field representations. It is an example of a "divide-and-conquer" strategy, which *decomposes the operator space and relieves the discretization process of tasks that it is not well-equipped to handle in a robust and efficient manner*. Due to the limited space, demonstration of the framework will be restricted to preservation of physical properties in a single physics setting.

2.1 Optimization-based reformulation of multiphysics operators

We reformulate the multiphysics model (1) into a multi-objective constrained optimization problem in three stages. For simplicity, we assume that all necessary spaces are Hilbertian and postpone the discussion of data assimilation to the end of the section. In the first stage we modify (1) into the equivalent problem

$$\mathcal{L}_1(u_1, u_2; d_1) + \mathcal{R}(\theta) + \mathcal{L}_2(u_2, u_1; d_2) - \mathcal{R}(\theta) = 0\,, \tag{2}$$

where X is a Hilbert space, $\theta \in X$ is a control function, and $\mathcal{R} : X \mapsto Y$ is a suitable operator. At the second stage we fix $\theta \in X$, $u_{12} \in \mathcal{U}_2$, and $u_{21} \in \mathcal{U}_1$ and split (2) into two independent problems: seek $u_{11} \in X_1$ and $u_{22} \in X_2$ such that

$$\mathcal{L}_1(u_{11}, u_{12}; d_1) + \mathcal{R}(\theta) = 0 \quad \text{and} \quad \mathcal{L}_2(u_{22}, u_{21}; d_2) - \mathcal{R}(\theta) = 0 \tag{3}$$

The third stage, reconnects these problems using the multi-objective functional

$$J_{\vec{\alpha}}\big(u_{11}, u_{12}; u_{22}, u_{21}; \theta\big) = \frac{1}{2}\big(\alpha_1 \|u_{11} - u_{21}\|_W^2 + \alpha_2 \|u_{22} - u_{12}\|_W^2 + \alpha_3 \|\theta\|_X^2\big)\,, \tag{4}$$

where $\vec{\alpha} = \{\alpha_1, \alpha_2, \alpha_3\}$, and W is such that $X_i \subseteq W$. In this stage we replace (1) by the constrained optimization problem[3]:

$$\min \;\; J_{\vec{\alpha}}(u_{11}, u_{12}; u_{22}, u_{21}; \theta) \quad \text{subject to} \quad \begin{cases} \mathcal{L}_1(u_{11}, u_{12}; d_1) + \mathcal{R}(\theta) = 0 \\ \mathcal{L}_2(u_{22}, u_{21}; d_2) - \mathcal{R}(\theta) = 0 \\ u_{i1} \in \mathcal{U}_1 \, ; u_{i2} \in \mathcal{U}_2 \, , i = 1, 2 \end{cases} . \quad (5)$$

The first two constraints in (5) are defined by the physics operators, and the third enforces the physical properties on the optimal solution. Its structure depends on these properties and can include both equality and inequality constraints.

2.2 Discretization of the reformulated problem

The gist of our strategy is to use the optimization problem (5) as an instrument to fuse stable and accurate discretizations $\mathcal{L}_i^h$ of the constituent physics operators into feature-preserving discretizations of the multiphysics problem (1). We assume that X_{ij}^h and $\mathcal{L}_i^h$ are as in A.1-A.4. Stable and accurate discretizations of the component operators may require mutually exclusive discrete spaces $X_{11}^h \neq X_{21}^h$ and $X_{22}^h \neq X_{12}^h$. This is a serious problem for monolithic discretizations of (1) but is *completely benign* for the discretization of (5) where physics operators are decoupled and can be approximated independently.

