Los Alamos NATIONAL LABORATORY
research note
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Date: May 22, 2008

Subject: Semi-Implicit Transport Schemes for Two-Dimensional Geometries

Executive Summary

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1 Deterministic Forms of the Transport Equation

The one-speed transport equation for isotropic scattering is given by [1]

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \hat{\Omega}\cdot\nabla\psi + \sigma_t\psi = \sigma_s\frac{\phi}{4\pi} + \frac{Q}{4\pi}. \tag{1}$$

Here, the angular flux is denoted by $\psi(\mathbf{x},\hat{\Omega},t)$, the scalar flux is $\phi(\mathbf{x},t) = \frac{1}{4\pi}\int_{4\pi} d\hat{\Omega}\,\psi$, $\hat{\Omega}$ is a unit vector that denotes the direction-of-flight variable, and σ_t, σ_s are the total, and scattering cross-sections that may vary in space and time. For a spatial domain denoted by $\mathcal{V}$ with boundary $\partial\mathcal{V}$ and normal to the boundary $\mathbf{n}(\mathbf{x})$, the boundary and initial conditions for Eq.(1) are

$$\psi(\mathbf{x},\hat{\Omega},t) = \Gamma(\mathbf{x},\hat{\Omega}), \qquad \mathbf{x}\in\partial\mathcal{V}, \quad \mathbf{n}(\mathbf{x})\cdot\hat{\Omega} > 0, \tag{2}$$

$$\psi(\mathbf{x},\hat{\Omega},0) = \Psi(\mathbf{x},\hat{\Omega}). \tag{3}$$

Two common methods for treating the direction-of-flight variable are the discrete ordinates method (S_n) and the spherical harmonics method (P_n). The S_n method solves for the angular flux along particular directions and uses a quadrature rule to approximate the scalar flux given the angular flux along particular directions [2]. In two-dimensional geometry the S_n method can be written as

$$\frac{1}{v}\frac{\partial \psi_l}{\partial t} + \eta_l\frac{\partial \psi_l}{\partial x} + \mu_l\frac{\partial \psi_l}{\partial z} + \sigma_t\psi_l = \sigma_s\sum_{m=1}^{N} w_m\psi_m + \frac{Q}{4\pi} \qquad \text{for } l = 1\ldots N, \tag{4}$$

where $\psi_l = \psi(x,z,\eta_l,\mu_l,t)$, η_l is the x-direction cosine for the l^{th} ordinate, while μ_l is the z-direction cosine; the quadrature weights are denoted by w_m. The number of ordinates, N, is given by $\frac{1}{2}(n(n+2))$ for a given S_n order. The quadrature rules that we will deal with in this study are level symmetric and satisfy

$$\frac{1}{4\pi}\sum_{l=1}^{N} w_l\mu_l^k = \begin{cases} 1, & k=0, \\ 0, & k=1, \\ \frac{1}{3}, & k=2, \end{cases} \tag{5}$$

and an identical conditions for η_l. The boundary and initial conditions for S_n are

$$\psi_l(\mathbf{x}) = \Gamma_l(\mathbf{x}), \qquad \mathbf{x}\in\partial\mathcal{V}, \quad \mathbf{n}(\mathbf{x})\cdot(\mu_l,\eta_l) > 0, \tag{6}$$

$$\psi_l(\mathbf{x},0) = \Psi_l(\mathbf{x}), \tag{7}$$

where Γ_l and Ψ_l are the continuous-in-angle functions Γ and Ψ evaluated at $\hat{\Omega} = (\mu_l, \eta_l)$.

The P_n method involves taking spherical harmonic moments of (1) and truncating the expansion. Using spherical harmonics functions given by

$$Y_l^m(\hat{\Omega}) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\mu) e^{im\varphi}\ , \tag{8}$$

with P_l^m the associated Legendre function and φ the azimuthal part of the direction of flight. Using the spherical harmonics functions we define a spherical harmonic moment of the angular flux,

$$\psi_l^m = \int_{4\pi} d\hat{\Omega}\, Y_l^{m*}(\hat{\Omega})\psi, \tag{9}$$

where we have denoted the complex conjugate using an asterisk. Taking moments of the two-dimensional form of (1) we get [3,4]

$$\begin{aligned}\frac{1}{v}\frac{\partial \psi_l^m}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}\left(-C_{l-1}^{m-1}\psi_{l-1}^{m-1} + D_{l+1}^{m-1}\psi_{l+1}^{m-1} + E_{l-1}^{m+1}\psi_{l-1}^{m+1} - F_{l+1}^{m+1}\psi_{l+1}^{m+1}\right) \\ + \frac{\partial}{\partial z}\left(A_{l-1}^{m}\psi_{l-1}^{m} + B_{l+1}^{m}\psi_{l+1}^{m}\right) + \sigma_t\psi_l^m = 0 \qquad \text{for } l = 1\dots n,\ m = 1\dots l\end{aligned} \tag{10a}$$

