Journal of Computational Physics 231 (2012) 6801–6826

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A non-negative moment-preserving spatial discretization scheme for the linearized Boltzmann transport equation in 1-D and 2-D Cartesian geometries

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ARTICLE INFO

Article history:
Received 24 August 2011
Received in revised form 8 March 2012
Accepted 12 June 2012
Available online 26 June 2012

Keywords:
Strictly non-negative closure
Discrete ordinates method
Radiation transport
Discontinuous finite elements

ABSTRACT

We present a new nonlinear spatial finite-element method for the linearized Boltzmann transport equation with S_n angular discretization in 1-D and 2-D Cartesian geometries. This method has two central characteristics. First, it is equivalent to the linear-discontinuous (LD) Galerkin method whenever that method yields a strictly non-negative solution. Second, it always satisfies both the zeroth and first spatial moment equations. Because it yields the LD solution when that solution is non-negative, one might interpret our method as a classical fix-up to the LD scheme. However, fix-up schemes for the LD equations derived in the past have given up solution of the first moment equations when the LD solution is negative in order to satisfy positivity in a simple manner. We present computational results comparing our method in 1-D to the strictly non-negative linear exponential-discontinuous method and to the LD method. We present computational results in 2-D comparing our method to a recently developed LD fix-up scheme and to the LD scheme. It is demonstrated that our method is a valuable alternative to existing methods.

1. Introduction

The linearized Boltzmann transport equation describes the transport of radiation or particles that interact with a background medium but have no self interactions. Examples of such particles include neutrons and gamma rays. The S_n or discrete-ordinates method is perhaps the most popular and widely used angular discretization for this equation. Spatial discretization methods for the S_n equations can produce negative angular flux solutions, which are clearly non-physical. Such negativities can arise in 1-D Cartesian geometry calculations only in optically thick cells but, in multidimensional Cartesian geometries, negativities can also arise in voids. Characteristic methods based upon polynomial scattering source representations of degree greater than zero, such as the Linear Characteristic method (LC) are always non-negative in 1-D geometry as long as the projected scattering source remains non-negative. In 2-D such methods are always positive as long as the projected scattering source and projected outflow boundary fluxes remain positive [1]. The Step Characteristic method (SC), which is based upon a constant scattering source representation [1], is strictly positive and formally second-order accurate, but it can be particularly inaccurate in multidimensional calculations due to a high degree of numerical diffusion resulting from the constant dependence of the angular flux that is assumed on cell faces. Furthermore, unlike most higher-order characteristic methods, the step method possesses neither the intermediate [2] nor the thick diffusion limit [3,4]. This can make it require an over-resolved mesh for even mildly diffusive problems.

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http://dx.doi.org/10.1016/j.jcp.2012.06.018

Several methods to eliminate or mitigate negativities have been devised in the past. Such methods can generally be divided into two categories: (1) so-called ad-hoc "fix-ups" and (2) inherently non-negative nonlinear moments methods. An example of the former type is the diamond difference scheme with set-to-zero fix-up [5], while examples of the latter include various exponential characteristic methods [6–8].

Ad-hoc fix-up schemes have been traditionally related to moments methods with non-smooth closures. Hence, their associated equations have generally been solved via a fixed-point iteration rather than Newton's method. This fixed-point approach is always effective for purely absorbing problems, but when scattering is present, it has been found to interact poorly with sophisticated convergence acceleration schemes such as the diffusion-synthetic acceleration (DSA) method [9], particularly in problems where acceleration is most needed [10]. If acceleration techniques are not applied, the fixed-point approach is generally effective, but unacceptably slow convergence is obtained in highly diffusive problems.

Inherently non-negative nonlinear methods, such as the linear exponential characteristic method and the linear exponential discontinuous finite-element method (ED) [11], have smooth nonlinearities and thus can be solved using Newton's method. However, characteristic methods are expensive, particularly on non-orthogonal meshes, and cannot be applied in curvilinear coordinates. Although exponential finite-element methods are less complicated than characteristic methods and can be applied in curvilinear coordinates (assuming an exponential representation in angle as well as in space), they can suffer from a lack of fine-mesh accuracy relative to analogous polynomial-based discontinuous finite-element schemes. For instance, Wareing showed that, in 1-D slab-geometry, ED can be less accurate than the linear-discontinuous Galerkin finite-element method (LD) when the mesh is highly refined [11].