To separate the accuracy considerations from the preservation of physical properties we treat the discrete solutions u_{ij}^h of $\mathcal{L}_i^h$ as *targets* that provide the best possible accuracy and impose the constraints on a separate set of variables $\widehat{u}_{ij}^h$. To this end, we modify the multi-objective functional by adding terms which force these new variables $\widehat{u}_{ij}^h$ close to the optimally accurate targets u_{ij}^h:

$$\widehat{J}_{\vec{\alpha}}(\widehat{u}_{ij}^h, u_{ij}^h; \theta^h) = \frac{1}{2}\Big(\sum_{i,j=1}^{2} \widehat{\alpha}_{ij} \|\widehat{u}_{ij}^h - u_{ij}^h\|_W^2 + \sum_{j=1}^{2} \alpha_j \|u_{1j}^h - u_{2j}^h\|_W^2 + \alpha_3 \|\theta^h\|_X^2 \Big) , \quad (6)$$

where $\vec{\alpha} = \{\{\widehat{\alpha}_{ij}\}, \alpha_1, \alpha_2, \alpha_3\}$. The discrete optimization problem then reads

$$\min \quad \widehat{J}_{\vec{\alpha}}(\widehat{u}_{ij}^h, u_{ij}^h; \theta^h) \quad \text{subject to} \quad \begin{cases} \mathcal{L}_1^h(u_{11}^h, u_{12}^h; d_1) + \mathcal{R}^h(\theta^h) = 0 \\ \mathcal{L}_2^h(u_{22}^h, u_{21}^h; d_2) - \mathcal{R}^h(\theta^h) = 0 \\ \widehat{u}_{i1}^h, \in \mathcal{U}_1 \, ; \;\; \widehat{u}_{i2}^h \in \mathcal{U}_2 \, ; \;\; i = 1, 2 \end{cases} . \quad (7)$$

The discrete optimization problem (7) retains the key features of (5) and thus, it can be used both for the ***synthesis*** of approximate multiphysics operators from discretizations of their constituent physics components, and for the ***decomposition*** of such operators into simpler parts.

[3] Problem (5) differs from those encountered in conventional PDE-constrained optimization. For instance, because θ is a virtual control, it is not subject to constraints, and does not reduce solution regularity relative to the original problem (1).

3 Application to transport problems

We use the optimization framework in Sections 2.1–2.2 to develop a new class of conservative, monotone and bounds preserving methods for the scalar transport equation

$$\partial_t \rho + \nabla \cdot \rho \mathbf{v} = 0 \quad \text{on } \Omega \times [0,T] \quad \text{and} \quad \rho(\mathbf{x},0) = \rho^0(\mathbf{x})\,, \tag{8}$$

where $T > 0$ is the final time, $\rho(\mathbf{x},t)$ is a positive density function (the primitive variable) on $\Omega \times [0,T]$ with initial distribution $\rho^0(\mathbf{x})$, and $\mathbf{v}$ is a velocity field. For simplicity, we assume that $\rho(\mathbf{x},t) = 0$ on $\partial\Omega \times [0,T]$. Let $K_h(\Omega)$ denote a partition of Ω into cells κ_i, $i = 1,\ldots,K$. We solve (8) using a cell-centered discretization of the density. The degrees of freedom ρ_i^n approximate the mean cell density at time $t = t_n$:

$$\rho_i(t_n) = \frac{\int_{\kappa_i} \rho(\mathbf{x},t_n) dV}{\int_{\kappa_i} dV} = \frac{\int_{\kappa_i} \rho(\mathbf{x},t_n) dV}{\mathrm{vol}(\kappa_i)}\,.$$

The approximate mass in cell κ_i at time t_n is $m_i^n = \rho_i^n \mathrm{vol}(\kappa_i)$.

To solve (8) we proceed as follows. Numerical integration of $\rho^0(\mathbf{x})$ on each grid cell κ_i yields the initial cell masses $\vec{m}^{\,0} = (m_1^0,\ldots,m_K^0)$ and the initial density distribution $\vec{\rho}^{\,0} = (\rho_1^0,\ldots,\rho_K^0)$ on $K_h(\Omega)$, where $\rho_i^0 = m_i^0/\mathrm{vol}(\kappa_i)$. Suppose that the approximate solution $\vec{\rho}^{\,n} = (\rho_1^n,\ldots,\rho_K^n)$ is known on $K_h(\Omega)$ at time $0 \le t_n < T$ and Δt_n is an admissible *explicit* time step. To find the approximate density distribution $\vec{\rho}^{\,n+1} = (\rho_1^{n+1},\ldots,\rho_K^{n+1})$ on $K_h(\Omega)$ at the new time step $t_{n+1} = t_n + \Delta_n$, we apply the forward *incremental remapping* algorithm [5]. This algorithm advances the solution of (8) to the next time step using that the mass of a Lagrangian volume $V_L(t)$ is conserved along the trajectories $d\mathbf{x}/dt = \mathbf{v}$:

