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Parallel sweep-based preconditioner for the solution of the linear Boltzmann transport equation

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ABSTRACT

The Boltzmann transport equation is solved in the context of radiative heat transfer, for an isotropically scattering medium with reflecting boundaries. Under these circumstances, the different ordinates of the angular flux are mutually coupled. We explore here the use of a parallel sweep-based block diagonal preconditioner as a complement of the GMRES solver on the solution of the discretization matrix (which includes all the inter-ordinate couplings). The validity of this approach, when compared to the standard source iteration scheme, is successfully assessed for a significant range of the coupling parameters.

1. Introduction

The Boltzmann transport equation (BTE) is used to model many phenomena of interest where a physical magnitude is transported by independent particles. In many applications, the scattering effect of the medium plays a significant role in the process and needs to be well resolved. For example, in the area of radiative heat transfer, photon scattering needs to be considered in many situations [1]; some medical physics applications, like the external beam therapy, rely on photon–electron scattering to reveal density variations of a tissue [2]; and nuclear power reactor design also requires neutron scattering to be included in the model. The solution of the time dependent Boltzmann equation can also be seen as a low density limit of continuum equations like the heat diffusion equation or the Navier–Stokes equations [3,4]. In this work, scattering effects are considered from a mathematical point of view, as a part of the couplings contained in a single discretization matrix of dimension $n \times m$, where n and m are the number of spatial and angular elements of the discretization, respectively.

The simplest method to deal with the angular couplings induced by scattering media is the source iteration (SI) scheme: the angular couplings are deferred to the source term, decoupling the system into m subsystems of dimension n, one for the spatial couplings of each angular ordinate. However, the convergence rate of the SI has been shown to be highly sensitive to the scattering/extinction ratio [5,6] and, being a stationary method, it can be affected by the false convergence phenomenon. False convergence is produced when the convergence is so slow that it is difficult to determine when the iterations have suitably converged [5].

The convergence rate of the SI method can be improved by using accelerators [7–9]. However, more sophisticated iterative methodologies can also be considered. Among the most prominent options there are the Krylov subspace projection methods [10]. In particular, in this work, the GMRES is considered to deal with this highly sparse linear system derived from de discretization of the BTE. Previous works using similar strategies are outlined in the next paragraphs.

An example of using the GMRES method on the solution of the discrete BTE can be found in the work by Patton and Holloway [6]. They used a GMRES solver with an ILU preconditioner, and compared it to a standard SI based on transport sweeps to solve each ordinate and diffusion synthetic acceleration (DSA) schemes to improve its convergence. They showed that the GMRES strategy performs well on a wide range of test cases, matching the SI + DSA performance or even surpassing it, especially for highly anisotropic cases. They also used the GMRES to accelerate fixed point iteration methods, such as the SI, on the solution of the scalar flux. In this case, the performance of the GMRES was not as good as the one provided by the DSA. Moreover, they note that using the GMRES the computational time grows super-linearly with the number of ordinates, because of preconditioning set-up costs. They concluded

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that the use of an ILU preconditioner is only justified if its cost can be amortized. This last remark, together with the performance exhibited by the GMRES, suggests that a highly scalable and efficient preconditioner with low set-up costs would be highly valuable.

Drumm and Fan [11] proposed a preconditioner obtained by discarding the scattering terms of the BTE, referred by them as an uncollided-flux preconditioner. Their work shows that this preconditioner is especially well suited for the solution of coupled electron-photon transport problems. They solved the weak form of the even parity transport equation, which results in a symmetric positive definite matrix solvable with the CG [10] method. The uncollided-flux preconditioner was also inverted with the CG. For the test problem considered in their work, significant improvements in number of iterations and computation time were observed.

Pautz et al. [12] explored the use of preconditioning algorithms for second order discretizations of the Boltzmann transport equation. The matrix resulting from their discretization is symmetric positive definite. Two different preconditioners are considered, the CG and a KLU. They reported that the number of iterations decreases significantly with respect to the non-preconditioned case. The smallest number of iterations is achieved using the KLU, although this variant shows a poor parallel efficiency. This work, however, did not address the possibility of using Krylov methods on first order discretizations.

Oliveira and Deng [13] used different solvers and preconditioners to solve transport equations. They considered the angular flux on a one dimensional slab. They used different Krylov methods (CGS, GMRES, CGNE), with ILU and spatial and angular multigrid preconditioners. They showed that the use of preconditioning techniques dramatically reduces the number of iterations required to achieve the desired degree of accuracy. The performance observed for the different methods is sensible to the ratio absorption/scattering of the considered test case.

