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Flux-corrected transport algorithms preserving the eigenvalue range of symmetric tensor quantities

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A B S T R A C T

This paper presents a new approach to constraining the eigenvalue range of symmetric tensors in numerical advection schemes based on the flux-corrected transport (FCT) algorithm and a continuous finite element discretization. In the context of element-based FEM-FCT schemes for scalar conservation laws, the numerical solution is evolved using local extremum diminishing (LED) antidiffusive corrections of a low order approximation which is assumed to satisfy the relevant inequality constraints. The application of a limiter to antidiffusive element contributions guarantees that the corrected solution remains bounded by the local maxima and minima of the low order predictor.

The FCT algorithm to be presented in this paper guarantees the LED property for the maximal and minimal eigenvalues of the transported tensor at the low order evolution step. At the antidiffusive correction step, this property is preserved by limiting the antidiffusive element contributions to all components of the tensor in a synchronized manner. The definition of the element-based correction factors for FCT is based on perturbation bounds for auxiliary tensors which are constrained to be positive semidefinite to enforce the generalized LED condition. The derivation of sharp bounds involves calculating the roots of polynomials of degree up to 3. As inexpensive and numerically stable alternatives, limiting techniques based on appropriate estimates are considered. The ability of the new limiters to enforce local bounds for the eigenvalue range is confirmed by numerical results for 2D advection problems.

1. Introduction

During the last decades, advanced flux-corrected transport (FCT) algorithms have been developed for the numerical solution of convection-dominated transport problems using finite element approximations on unstructured meshes [9]. High-resolution schemes of FCT type distinguish themselves from traditional stabilization techniques like the streamline upwind Petrov–Galerkin (SUPG) method in that local maximum principles are enforced algebraically and the high order of accuracy is preserved in regions where the solution is smooth. This design philosophy ensures monotonicity of the solution and leads to robust algorithms.

While the FCT methodology has been successfully extended to systems of conservation laws like the Euler equations, current research challenges include limiting of (symmetric) tensor quantities which occur, e.g., in context of orientation and stress tensors to be discussed in this paper. In contrast to scalar variables, it is not entirely clarified which properties of tensor fields should be monitored and constrained to satisfy a relevant local maximum principle. The use of algorithms

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that limit each tensor component separately is not recommended since such limiting techniques are frame dependent and may fail to preserve physical properties like positive semidefiniteness. The objective limiter developed by Maire et al. [17] constrains the tensor components along flow-related directions. Luttwak and Falcovitz [16] proposed a tensor image polyhedron (TIP) approach based on the convex hull criterion initially developed for vectors [15]: The scaled/modified quantity of interest must lie in the convex hull of neighboring vectors/tensors. This limiting strategy guarantees that tensor components are constrained in a frame invariant manner and, hence, preserves the symmetry of numerical solutions. Related and more efficient extensions are proposed in [14], where bounding boxes (BB) enclosing the convex hull are exploited. In the context of bounds preserving reconstruction (remapping), tailor-made slope limiters for stress tensors were recently developed in [8,19] using principal invariants as quantities of interest: After separating the trace and limiting it as a scalar quantity, the second (and third) principal invariant of the traceless part are constrained separately. This strategy makes it possible to preserve low order bounds for the elastic energy density, an important conserved quantity proportional to the second invariant of the deviatoric stress tensor [8]. In addition, eigenvalues are implicitly constrained because of their relation to principal invariants.

In the context of orientation tensors which are defined as moments of an orientation distribution function, eigenvalues have a more important physical meaning: The eigenvectors represent the principal orientation directions, while the corresponding rates of alignment are represented by the eigenvalues [1,2]. This calls for the use of numerical methods that preserve the range of eigenvalues and motivates the following definition of local maximum principles in the present paper: *The minimal/maximal eigenvalue of a constrained orientation tensor should be bounded below/above by the local minimum/maximum of eigenvalues corresponding to an eigenvalue range preserving low order approximation.* In practice, the need for calculation or estimation of eigenvalues can be avoided using sufficient conditions which boil down to root isolation for polynomials of degree up to 3. The resulting *eigenvalue range limiters* preserve physical properties of orientation tensors and maintain their positive semidefiniteness. In simulations of fiber-reinforced polymers, a failure to control the range of eigenvalues may result in unphysical orientation states leading to unrealistic stresses and spurious velocities [23].