$$\int_{V_L(t_{n+1})} \rho dV = \int_{V_L(t_n)} \rho dV\,. \tag{9}$$

In particular, if $V_L(t_n) = \Omega$, and $\widetilde{\Omega} = V_L(t_{n+1})$ is the deformed region, the total mass is conserved:

$$M(\Omega) = \int_{\Omega} \rho(\mathbf{x},t) dV = \int_{\widetilde{\Omega}} \rho(\mathbf{x},t) dV = M(\widetilde{\Omega})\,.$$

The idea of the incremental remap approach is to evolve the computational grid $K_h(\Omega)$ into a grid $\widetilde{K}_h(\widetilde{\Omega})$ on the deformed region $\widetilde{\Omega}$ at t_{n+1}, compute the mean density on this grid and interpolate it back to $K_h(\Omega)$. Specifically, if we set $V_L(t_n) = \kappa_i$ then, according to (9) the mass $\widetilde{m}_i$ in $V_L(t_{n+1})$ equals the mass m_i^n in $V_L(t_n)$ and the mean density on $V_L(t_{n+1})$ is $\widetilde{\rho}_i = m_i^n/\mathrm{vol}(V_L(t_{n+1}))$.

In practice, $V_L(t_{n+1})$ is not known exactly and must be approximated. A simple strategy is to evolve the vertices $\{\mathbf{x}_p\}$ of κ_i along the trajectories using, e.g., an explicit Euler method. This yields a cell $\widetilde{\kappa}_i$ with vertices $\widetilde{\mathbf{x}}_p = \mathbf{x}_p + \Delta t_n \mathbf{v}$, which approximates $V_L(t_{n+1})$. The mass $\widetilde{m}_i$ and the mean density $\widetilde{\rho}_i$ on $\widetilde{\kappa}_i$ are

$$\widetilde{m}_i = m_i^n \quad \text{and} \quad \widetilde{\rho}_i = \frac{m_i^n}{\mathrm{vol}(\widetilde{\kappa}_i)}\,; \quad i = 1,\ldots,K\,.$$

Algorithm 1: One forward step of incremental remapping

input : Density approximation $\vec{\rho}^{\,n} = (\rho_1^n, \ldots, \rho_K^n)$ at time t_n, time step Δt_n
output: Density approximation $\vec{\rho}^{\,n+1} = (\rho_1^{n+1}, \ldots, \rho_K^{n+1})$ at time t_{n+1}

1 Project grid: $K_h(\Omega) \ni \mathbf{x}_p \mapsto \mathbf{x}_p + \Delta t_n \mathbf{v} = \widetilde{\mathbf{x}}_p \in \widetilde{K}_h(\widetilde{\Omega})$

2 Transport m and ρ: $\forall \widetilde{\kappa}_i \in \widetilde{K}_h(\widetilde{\Omega})$ set $\widetilde{m}_i = m_i^n$ and $\widetilde{\rho}_i = \widetilde{m}_i / \mathrm{vol}(\widetilde{\kappa}_i)$

3 Remap density: $\vec{\rho}^{\,n+1} = \mathcal{R}(\{\widetilde{\rho}_1, \ldots, \widetilde{\rho}_K\})$

Conservative interpolation (remap) of the mean density values $\widetilde{\rho}_i$ from the deformed mesh $\widetilde{K}_h(\widetilde{\Omega})$ onto the original mesh $K_h(\Omega)$ gives the approximate mean cell density $\vec{\rho}^{\,n+1} = (\rho_1^{n+1}, \ldots, \rho_K^{n+1})$ at the next time level; see Algorithm 1.