Our purpose here is to devise a new nonlinear spatial finite-element method for the S_n equations in 1-D and 2-D Cartesian geometries. This method has two central characteristics. First, it is equivalent to the LD scheme whenever LD yields a strictly non-negative solution. Second, the new scheme always satisfies both the zeroth and first spatial moment equations. Because it yields the LD solution when that solution is non-negative, one could interpret our method as a fix-up scheme. However, fix-up schemes defined in the past for the LD equations do not satisfy the first moment equation when the LD solution is negative in order to satisfy positivity in a simple manner [12].

The equations associated with our scheme are not smooth, but they are everywhere continuous and the Jacobian matrix is discontinuous at only a finite number of points. Since our equations do not have a continuous Jacobian, the applicability of Newton's method might seem to be questionable. However, Fichtl, et al., [13] have recently been able to reliably apply Newton's method to the LD equations using a traditional fix-up scheme having a continuous set of equations with a pointwise-discontinuous Jacobian.

Work for this paper originally began as the 2-D extension of another strictly non-negative finite-element closure for the zeroth and first S_n moment equations [14]. However, some practical implementation difficulties together with the results of Fichtl, et al., motivated us to develop the present approach, yielding an inherently non-negative finite-element scheme. The new method presented herein represents the discontinuous finite-element analog of a characteristic scheme originally developed for both slab and rectangular geometries by Mathews and Minor [15,16]. Qualitatively, the new method assumes an angular flux distribution within a cell that is defined to be equal to a linear function at all points for which that linear function is non-negative, and zero at all points for which that linear function is negative. Given a valid set of spatial moments, an angular flux representation having those moments can be uniquely constructed using this formulation. While we have not formally proved this property, we have successfully tested it numerically. In particular, we have been able to specify a valid set of moments and then solve for the corresponding representation having those moments. The only caveat is that the method becomes increasingly ill-conditioned as the specified moments approach those of a delta-function at either of the cell endpoints. This same type of ill-conditioning occurs with the exponential discontinuous representation, and can be expected to occur with essentially any representation that does not explicitly contain delta-functions. Since our general angular flux representation is obtained from a linear function via a set-to-zero procedure, we refer to our new technique as the consistent set-to-zero method (CSZ).

The linear S_n equations are generally solved via source iteration [5]. Each source iteration requires the inversion of an independent block lower-triangular system for each direction and energy in a process known as a sweep. Since our equations are nonlinear, we use Newton's method to solve our equations. There are two ways to implement this method. The first is to apply Newton's method to each independent set of sweep equations, effectively solving a nonlinear system for each scattering source iterate. In this case, Newton's method is nested within the source iteration process. An important property of this approach is that the independent nonlinear sweep equations for each direction and energy can be solved one spatial cell at a time. Hence the nonlinear systems that must be individually solved are quite small. In addition, storing the full angular flux iterate can be avoided simply by re-starting the nonlinear iterations with a zero guess for each source iteration. More specifically, once the angular flux solution for a single cell, direction, and energy is obtained and the associated contributions to both the scattering source in that cell and the inflow source for the next downstream cell are computed, the angular flux solution for that cell, direction, and energy can be discarded. The ability to avoid storage of the full angular flux iterate is the primary advantage of this approach. This approach has traditionally been used to solve nonlinear S_n equations. For many years after the introduction of S_n codes, storage of the full angular flux solution was simply not practical, and it is still often avoided today. The primary disadvantage of this approach is that if one is to apply convergence acceleration techniques to the source iteration process, they must be applied to a nonlinear system. DSA has been applied to nonlinear forms of the transport equation [17], but nonlinear DSA is far less theoretically understood and potentially much less robust than linear DSA.