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Diffusion synthetic methods for computational modeling of one-speed slab-geometry transport problems with linearly anisotropic scattering

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ABSTRACT

Two diffusion synthetic methods are described for computational modeling of one-speed, slab-geometry transport problems with linearly anisotropic scattering. These methods are referred to as diffusion synthetic methods, since the lower-order diffusion is used to *simplify* numerical solutions to the higher-order transport equation. In part I of this paper the word *simplify* is used in the sense of reducing the number of iterations to a prescribed stopping criterion; in other words, in the sense of accelerating the iteration on the scattering source in discrete ordinates (S_N) calculations, by generating an improved initial guess. In part II, the word *simplify* is used in the sense of generating numerical results for the angular flux by solving analytically the first-order form of the transport equation in slab geometry with diffusion approximation for the scattering source integral terms. As with these two offered synthetic methods, special approximate boundary conditions are used in the diffusion equation to account for prescribed incident flux on the outer boundaries of the slab, including vacuum boundary conditions. Numerical results are given to illustrate the application of these two synthetic methods.

1. Introduction

Deterministic computational modeling of particle transport classically leads to the discretization of the linearized Boltzmann equation into a system of linear algebraic equations. Since this system has typically large size, iterative schemes are usually chosen, instead of direct methods. The most basic transport iteration scheme is source iteration (SI) (Lewis and Miller, 1993). For slabs composed of optically thick (low leakage) and scattering-dominated spatial regions, particles typically undergo many collisions before they are captured or leak out. For such systems, the SI scheme converges slowly and efficient acceleration strategies are of great interest for computational modeling (Adams and Larsen, 2002). In this context, it is well known that synthetic acceleration techniques are very efficient (Koop, 1963; Reed, 1971; Alcouffe, 1977; Duderstadt and Martin, 1979; Adams and Larsen, 2002; Santos et al., 2011; Ficht et al., 2011; Anistratov, 2011).

The class of problems soluble in closed form in transport theory is rather limited (Case and Zweifel, 1967); therefore, we offer in this paper a synthetic technique based on diffusion theory for approximate solution of the first-order form of one-speed, slab-geometry transport equation with linearly anisotropic scattering.

We divide this paper into two major parts. In part I, we describe an acceleration scheme based on an improved initial guess for the scattering source terms within the slab. In other words, as initial guess for the fine-mesh scattering source terms, we use the coarse-mesh solution of diffusion equation with special boundary conditions to account for the prescribed boundary conditions in the discrete ordinates (S_N) formulation of the transport equation (Lewis and Miller, 1993). To achieve this goal, we first implement a spectral nodal method (SND) that generates coarse-mesh diffusion solution that is completely free from spatial truncation errors, then we reconstruct this coarse-mesh solution within each spatial cell of the coarse discretization grid, to further yield the initial guess for the fine-mesh scattering source in the first S_N transport sweep across the fine spatial grid ($\mu_m > 0$ and $\mu_m < 0$, $m = 1{:}N$), as is conventional in the SI scheme. At this point we remark that spatial discretization is not essential, as one can set up a spatial grid composed of one single node per region of a multilayer slab, since the present SND method is absolutely free from spatial truncation errors. In part II,

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we describe a synthetic method to solve the one-speed slab-geometry transport problems with linearly anisotropic scattering, wherein we approximate the scattering source terms by the diffusion solution generated by the coarse-mesh SND method coupled with the aforementioned spatial reconstruction scheme. We refer to this numerical scheme as the diffusion synthetic angular reconstruction scheme.

In Sections 2 and 3, we present parts I and II, as briefly summarized above, and a brief discussion is given in Section 4. We describe the SND method with the spatial reconstruction scheme for diffusion numerical solution in the Appendix.

2. Part I: diffusion synthetic method for the initial guess in scattering source iterations

Let us consider the one-speed, fixed-source, slab geometry, S_N problems with linearly anisotropic scattering

$$\begin{aligned}\mu_m\frac{\mathrm{d}}{\mathrm{d}x}\psi_m(x)+\sigma_T(x)\psi_m(x) &= \frac{1}{2}\sigma_{S0}(x)\sum_{n=1}^{N}\psi_n(x)\omega_n \\ &+\frac{3}{2}\mu_m\sigma_{S1}(x)\sum_{n=1}^{N}\mu_n\psi_n(x)\omega_n+Q(x), \\ 0\le x\le X,\ \ m &= 1:N,\end{aligned} \tag{1}$$

with isotropic boundary conditions

$$\psi_m(0) = f,\ \ \mu_m>0, \tag{2}$$

and

$$\psi_{\mathrm{m}}(\mathrm{X}) = g,\ \ \mu_m<0. \tag{3}$$

Our notation is standard (Lewis and Miller, 1993): $\psi_m(x)=\psi(x,\mu_m)$ is the angular flux of particles traveling in direction μ_m; ω_m is the angular weight for direction μ_m; σ_T is the total macroscopic cross section; σ_{S0} and σ_{S1} are respectively the isotropic and the linearly anisotropic components of the differential scattering macroscopic cross section; and Q is the prescribed interior source.