The conservative interpolation (remap) operator $\mathcal{R}$ is the key ingredient of Algorithm 1. To state the requirements on $\mathcal{R}$ without going into unnecessary technical details, it is convenient to assume that $\mathbf{v} \cdot \mathbf{n} = 0$. In this case the original and deformed regions coincide: $\Omega = \widetilde{\Omega}$, and the mass is conserved at all times. Let $\widetilde{N}_i$, and N_i denote the neighborhoods of $\widetilde{\kappa}_i \in \widetilde{K}_h(\widetilde{\Omega})$, and $\kappa_i \in K_h(\Omega)$, resp., i.e., all cells that share vertex or an edge or a face with $\widetilde{\kappa}_i$ or κ_i. Define

$$\widetilde{\rho}_i^{\min} = \min_{j \in \widetilde{N}_i} \widetilde{\rho}_j \,; \qquad \widetilde{\rho}_i^{\max} = \max_{j \in \widetilde{N}_i} \widetilde{\rho}_j \,;$$

Under the assumptions stated above, $\mathcal{R}$ must satisfy the following requirements:

R.1 local bounds are preserved: $\widetilde{\rho}_i^{\min} \le \rho_i^{n+1} \le \widetilde{\rho}_i^{\max}$;

R.2 total mass is conserved: $\sum_{i=0}^K m_i^{n+1} = \sum_{i=0}^K \widetilde{m}_i = \sum_{i=0}^K m_i^n$;

R.3 linearity is preserved: $m_i^{n+1} = \int_{\kappa_i} \rho(\mathbf{x}, t_{n+1}) dV$ if $\rho(\mathbf{x}, t)$ is linear in $\mathbf{x}$.

We use the optimization framework in Section 2.2 to define a constrained interpolation operator that satisfies R.1–R.3. The starting point is the flux-form formula[4] for the cell masses on $K_h(\Omega)$ corresponding to the new time level:

$$m_i^{n+1} = \widetilde{m}_i + \sum_{\widetilde{\kappa}_j \in \widetilde{N}_i} \widetilde{F}_{ij}^h \,; \quad i = 1, \ldots, K \,. \tag{10}$$

The mass fluxes $\widetilde{F}_{ij}^h$ approximate the mass exchanges between the cells in the neighborhood $\widetilde{N}_i$ of $\widetilde{\kappa}_i$. We specialize the abstract optimization problem (7) as follows. Clearly, (8) is a "single-physics" equation and it suffices to consider a single "physics" operator with a single target field u^h and a single approximation field $\widehat{u}^h$. We identify $\widehat{u}^h$ with the mass fluxes in (10) and u^h – with a target flux $\widetilde{F}_{ij}^T$ which is *exact for linear density functions*. In this context, the single "physics" operator $\mathcal{L}^h(u^h)$ is the target flux reconstruction

$$\mathcal{L}^h(\widetilde{F}_{ij}^T) = \widetilde{F}_{ij}^T = \int_{\kappa_i \cap \widetilde{\kappa}_j} \widetilde{\rho}_j^{\,\ell}(\mathbf{x}) dV - \int_{\widetilde{\kappa}_i \cap \kappa_j} \widetilde{\rho}_i^{\,\ell}(\mathbf{x}) dV \,; \quad \widetilde{\kappa}_j \in \widetilde{N}_i \,; \kappa_j \in N_i$$

[4] The conditions under which this formula holds [9] can be always satisfied for the settings of interest to us.

where $\widetilde{\rho}_i^{\ell}(\mathbf{x})$ is density reconstruction on cell $\widetilde{\kappa}_i$, which is exact for linear functions. Finally, from R.1 we obtain bounds for the mass on the new time level:

$$\widetilde{\rho}_i^{\min}\mathrm{vol}(\kappa_i) = m_i^{\min} \le m_i^{n+1} \le m_i^{\max} = \widetilde{\rho}_i^{\max}\mathrm{vol}(\kappa_i)$$

Thus, the abstract discrete problem (7) specializes to the following QP:

$$\underset{\widetilde{F}_{ij}^h}{\text{minimize}} \ \sum_{i=1}^{K}\sum_{\widetilde{\kappa}_j\in\widetilde{N}_i}(\widetilde{F}_{ij}^h - \widetilde{F}_{ij}^T)^2 \quad \text{subject to}$$

$$\begin{cases} \widetilde{F}_{ij}^T = \displaystyle\int_{\kappa_i\cap\widetilde{\kappa}_j}\widetilde{\rho}_j^{\ell}(\mathbf{x})dV - \int_{\widetilde{\kappa}_i\cap\kappa_j}\widetilde{\rho}_i^{\ell}(\mathbf{x})dV & \leftarrow \text{“physics” operator} \\ \widetilde{F}_{ij}^h = -\widetilde{F}_{ji}^h & \leftarrow \text{mass conservation} \\ m_i^{\min} \le \widetilde{m}_i + \displaystyle\sum_{\widetilde{\kappa}_j\in\widetilde{N}_i}\widetilde{F}_{ij}^h \le m_i^{\max} & \leftarrow \text{local bounds}\,. \end{cases} \tag{11}$$

