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The adaptive collision source method for discrete ordinates radiation transport

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ABSTRACT

A novel collision source method has been developed to solve the Linear Boltzmann Equation (LBE) more efficiently by adaptation of the angular quadrature order. The angular adaptation method is unique in that the flux from each scattering source iteration is obtained, with potentially a different quadrature order used for each. Traditionally, the flux from every iteration is combined, with the same quadrature applied to the combined flux. Since the scattering process tends to distribute the radiation more evenly over angles (i.e., make it more isotropic), the quadrature requirements generally decrease with each iteration. This method allows for an optimal use of processing power, by using a high order quadrature for the first iterations that need it, before shifting to lower order quadratures for the remaining iterations. This is essentially an extension of the first collision source method, and is referred to as the adaptive collision source (ACS) method. The ACS methodology has been implemented in the 3-D, parallel, multigroup discrete ordinates code TITAN. This code was tested on a several simple and complex fixed-source problems. The ACS implementation in TITAN has shown a reduction in computation time by a factor of 1.5–4 on the fixed-source test problems, for the same desired level of accuracy, as compared to the standard TITAN code.

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1. Introduction

The discrete ordinates (S_N) method is one of the standard methods to discretize the angular variable in the Linear Boltzmann Equation (LBE) that governs radiation transport, and is used in many production radiation transport codes (Sjoden and Haghighat, 1997; Yi and Haghighat, 2010; Rhoades and Childs, 1987; Wareing et al., 1997). In the discrete ordinates method, the LBE is solved over a set of angular directions Ω_i (also called ordinates), with corresponding weights w_i (Chandrasekhar, 1950; Carlson, 1970). This combination of (Ω_i, w_i) is called an angular quadrature set. A quadrature set allows the angular integrals to be converted into sums over the angles of the set. Selection of an appropriate angular quadrature set is one of the difficulties with the discrete ordinates method (Lathrop, 1971; Lewis and Miller, 1984). Depending on the problem, the flux may vary greatly in direction (that is, very anisotropic). An anisotropic function would require many quadrature points in order to properly resolve the integrals. Using a quadrature order that is too low will result in large errors from so-called "ray effects", while using an order too high greatly increases computation time (Lathrop, 1968).

There have been several methods developed to optimize the efficiency of the angular quadrature in discrete ordinates calculations. The first is simply in the selection of better general quadrature sets that can more accurately integrate the angular flux for the same total number of directions (Jarrell and Adams, 2011; Ahrens, 2012; Manalo et al., 2015). Another method is local angular refinement (Longoni and Haghighat, 2001, 2002a,b; Longoni, 2004), which involves adding quadrature points in angular directions of high anisotropy, while leaving a coarse distribution of points in the more isotropic directions. This has been implemented in the static, user defined case in production codes (Sjoden and Haghighat, 1997; Yi and Haghighat, 2010) and some work has been done to perform this refinement adaptively (Stone and Adams, 2003; Stone, 2007; Jarrell, 2010; Jarrell and Adams, 2011). There is also the so-called first-collision source method (Alcouffe, 1985; Alcouffe et al., 1990), which is more closely related to the subject of this paper. This involves calculating the un-collided flux using a high-order transport method and then using this to generate a first-collision source, which is used to start a low order transport calculation to solve for the collided flux and thus save on computation time. This method has been implemented with success into

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several transport codes (Wareing et al., 1997, 1998; Lathrop, 1971; Lillie, 1998).

The new adaptive collision source (ACS) method described in this paper builds off the first-collision source method by separating not just the uncollided flux, but also the once-collided flux, twice-collided flux, etc. At each transport iteration, only the i'th collided flux is solved for, and the possibility of using different angular quadrature orders for each is allowed. An intelligent scheme is also developed with which to choose, on-the-fly, an appropriate angular quadrature for each iteration. This can achieve the good speed-ups of the first-collision source method, but is more robust to a wide variety of problems for which the first collision source is not as effective.

This paper is organized as follows: first, some background theory is given. Next the first-collision source method is discussed, followed by its extension to the new adaptive collision source (ACS) method (Walters and Haghighat, 2013a,b, 2014). For the ACS method, the general theory will be discussed followed by the implementation of the ACS algorithm into the TITAN transport code. Finally, the results of the ACS method will be compared to the standard TITAN source iteration on several test problems.