The work by Gupta and Modak [14] is a useful reference on iterative methods for the neutron transport equation. Several iterative algorithms, based on the conjugate gradient (CG) method, are discussed for the solution of the scalar flux. A sequential sweep procedure is used within the general iterative algorithm, increasing the efficiency of the computations. They compared these schemes to the traditional source iteration method for a number of problems. Using the improved iterative methods, the number of iterations decreased and the computation time shortened significantly.

In this paper we are considering the PSD-b method [15] (parallel sweep by directions using buffering) as a block diagonal preconditioner for the GMRES solver on the solution of the BTE. The sweep-based strategy is applicable when upwind-like schemes are used for the spatial discretization, deriving into a triangular subsystem for each ordinate. The motivation to use this strategy has been the notable performance achieved with the PSD-b on the parallel solution of the block diagonal subsystems, obtained when the inter-ordinate couplings are discarded. With this new method, the number of iterations is greatly reduced respect to the standard sweep-based SI algorithm, without increasing the iteration costs. The usefulness of this approach is shown for an homogeneous medium with isotropic scattering and reflecting boundary conditions.

2. Mathematical model

2.1. Boltzmann transport equation

The time independent Boltzmann Transport Equation (BTE) is a conservation equation that accounts for the number ψ of straight-propagating particles crossing a unit area normal to a given direction per unit time, and their interaction with the medium where they are propagating in. The angular flux ψ depends on the location $x \in \mathbb{R}^3$ and the angular direction $s \in S^2$. In a general form, and omitting the spatial dependence in all terms for clarity, the BTE can be written as [16]

$$\frac{d\psi^s}{d\ell(s)} + \beta_1\psi^s = \beta_0 + \beta_2 \int_{4\pi} \psi^{s'} f^{s's} d\Omega'. \quad (1)$$

This equation describes the variation of ψ in a straight path along direction s, through a unit area normal to s, where the variable $\ell(s)$ is the length of such path. This variation is divided into three contributions, with different functional dependence on ψ, to better capture the behavior of different physical phenomena. Note that in the integral term the angular flux $\psi^{s'}$ is multiplied by the *phase function* $f^{s's}$, that accounts for the probability of a particle changing its propagation direction from s' to s, subject to $\int_{4\pi} f^{s's} d\Omega = 1$ for each direction s'. The possible dependences of ψ on time or on different velocities of the particles is not considered. To take this into account additional terms must be added.

The boundary conditions for the BTE are summarized in the following equation:

$$\psi^s = b^s - \beta_3 \int_{\cos\theta<0} \psi^{s'} \cos\theta d\Omega', \quad (2)$$

where b^s is a prescribed value at the boundary, and the integral term accounts for the (diffuse) reflection of particles at the boundary, being θ the angle between the inward normal to the surface and the direction s'.

The meaning of the various coefficients $\{\beta_i\}$ depends on the phenomena being modeled. In the context of radiative heat transfer, the coefficients $\beta_{0,1,2,3}$ represent the emission, extinction, scattering, and reflection processes, respectively. In particular:

$$\beta_0 = \kappa I_b, \quad \beta_1 = \kappa + \sigma, \quad \beta_2 = \sigma, \quad \beta_3 = \rho/\pi.$$

where κ and σ are the absorption and scattering coefficients, respectively, ρ is the reflectivity of the walls, I_b the black body emission function (that depends on the temperature and photon wavelength), and b^s is the surface emission (that depends on the temperature and surface properties). In the case of isotropically scattering $f^{s's} = 1/4\pi$ for all s' and s. Additional details of these coefficients can be found in [16].

2.2. Discretization

The Discrete Ordinates Method (DOM) and an unstructured finite volume method are used for the discretization of the BTE over the angular and spatial subdomains, respectively. The angular integrals are approximated by means of an m-point quadrature, where the integrand is evaluated at some prescribed directions, represented by the unitary vectors $\hat{\mathbf{s}}_i$, and weighted accordingly:

$$\int_{4\pi} \phi^s d\Omega \simeq \sum_{i=1}^{m} \omega^i \psi^i, \quad (3)$$

where ψ^i and ω^i are the flux and the weighting coefficient for ordinate i, respectively. Götz [17] gives an overview on different quadrature sets. In this paper we are using the quadrature sets S_4, S_8 [16], and S_{12} [18], with 24, 80, and 168 ordinates respectively. Therefore, the BTE becomes a system of m differential equations coupled together, one equation for each quadrature point:

$$\frac{d\psi^i}{d\ell(s_i)} = \hat{\mathbf{s}}_i \cdot \nabla\psi^i = -(\beta_1 - \beta_2\omega^i f^{ii})\psi^i + \beta_0 + \beta_2 \sum_{j\neq i} \omega^j f^{ji} \psi^j. \quad (4)$$

The spatial discretization on unstructured meshes is carried out by means of a finite volume approach. Integrating the left hand side