The optimization-based formulation (11) for constrained interpolation is of independent interest for Arbitrary Lagrangian-Eulerian methods [6]. It separates enforcement of the physical properties R.1 and R.2, which is done through the constraints, from the enforcement of the accuracy R.3, which is achieved through the objective functional. As a result, (11) is impervious to cell shapes and can be used on arbitrary grids. We conclude Part 1 with a proof that (11) has optimal solution. Part 2 [1] develops efficient algorithms for (11) and Part 3 [2] presents implementation of Algorithm 1 and computational studies.

Theorem 1. *Assume that $K_h(\Omega)$ and $\widetilde{K}_h(\widetilde{\Omega})$ are such that every cell $\kappa_i \in K_h(\Omega)$ is contained in the neighborhood $\widetilde{N}_i$ of its image $\widetilde{\kappa}_i \in \widetilde{K}_h(\widetilde{\Omega})$. For any given set of masses $\widetilde{m}_i$ and associated densities $\widetilde{\rho}_i = \widetilde{m}_i/\mathrm{vol}(\widetilde{\kappa}_i)$ on $\widetilde{K}_h(\widetilde{\Omega})$ there exist antisymmetric fluxes $\{\widetilde{F}_{ij}\}$ which satisfy the inequality constraints in (11).*

Proof. We need to show that there are antisymmetric fluxes $\widetilde{F}_{ij}$ such that

$$\widetilde{\rho}_i^{\min}\mathrm{vol}(\kappa_i) \le \widetilde{\rho}_i\mathrm{vol}(\widetilde{\kappa}_i) + \sum_{\widetilde{\kappa}_j\in\widetilde{N}_i}\widetilde{F}_{ij} \le \widetilde{\rho}_i^{\max}\mathrm{vol}(\kappa_i)$$

Fix a cell index $1 \le i \le K$, and choose $\widehat{\rho}_j$, for $\widetilde{\kappa}_j \in \widetilde{N}_j$ according to

$$\widetilde{\rho}_i^{\min} \le \widehat{\rho}_j \le \widetilde{\rho}_i^{\max} \quad \text{for } j \ne i \quad \text{and} \quad \widehat{\rho}_i = \widetilde{\rho}_i\,. \tag{12}$$

Define the fluxes

$$\widetilde{F}_{ij} = \widehat{\rho}_j\mathrm{vol}(\kappa_i\cap\widetilde{\kappa}_j) - \widehat{\rho}_i\mathrm{vol}(\widetilde{\kappa}_i\cap\kappa_j)\,. \tag{13}$$

Clearly, $\widetilde{F}_{ij} = -\widetilde{F}_{ji}$. Using the definition (13)

$$\begin{aligned}\widetilde{\rho}_i\mathrm{vol}(\widetilde{\kappa}_i) + \sum_{\widetilde{\kappa}_j\in\widetilde{N}_i}\widetilde{F}_{ij} &= \widetilde{\rho}_i\Big[\mathrm{vol}(\widetilde{\kappa}_i) - \sum_{j\ne i}\mathrm{vol}(\widetilde{\kappa}_i\cap\kappa_j)\Big] + \sum_{j\ne i}\widehat{\rho}_j\mathrm{vol}(\kappa_i\cap\widetilde{\kappa}_j) \\ &= \widetilde{\rho}_i\mathrm{vol}(\widetilde{\kappa}_i\cap\kappa_i) + \sum_{j\ne i}\widehat{\rho}_j\mathrm{vol}(\kappa_i\cap\widetilde{\kappa}_j) = \sum_{\widetilde{\kappa}_j\in\widetilde{N}_i}\widehat{\rho}_j\mathrm{vol}(\kappa_i\cap\widetilde{\kappa}_j)\,.\end{aligned}$$