2. Theory

2.1. The linear Boltzmann equation

The steady-state LBE (Bell and Glasstone, 1970) for a fixed source problem describes the balance of the angular flux $\Psi(\vec{r}, E, \Omega)$ in a phase space $(d^3\vec{r}\, dE\, d\Omega)$.

$$\hat{\Omega} \cdot \nabla\Psi(\vec{r}, E, \Omega) + \sigma(\vec{r}, E)\Psi(\vec{r}, E, \Omega) = Q_0(\vec{r}, E, \Omega) + \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega})\Psi(\vec{r}, E, \Omega) \quad (1)$$

An important quantity derived from the angular flux is the scalar flux ϕ, defined in Eq. (2).

$$\phi(\vec{r}, E) = \int_{4\pi} d\Omega \Psi(\vec{r}, E, \Omega) \quad (2)$$

2.2. Angular quadrature

For the discrete ordinates method, consider that the LBE holds over a set of discrete angles (or ordinates). This allows an integral over angle to be replaced by a weighted sum over the discrete ordinates:

$$\int_{4\pi} d\Omega f(\Omega) = \sum_m^M w_m f(\Omega_m) \quad (3)$$

where m is the ordinate index, M is the total number of ordinates, Ω_m is the angle of the m'th ordinate and w_m is the weight of the m'th ordinate. The set of weights and angles (called a quadrature set) must be chosen carefully to ensure conservation of various integral properties such as current and scalar flux moments. In this work, Legendre-Chebyshev quadrature sets are used (Longoni, 2004; Longoni and Haghighat, 2002b), denoted by S_N where N is called the quadrature order. The total number of ordinates M in the set in a 3-D geometry given by $M = N(N+2)$. For example, the S_{20} quadrature set has $M = 20(20+2) = 440$ ordinates, while S_6 has only 48. This can mean a huge difference in computation time between these sets.

2.3. Source iteration

The LBE can be written in operator form as:

$$H\Psi = S\Psi + Q_0 \quad (4)$$

where the streaming-collision operator H is defined as in Eq. (5).

$$H = \hat{\Omega} \cdot \nabla + \sigma(\vec{r}, E) \quad (5)$$

The scattering operator S is defined in Eq. (6).

$$S = \int_0^\infty dE' \int_{4\pi} d\Omega \sigma_s(\vec{r}, E' \to E, \Omega' \cdot \Omega) \quad (6)$$

In the standard source iteration method, an initial flux $\Psi^{(0)}$ (usually 0) is assumed, then the flux is calculated assuming a constant scattering source $S\Psi$, then the source is updated and the flux recalculated.

$$H\Psi^{(i)} = S\Psi^{(i-1)} + Q_0 \quad (7)$$

where $\Psi^{(i)}$ is the flux after iteration i. This operation, the solving of Eq. (7), is commonly referred to as a transport sweep. After a sufficient iteration, both sides of the equation will converge to within some given tolerance.

2.4. First collision source method

In the first-collision source (FCS) method, the flux is split into the uncollided (Ψ_u) and collided (Ψ_c) fluxes, as in Eq. (8).

$$\Psi = \Psi_c + \Psi_u \quad (8)$$

If we insert the above Eq. (8) into Eq. (4), we can arrive at a set of coupled transport equations in Eq. (9) and Eq. (10)

$$H\Psi_u = Q_0 \quad (9)$$

$$H\Psi_c = Q_c + S\Psi_c \quad (10)$$

where the first-collision source Q_c is defined in Eq. (11)

$$Q_c = S\Psi_u \quad (11)$$

Eq. (9) requires no iterations on the scattering source, and could be solved relatively quickly using a high-order method (e.g., high order S_N or ray-tracing). Eq. (10) looks exactly like the standard LBE, except the independent source Q_0 is replaced with the first-collision source derived from the un-collided flux. This collided flux can then be solved using a lower quadrature order S_N in a standard source iteration method relatively quickly. Again, the motivation behind this is that the un-collided flux has a much higher angular variation than the collided flux, so generally requires a more robust treatment of the angular variable than does the collided flux.

3. Adaptive collision source (ACS) methodology

The new ACS methodology builds on the first-collision source method to a type of n'th-collision source method using discrete ordinates. Instead of splitting the flux up into uncollided flux and collided flux, we expand the total flux (denoted as $\Psi_{t,n}$) into the fluxes of different collision source order (i.e., 0 to n).

$$\Psi_{t,n} = \Psi_0 + \Psi_1 + \Psi_2 + \cdots \Psi_n \quad (12)$$

We truncate the series at the n'th collision. The uncollided flux and collided flux can be defined in terms of the i'th collided fluxes as follows:

$$\Psi_u = \Psi_0 \quad (13)$$

$$\Psi_c = \Psi_1 + \Psi_2 + \cdots \Psi_n \quad (14)$$

Now we arrive at a similar formulation as the first-collision source method:

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