The paper is organized as follows: After motivating limiting based on (the range of) the eigenvalues (Sec. 2), an upwind-biased low order method originally developed for scalar transport equations is extended to tensorial variables and the corresponding local extremum diminishing (LED) property is proved for the semidiscrete and fully discrete problem (Sec. 3). Eigenvalue range preserving limiters for the antidiffusive element contributions (as defined in Sec. 4) are designed using sufficient conditions of positive semidefiniteness for auxiliary tensors (Sec. 5). The straightforward approach to enforcing these conditions involves worst case estimates or the use of a theorem by Caron et al. [4]. As an alternative to eigenvalue calculations, a criterion based on nonnegativity of the principle invariants is introduced in Sec. 5.3. It yields sharp estimates at the cost of root finding for cubic polynomials. Simplified criteria of positive semidefiniteness are derived using appropriate approximations which lead to cost-effective limiting procedures. Additionally, local maximum principles for the trace are enforced using the limiter presented in Sec. 6. This paper concludes with a numerical study and evaluation of the proposed limiting algorithms. The test problems considered in Sec. 7 represent tensorial extensions of well-known benchmark problems for linear advection of scalar quantities in incompressible flows.

1.1. Index convention for tensors

Without loss of generality, let the (real-valued) eigenvalues of a symmetric tensor $A \in \mathbb{R}^{d\times d}$, $d = 2, 3$, be sorted in increasing order. The notation $\lambda_1(A) \le \ldots \le \lambda_d(A)$ can be shortened by using the abbreviations $a_1 := \lambda_1(A), \ldots, a_d := \lambda_d(A)$ for the sorted eigenvalues. The double subscript notation a_{kl}, $1 \le k, l \le d$ will be used to identify components of A. The eigenvalues and entries of a tensor A_i will be referred to as $a_{i,k}$ and $a_{i,kl}$, respectively. Inequalities involving tensors are meant to hold for each eigenvalue. For example, the notation $A \ge 0$ will be used if A is positive semidefinite (similarly for $A \le 0$, $A > 0$, and $A < 0$).

2. Properties of interest

The problem to be considered is given by the linear transport equation

$$\begin{cases} \partial_t U + \operatorname{div}(\mathbf{v}U) = 0 & \text{in } \Omega, & \text{(a)} \\ U(\cdot,t) = U_{\text{in}} & \text{on } \Gamma_{\text{in}} = \{\mathbf{x} \in \partial\Omega : \mathbf{n}(\mathbf{x})\cdot\mathbf{v} < 0\}, & \text{(b)} \\ U(\cdot,0) = U_0 & \text{in } \Omega, & \text{(c)} \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ is a bounded domain, Γ_{in} is the inflow part of the boundary $\partial\Omega$, $\mathbf{n} : \partial\Omega \to \mathbb{R}^d$ is the unit outward normal vector, $\mathbf{v} : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^d$ is the velocity field, and $U : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^{d\times d}$ is the unknown symmetric tensor and variable of interest. The initial and boundary conditions are given by the (symmetric) tensor fields $U_0 : \Omega \to \mathbb{R}^{d\times d}$ and $U_{\text{in}} : \Gamma_{\text{in}} \times \mathbb{R}_0^+ \to \mathbb{R}^{d\times d}$.

At the continuous level, a solution of the scalar transport equation (1) is positivity preserving and satisfies the maximum principle if $\operatorname{div}(\mathbf{v}) = 0$. When tensorial unknowns are convected by divergence-free velocity fields, each scalar quantity $f : \mathbb{R}^{d\times d} \to \mathbb{R}$ corresponding to a differentiable function of the tensor entries evolves in the same manner as the solution of the scalar transport equation