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Flux-corrected transport techniques applied to the radiation transport equation discretized with continuous finite elements

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ABSTRACT

The Flux-Corrected Transport (FCT) algorithm is applied to the unsteady and steady-state particle transport equation. The proposed FCT method employs the following: (1) a low-order, positivity-preserving scheme, based on the application of M-matrix properties, (2) a high-order scheme based on the entropy viscosity method introduced by Guermond [1], and (3) local, discrete solution bounds derived from the integral transport equation. The resulting scheme is second-order accurate in space, enforces an entropy inequality, mitigates the formation of spurious oscillations, and guarantees the absence of negativities. Space discretization is achieved using continuous finite elements. Time discretizations for unsteady problems include theta schemes such as explicit and implicit Euler, and strong-stability preserving Runge–Kutta (SSPRK) methods. The developed FCT scheme is shown to be robust with explicit time discretizations but may require damping in the nonlinear iterations for steady-state and implicit time discretizations.

1. Introduction

The radiation transport equation, or linear Boltzmann equation, describes the transport of particles interacting with a background medium [2]. Some of its applications include the modeling of nuclear reactors, radiation therapy, astrophysical applications, radiation shielding, and high energy density physics [2–6]. This paper focuses on solution techniques applicable to the first-order form of the transport equation in Cartesian geometries, recalled below in Equation (1). The transport equation is a particle balance statement in a six-dimensional phase-space volume where $\mathbf{x}$ denotes the particle's position, $\mathbf{\Omega}$ its direction of flight, and E its energy:

$$\frac{1}{v(E)}\frac{\partial \psi}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(\mathbf{x},\mathbf{\Omega},E,t) + \Sigma_t(\mathbf{x},E,t)\psi(\mathbf{x},\mathbf{\Omega},E,t) = Q_{\text{tot}}(\mathbf{x},\mathbf{\Omega},E,t)\,. \tag{1}$$

$Q_{\text{tot}}(\mathbf{x},\mathbf{\Omega},E,t)$ denotes the total particle source gains in an infinitesimal phase-space volume due to particle scattering, extraneous source of particles (if any), and fission sources (in the case of neutron transport in multiplying media):

$$Q_{\text{tot}}(\mathbf{x},\mathbf{\Omega},E,t) \equiv Q_{\text{sca}}(\mathbf{x},\mathbf{\Omega},E,t) + Q_{\text{ext}}(\mathbf{x},\mathbf{\Omega},E,t) + Q_{\text{fis}}(\mathbf{x},\mathbf{\Omega},E,t)\,. \tag{2}$$

The source terms Q_{sca} and Q_{fis} linearly depend on the solution variable, the angular flux, denoted by ψ. Only simple configurations are amenable to an analytical solution of Equation (1). In most cases of relevance, the transport equation

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must be solved numerically; transport calculations fall under two main categories: stochastic calculations and deterministic calculations. The former category is referred to as Monte Carlo and relies on sampling large numbers of particle histories using random number generators [2], and the latter involves discretization of the phase-space and the use of iterative techniques. This work applies to the latter category. One common angular discretization is the discrete-ordinate or S_N method [2,5,7]; it is a collocation method in angle whereby the transport equation is solved only along discrete directions $\mathbf{\Omega}_d$ ($1 \leq d \leq n_{\mathbf{\Omega}}$, with $n_{\mathbf{\Omega}}$ the total number of discrete directions). One of the main advantages of the S_N technique is that it enables an iterative approach, called source iteration in the transport literature [2,5,7], to resolve both the particle's streaming and interaction processes and the scattering events as follows:

$$\frac{1}{v}\frac{\partial \psi_d^{(\ell)}}{\partial t} + \mathbf{\Omega}_d \cdot \nabla \psi_d^{(\ell)} + \Sigma_t \psi_d^{(\ell)} = Q_{\text{tot},d}^{(\ell-1)} \quad \forall d \in [1, n_{\mathbf{\Omega}}], \tag{3}$$

where ℓ is the iteration index and $\psi_d^{(\ell)}(\mathbf{x}, E, t) = \psi^{(\ell)}(\mathbf{x}, \mathbf{\Omega}_d, E, t)$. Hence, a system of $n_{\mathbf{\Omega}}$ decoupled equations are to be solved at a given source iteration index ℓ. For curvilinear geometries, an angular derivative term is present at iteration ℓ, and thus the equations are not decoupled; in this case, the scalar FCT methodology discussed in this work requires amendment. This allows solution techniques for scalar conservation laws to be leveraged in solving the system given by Equation (3). For brevity, the discrete-ordinate subscript d will be omitted hereafter and our model transport equation will consist in one of the $n_{\mathbf{\Omega}}$ transport equations for a given fixed source (right-hand side).

