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Synchronized flux limiting for gas dynamics variables

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ABSTRACT

This work addresses the design of failsafe flux limiters for systems of conserved quantities and derived variables in numerical schemes for the equations of gas dynamics. Building on Zalesak's multidimensional flux-corrected transport (FCT) algorithm, we construct a new positivity-preserving limiter for the density, total energy, and pressure. The bounds for the underlying inequality constraints are designed to enforce local maximum principles in regions of strong density variations and become less restrictive in smooth regions. The proposed approach leads to closed-form expressions for the synchronized correction factors without the need to solve inequality-constrained optimization problems. A numerical study is performed for the compressible Euler equations discretized using a finite element based FCT scheme.

1. Introduction

The ability to enforce local discrete maximum principles and/or positivity preservation for a set of coupled gas dynamics variables is a highly desired property of high-resolution schemes for the compressible Euler equations [13,17,21] and constrained interpolation (remapping) algorithms [2,15,16,24] for systems of conserved quantities. Many existing tools for constraining the quantities of interest are based on the use of limiting techniques for numerical fluxes associated with oscillatory antidiffusive components of a high-order approximation. The underlying design principles trace their origins to the classical *flux-corrected transport* (FCT) algorithm introduced by Boris and Book [3–5] and Zalesak [26] in the 1970s. Löhner et al. [18] extended the FCT methodology to unstructured grid finite element methods and systems of conservation laws. The first use of flux limiters in the context of remapping goes back to the work of Smolarkiewicz and Grell [22] who proposed a class of nonconservative monotone interpolation schemes. Conservative flux-corrected remap (FCR) methods were developed in [14,17,15,24]. As shown by Bochev et al. [2], the FCR approach to calculating the correction factors is equivalent to solving an optimization problem with simple box constraints corresponding to a worst-case scenario. Advanced algorithms for constrained optimization-based data transfer were proposed in [1,2,16].

Flux limiting techniques for systems of coupled variables can be classified into sequential [15] and synchronized [14,17,16,21] algorithms. A sequential limiter constrains each quantity of interest under worst-case assumptions regarding the fluxes that depend on other variables. In synchronized FCT algorithms [13,14,18,17], the antidiffusive fluxes are multiplied by the minimum of the correction factors for selected control variables. Due to the involved linearizations, such algorithms may require additional a posteriori corrections to guarantee the nonnegativity of the pressure and internal energy [14,27]. In optimization-based synchronized algorithms, different correction factors may be used in different conservation laws provided that the imposed constraints are satisfied for each quantity of interest [16]. However, the cost of coupled flux

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optimization is rather high, which has led Bochev et al. [1] to favor globally conservative formulations of the constrained remap problem.

In this paper, we improve the synchronized FCT algorithm presented in [13,14] by introducing new limiters for the energy and pressure. In contrast to approaches that rely on linearized transformations of variables, the proposed limiting strategy does not involve any linearizations and guarantees positivity preservation without a posteriori fixes. Moreover, the bounds for FCT are designed to prevent unnecessary limiting in regions of constant pressure. The calculation of correction factors for the synchronized FCT limiter does not require solving inequality-constrained optimization problems, which makes it an inexpensive alternative to synchronized optimization-based limiters [2,16]. The ability of the proposed algorithm to handle shocks and contact discontinuities is illustrated by a numerical study for the Euler equations.

2. Synchronized flux limiting

Consider a system of conservation laws for $U = [\rho, \rho\mathbf{v}, \rho E]^T$, where ρ is the density, $\mathbf{v}$ is the velocity and E is the total energy. In the case of an ideal polytropic gas, the pressure p is given by the equation of state

$$p = (\gamma - 1)\left(\rho E - \frac{|\rho\mathbf{v}|^2}{2\rho}\right), \tag{1}$$

where γ stands for the constant ratio of specific heats ($\gamma = 1.4$ for air).

Let U_i denote a numerical approximation to the vector U of gas dynamics variables at the ith nodal point or control volume. The simplest representatives of flux-corrected transport (FCT) and flux-corrected remapping (FCR) algorithms are based on the following predictor–corrector strategy:

1. Calculate a low-order approximation U_i^L using a numerical scheme which is guaranteed to satisfy all relevant maximum principles.
2. Decompose the difference between U_i^L and a high-order approximation U_i^H into a sum of antidiffusive fluxes $F_{ij} = [f_{ij}^{\rho}, \mathbf{f}_{ij}^{\rho v}, f_{ij}^{\rho E}]^T$ such that

$$m_i U_i^H = m_i U_i^L + \sum_{j\neq i} F_{ij}, \qquad F_{ji} = -F_{ij}, \tag{2}$$

   where m_i is a positive diagonal entry of the (lumped) mass matrix.
3. Multiply F_{ij} and its companion F_{ji} by a solution-dependent correction factor $\alpha_{ij} \in [0, 1]$ such that the flux-corrected approximation

$$m_i U_i = m_i U_i^L + \sum_{j\neq i} \alpha_{ij} F_{ij}, \qquad \alpha_{ji} = \alpha_{ij} \tag{3}$$

   satisfies inequality constraints of the form

$$u_i^{\min} \le u_i \le u_i^{\max} \tag{4}$$

   for each scalar quantity of interest u (density, energy, pressure etc.).

Following [14,18], we will limit all components of F_{ij} using the same scalar correction factor α_{ij}. The choice $\alpha_{ij} \equiv 1$ corresponds to the high-order approximation U_i^H, whereas $\alpha_{ij} \equiv 0$ corresponds to the low-order approximation U_i^L. Since the latter is assumed to satisfy the maximum principles, the bounds for (4) are commonly defined in terms of U^L as follows:

$$u_i^{\max} = \max_{j\in\mathcal{N}(i)} u_j^L, \qquad u_i^{\min} = \min_{j\in\mathcal{N}(i)} u_j^L, \tag{5}$$

where u_i^L is the low-order approximation to the quantity of interest and $\mathcal{N}(i)$ is the set of nodes containing i and its nearest neighbors $j \neq i$. Throughout this paper, the shorthand notation "$j \neq i$" is used for $j \in \mathcal{N}(i)\backslash\{i\}$.

For a scalar conserved quantity u, nearly optimal correction factors α_{ij} can be calculated using Zalesak's multidimensional FCT limiter [26] which we use to constrain the density ($u = \rho$) in the next section. The design of FCT algorithms for systems is more involved because of the strong coupling between the quantities of interest [13,18]. For example, any antidiffusive correction to ρ_i may produce an undershoot or overshoot in $\mathbf{v}_i := \frac{(\rho\mathbf{v})_i}{\rho_i}$ and/or $E := \frac{(\rho E)_i}{\rho_i}$ even if the values of $(\rho\mathbf{v})_i$ and $(\rho E)_i$ remain unchanged. Similarly, any adjustment of the conservative variables may result in a violation of local bounds for the pressure p defined by the equation of state (1). Hence, possible changes in the values of derived quantities must be taken into account when it comes to limiting the changes in the conservative variables.

In the next three sections, we present a new synchronized FCT algorithm for constraining the density, energy, and pressure. After formulating the inequality constraints for each variable, we derive upper bounds for the correction factors α_{ij} and design practical algorithms for enforcing these bounds.