and

$$\frac{1}{v}\frac{\partial \psi_l^0}{\partial t} + \frac{\partial}{\partial x}\left(E_{l-1}^{1}\psi_{l-1}^{1} - F_{l+1}^{1}\psi_{l+1}^{1}\right) + \frac{\partial}{\partial z}\left(A_{l-1}^{0}\psi_{l-1}^{0} + B_{l+1}^{0}\psi_{l+1}^{0}\right) + \sigma_t\psi_l^0 = \delta_{l0}\left(\sigma_s\psi_l^0 + \frac{Q}{2\sqrt{\pi}}\right) \quad \text{for } l = 0\dots n, \tag{10b}$$

where

$$\begin{aligned} A_l^m &= \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+3)(2l+1)}} & B_l^m &= \sqrt{\frac{(l-m)(l+m)}{(2l+1)(2l-1)}} \\ C_l^m &= \sqrt{\frac{(l+m+1)(l+m+2)}{(2l+3)(2l+1)}} & D_l^m &= \sqrt{\frac{(l-m)(l+m-1)}{(2l+1)(2l-1)}} \\ \mathcal{E}_l^m &= \sqrt{\frac{(l-m+1)(l-m+2)}{(2l+3)(2l+1)}} & F_l^m &= \sqrt{\frac{(l+m)(l+m-1)}{(2l+1)(2l-1)}}. \end{aligned}$$

For the P_n method the scalar flux is given by $\phi = 2\sqrt{\pi}\psi_0^0$, and the number of unknowns in the P_n equations is $\frac{1}{2}(n^2+3n)+1$. The initial conditions for P_n are given by

$$\psi_l^m(\mathbf{x}) = \int_{4\pi} d\hat{\Omega}\, Y_l^{m*}(\hat{\Omega})\Psi(\mathbf{x},\hat{\Omega}). \tag{11}$$

The boundary conditions for P_n are more difficult to define than those for S_n . We will use a ghost cell boundary condition [3,5] that is equivalent to the Mark boundary condition. The details of the ghost cell boundary condition will be given in section 4.

1.1 Conservation law form

The S_n and P_n methods can both be written in the form of a linear conservation law, i.e.,

$$\frac{1}{v}\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A}_x\frac{\partial \mathbf{u}}{\partial x} + \mathbf{A}_z\frac{\partial \mathbf{u}}{\partial z} = \mathbf{C}\mathbf{u} + \mathbf{Q}. \tag{12}$$

For the S_n system these matrices are given by

$$\mathbf{A}_x = \mathsf{diag}(\eta_1, \ldots, \eta_N), \qquad \mathbf{A}_z = \mathsf{diag}(\mu_1, \ldots, \mu_N), \tag{13a}$$

where diag denotes a diagonal matrix, and

$$\mathbf{C} = \frac{\sigma_s}{4\pi} \begin{pmatrix} w_1 - \frac{4\pi\sigma_t}{\sigma_s} & w_2 & \ldots & w_N \\ \vdots & \ddots & & \\ w_1 & w_2 & \ldots & w_N - \frac{4\pi\sigma_t}{\sigma_s} \end{pmatrix}, \tag{13b}$$

$$\mathbf{Q} = \left(\frac{Q}{4\pi}, \cdots, \frac{Q}{4\pi} \right)^T. \tag{13c}$$

and $\mathbf{u}$ is given by

$$\mathbf{u} = \left(\psi_1, \cdots, \psi_N \right)^T. \tag{14}$$

Note that for S_n the matrices that govern the flow of information, the $\mathbf{A}$ matrices, are diagonal. This is the basis for the sweeping schemes that have been popular for solving the S_n equations implicitly. On the other hand, the P_n equations, as we will see, have a diagonal collision matrix, $\mathbf{C}$, and full $\mathbf{A}$ matrices.

The matrices for the P_n equations are more complicated. First, we must decide how to order $\mathbf{u}$; our ordering is in blocks of increasing l,

$$\mathbf{u} = \left(\psi_0^0, \psi_1^0, \psi_1^1, \psi_2^0, \psi_2^1, \psi_2^2, \cdots, \psi_n^n \right)^T. \tag{15}$$

Under this ordering, a given ψ_l^m moment is at position $m + \frac{1}{2}(l + l^2)$. Due to the large size of the $\mathbf{A}$ matrices and the fact there is no convenient way to write them, we shall omit explicitly writing out these matrices. However, given the indexing scheme just mentioned, these matrices can be easily generated. The collision matrix can be written succintly as

$$\mathbf{C} = \mathsf{diag}(\sigma_a, \sigma_t, \ldots, \sigma_t), \tag{16}$$

where the absorption cross-section is $\sigma_a = \sigma_t - \sigma_s$. The source term, $\mathbf{Q}$, is

$$\mathbf{Q} = \left(\frac{Q}{2\sqrt{\pi}}, 0, \cdots, 0 \right)^T. \tag{17}$$

Using the conservation law form we can write either the S_n or P_n systems in a general form on which we can apply spatial and temporal discretizations. In the next sections we will develop a semi-implicit, bilinear discontinuous discretization for this general form.