From $\kappa_i = \cup_k(\kappa_i \cap \widetilde{\kappa}_j)$ and the bounds in (12) it follows that

$$\sum_{\widetilde{\kappa}_j \in \widetilde{N}_i} \widehat{\rho}_j \mathrm{vol}(\kappa_i \cap \widetilde{\kappa}_j) \leq \widetilde{\rho}_i^{\max} \sum_{\widetilde{\kappa}_j \in \widetilde{N}_i} \mathrm{vol}(\kappa_i \cap \widetilde{\kappa}_j) = \widetilde{\rho}_i^{\max} \mathrm{vol}(\kappa_i)\,;$$
$$\sum_{\widetilde{\kappa}_j \in \widetilde{N}_i} \widehat{\rho}_j \mathrm{vol}(\kappa_i \cap \widetilde{\kappa}_j) \geq \widetilde{\rho}_i^{\min} \sum_{\widetilde{\kappa}_j \in \widetilde{N}_i} \mathrm{vol}(\kappa_i \cap \widetilde{\kappa}_j) = \widetilde{\rho}_i^{\min} \mathrm{vol}(\kappa_i)\,. \qquad \square$$

In [6] we prove that (11) preserves linear densities if the barycenter of κ_i remains in the convex hull of the barycenters of the cells in $\widetilde{N}_i$ for all $1 \leq i \leq K$. This condition is less restrictive than the one required for linearity preservation by Van Leer limiting [10] and is valid for any unstructured grid. In summary, using Algorithm 1 in conjunction with an operator $\mathcal{R}$ defined by the QP (11), yields a conservative and monotone transport algorithm that is applicable to *arbitrary cell shapes*, including polygons and polyhedra.

References

1. Young, J., Ridzal, D., Bochev, P.: Optimization–based modeling with applications to transport. Part 2. Optimization algorithm. In Lirkov, I., Margenov, S., Wasniewski, J., eds.: Proceedings of LSSC 2011. Springer Lecture Notes in Computer Science (Submitted 2011)
2. Ridzal, D., Bochev, P., Young, J., Peterson, K.: Optimization–based modeling with applications to transport. part 3. Implementation and computational studies. In Lirkov, I., Margenov, S., Wasniewski, J., eds.: Proceedings of LSSC 2011. Springer Lecture Notes in Computer Science (Submitted 2011)
3. Bochev, P., Ridzal, D.: An optimization-based approach for the design of PDE solution algorithms. SIAM Journal on Numerical Analysis **47**(5) (2009) 3938–3955
4. Bochev, P., Ridzal, D.: Additive operator decomposition and optimization–based reconnection with applications. In Lirkov, I., Margenov, S., Wasniewski, J., eds.: Proceedings of LSSC 2009. Volume 5910 of Springer Lecture Notes in Computer Science. (2009)
5. Dukowicz, J.K., Baumgardner, J.R.: Incremental remapping as a transport/advection algorithm. Journal of Computational Physics **160**(1) (2000) 318 – 335
6. Bochev, P., Ridzal, D., Scovazzi, G., Shashkov, M.: Formulation, analysis and numerical study of an optimization-based conservative interpolation (remap) of scalar fields for arbitrary lagrangian-eulerian methods. Journal of Computational Physics **Submitted** (2011)
7. Berger, M., Murman, S.M., Aftosmis, M.J.: Analysis of slope limiters on irregular grids. In: Proceedings of the 43rd AIAA Aerospace Sciences Meeting. Number AIAA2005-0490, Reno, NV, AIAA (January 10–13 2005)
8. Kucharik, M., Shashkov, M., Wendroff, B.: An efficient linearity-and-bound-preserving remapping method. Journal of Computational Physics **188**(2) (2003) 462 – 471
9. Margolin, L.G., Shashkov, M.: Second-order sign-preserving conservative interpolation (remapping) on general grids. Journal of Computational Physics **184**(1) (2003) 266 – 298
10. Swartz, B.: Good neighborhoods for multidimensional Van Leer limiting. Journal of Computational Physics **154**(1) (1999) 237 – 241