A common spatial discretization method for the S_N equations has been a Discontinuous Galerkin finite element method (DGFEM) with upwinding [8,9]. Here, however, a Continuous Galerkin finite element method (CGFEM) is applied. Some recent work by Guermond and Popov [1] on solution techniques for conservation laws with CGFEM addresses some of the main disadvantages of CGFEM versus DGFEM, including the formation of spurious oscillations. The purpose of the present paper is to demonstrate a proof of concept for the application of such solution techniques to the transport equation. Furthermore, some or all of the methodology explored in this paper can be later extended to DGFEM as well; see, for instance, Zingan et al. [10] where the techniques proposed by Guermond and Popov [1] have been ported to DGFEM schemes for Euler equations.

One of the main objectives of this paper is to present a method that precludes the formation of spurious oscillations and the negativities that result from these oscillations; these issues have been a long-standing issue in the numerical solution of the transport equation [11]. Not only are these negativities physically incorrect (a particle's distribution density must be non-negative), but they can cause simulations to terminate prematurely, for example in radiative transfer where the radiation field is nonlinearly coupled to a material energy equation. Many attempts to remedy the negativities in transport solutions rely on ad-hoc fix-ups, such as the set-to-zero fix-up for the classic diamond difference scheme [5]. Recent work by Hamilton introduced a similar fix-up for the linear discontinuous finite element method (LDFEM) that conserves local balance and preserves third-order accuracy [12]. Walters and Wareing developed characteristic methods [13], but Wareing later notes that these characteristic methods are difficult to implement and offers a nonlinear positive spatial differencing scheme known as the exponential discontinuous scheme [14]. Maginot has recently developed a consistent set-to-zero (CSZ) LDFEM method [15], as well as a non-negative method for bilinear discontinuous FEM [16,17].

In fluid dynamics, traditional approaches to remedy the issue of spurious oscillations include the flux-corrected transport (FCT) algorithm, introduced in 1973 as the SHASTA algorithm for finite difference discretizations by Boris and Book [18], where it was applied to linear discontinuities and gas dynamic shock waves. To the best of our knowledge, these FCT techniques have not been applied to the particle transport equation. The main idea of the FCT algorithm is to blend a low-order scheme having desirable properties with a high-order scheme which may lack these properties. Zalesak improved methodology of the algorithm and introduced a fully multi-dimensional limiter [19]. Parrott and Christie extended the algorithm to the finite element method on unstructured grids [20], thus beginning the FEM-FCT methodology. Löhner et al. applied FEM-FCT to the Euler and Navier–Stokes equations and began using FCT with complex geometries [21]. Kuzmin and Möller introduced an algebraic FCT approach for scalar conservation laws [22] and later introduced a general-purpose FCT scheme, which is designed to be applicable to both steady-state and transient problems [23]. In these FEM-FCT works and others [24–26], the high-order scheme used in the FCT algorithm was the Galerkin finite element method, but this work uses the entropy viscosity method developed by Guermond and others [1].

Recent work by Guermond and Popov addresses the issue of spurious oscillations for general conservation laws by using artificial dissipation based on local entropy production, a method known as entropy viscosity [1]. The idea of entropy viscosity is to enforce an entropy inequality on the weak solution, and thus filter out weak solutions containing spurious oscillations. However, entropy viscosity solutions may still contain spurious oscillations, albeit smaller in magnitude, and consequently negativities are not precluded. To circumvent this deficiency, Guermond proposed using the entropy viscosity method in conjunction with the FCT algorithm [27]; the high-order scheme component in FCT, traditionally the unmodified Galerkin scheme, is replaced with the entropy viscosity scheme. For the low-order scheme, Guermond also introduced a discrete maximum principle (DMP) preserving (and positivity-preserving) scheme for scalar conservation laws [28].

The algorithm described in this paper takes a similar approach to the algorithm described in the work by Guermond and Popov for scalar conservation laws, but is extended to allow application to the transport equation, which does not fit the precise definition of a conservation law but is instead a balance law since it includes sinks and sources, namely the reaction term $\Sigma_t \psi$ and the source term Q_{tot}. The presence of these terms is also a novelty in the context of the FCT algorithm.