Now, we consider a fine-mesh spatial grid composed of J_F discretization nodes on a slab of thickness X, as shown in Fig. 1, and we integrate Eq. (1) inside one spatial node. The result is the standard spatially discretized S_N balance equations

$$\begin{aligned}\frac{\mu_m}{h_j}\left(\psi_{m,j+1/2}-\psi_{m,j-1/2}\right)+\sigma_{Tj}\overline{\psi}_{m,j} &= \frac{1}{2}\sigma_{s0j}\sum_{n=1}^{N}\overline{\psi}_{n,j}\omega_n \\ &+\frac{3}{2}\mu_m\sigma_{s1j}\sum_{n=1}^{N}\mu_n\overline{\psi}_{n,j}\omega_n+Q_j, \\ m &= 1:N,\ \ j=1:J_F,\end{aligned} \tag{4}$$

where we have defined the node-average angular flux

$$\overline{\psi}_{m,j} = \frac{1}{h_j}\int_{x_{j-1/2}}^{x_{j+1/2}}\psi_m(x)\mathrm{d}x. \tag{5}$$

Using the angular quadrature formula, we approximate the node-average scalar flux and current respectively as

$$\overline{\phi} = \sum_{n=1}^{N}\overline{\psi}_{n,j}\omega_n \tag{6}$$

and

$$\overline{J}_j = \sum_{n=1}^{N}\mu_n\overline{\psi}_{n,j}\omega_n,\ \ j=1:J_F. \tag{7}$$

A simple count indicates that Eq. (4) for $m=1{:}N$ and $j=1{:}J_F$ has more unknowns than equations; therefore we need auxiliary equations that we write in the generalized form

$$\overline{\psi}_{m,j}=\frac{(1+\theta_{m,j})\psi_{m,j+1/2}+(1-\theta_{m,j})\psi_{m,j-1/2}}{2},\ m=1:N,\ j=1:J_F. \tag{8}$$

Here we define $\theta_{m,j}=0$ to obtain the conventional diamond difference (DD) method. To obtain the step method we use

$$\theta_{m,j} = \begin{cases}1, & \mu_m>0\\ -1, & \mu_m<0,\end{cases}\qquad m=1:N,\ j=1:J_F, \tag{9}$$

and to obtain the step characteristics method, which is the constant nodal method, we set

$$\theta_{m,j} = \mathrm{cotgh}\left(\frac{h_j\sigma_{Tj}}{2\mu_{\mathrm{m}}}\right)-\frac{2\mu_{\mathrm{m}}}{h_j\sigma_{Tj}},\ \ m=1:N,\ \ j=1:J_F. \tag{10}$$

Equation (10) is obtained from Eq. (8) by assuming that the scattering source is constant inside each node I_{j} of the spatial grid.

Now, we substitute Eq. (8) into the removal term by collision of Eq. (4) to write the S_N sweeping equations

$$\psi_{m,j\pm1/2}=\frac{\left[\frac{|\mu_m|}{h_j}-\frac{\sigma_{Tj}}{2}\left(1-|\theta_{m,j}|\right)\right]\psi_{m,j\mp1/2}+S_{m,j}+Q_j}{\left[\frac{|\mu_m|}{h_j}-\frac{\sigma_{Tj}}{2}\left(1+|\theta_{m,j}|\right)\right]},\mathrm{m}=1{:}N,j=1{:}\mathrm{J_F}, \tag{11}$$

where we have defined the node-average scattering source

$$S_{m,j} = \frac{1}{2}\sigma_{S0j}\overline{\phi}_j+\frac{3}{2}\mu_m\sigma_{S1j}\overline{J}_j,\ \ m=1:N,\ \ j=1:J_F, \tag{12}$$

with the S_N definitions given in Eqs. (6) and (7). Once one chooses the numerical method by defining $\theta_{m,j}$ as described above, and an initial guess for $\mathrm{S_{m,j}}$, Eq. (11) is used to sweep from left to right ($\mu_m>0$,$m=1{:}N/2$) and from right to left ($\mu_m<0$,$\mathrm{m}=\mathrm{N}/2+1,\mathrm{N}$), characterizing one source iteration. Then, the scattering source given in Eq. (12) is updated and the sweeping algorithm is repeated until a prescribed stopping criterion is satisfied. This is the conventional SI scheme.

In this section we offer a technique to define the initial guess for the scattering source $S_{m,j}$ in the SI scheme. This technique is based on the diffusion solution; therefore, we refer to it as a diffusion synthetic method for accelerating the SI scheme. In other words, we use the SND method to generate the coarse-mesh solution of the diffusion equation with approximate boundary conditions as

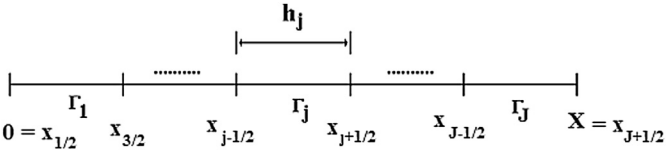

Fig. 1. Spatial discretization grid ($J=J_F$) for fine-mesh method and ($J=J_C$) for the SND method (viz Appendix), with ($J_F\ge J_C$).