2 Time Integration

To complete our numerical method we will now treat the time variable. We are interested in semi-implicit (also called implicit-explicit) time integration where we treat the streaming terms explicitly and the material interaction terms implicitly. In this work we look at two such approaches. Before introducing the time integration schemes we will write a simpler form of semi-discrete equations, either (58) or (60) for each degree of freedom, j, in cell k:

$$\frac{1}{v}\frac{d\mathbf{u}_j}{dt} + \mathbf{L}\mathbf{u}_j = \mathbf{C}\mathbf{u}_j + \mathbf{S}_j, \tag{18}$$

with the streaming terms collapsed into the matrix $\mathbf{L}$.

The first time integration method we consider will be a predictor-corrector method given by

$$\frac{1}{v}\frac{\mathbf{u}_j^{n+1/2} - \mathbf{u}_j^n}{\Delta t/2} + \mathbf{L}\mathbf{u}_j^n = \mathbf{C}\mathbf{u}_j^{n+1/2} + \mathbf{S}_j^{n+1/2}, \tag{19a}$$

$$\frac{1}{v}\frac{\mathbf{u}_j^{n+1}-\mathbf{u}_j^n}{\Delta t}+\mathbf{L}\mathbf{u}_j^{n+1/2}=\mathbf{C}\mathbf{u}_j^{n+1}+\mathbf{S}_j^{n+1}. \tag{19b}$$

In this method the streaming terms are treated using a second-order Runge-Kutta discretization and the material interaction terms are updated using the backward Euler method. One drawback of this method is that it requires each cell to be updated twice per timestep: once for the predictor and then again for the corrector. A simpler approach would be to use forward Euler for the streaming terms, however, it has been shown that forward Euler is not stable in the case of free streaming [6].

The other method we will investigate is the implicit-explicit (IMEX) BDF-2 scheme of Hundsdorfer and Jaffré [7]. Their method is given by

$$\frac{1}{v}\frac{1}{\Delta t}\left(\frac{3}{2}\mathbf{u}_j^{n+1}-2\mathbf{u}_j^n+\frac{1}{2}\mathbf{u}_j^{n-1}\right)+\mathbf{L}\left(2\mathbf{u}_j^n-\mathbf{u}_j^{n-1}\right)=\mathbf{C}\mathbf{u}_j^{n+1}+\mathbf{S}_j^{n+1}. \tag{20}$$

The IMEX scheme involves only one update per unknown to complete at timestep—at the cost of requiring the storage of the two previous time step's unknowns.

Both the above methods treat the streaming of radiation explicitly, hence, each method has a Courant limit for the time step. This limits are given by [6, 7]

$$\frac{v\Delta t}{h}\le\frac{1}{3}\qquad\text{predictor-corrector,} \tag{21}$$

$$\frac{v\Delta t}{h}\le\frac{1}{4}\qquad\text{IMEX BDF-2,} \tag{22}$$

where $h=\min(\Delta x,\Delta z)$.

3 Asymptotic Diffusion Limit

An important property of the transport equation, Eq. (1), is that in the limit of large values for the scattering cross-section and particle velocity and small sources the hyperbolic transport equation limits to a parabolic diffusion equation for the scalar flux [8]. Specifically, in this limit away from boundary and initial layers, the leading order scalar flux satisfies

$$\frac{1}{v}\frac{\partial\phi}{\partial t}-\nabla\cdot\frac{1}{3\sigma_t}\nabla\phi+\sigma_a\phi=Q\,, \tag{23}$$

and

$$\psi=\frac{1}{4\pi}\phi\,. \tag{24}$$

In the rest of this section we will examine the P_n and S_n equations with the predictor-corrector and IMEX BDF-2 methods in the asymptotic diffusion limit. To analyze this limit we use a small positive parameter ϵ to scale

$$\sigma_t\to\frac{\sigma_t}{\epsilon},\qquad \sigma_a\to\epsilon\sigma_a$$
$$v\to\frac{v}{\epsilon},\qquad Q\to\epsilon Q.$$

3.1 S_n Equations

Under this scaling, the collision matrix for the S_n equations becomes

$$\mathbf{C}_\epsilon=\frac{\sigma_t-\epsilon^2\sigma_a}{4\pi\epsilon}\begin{pmatrix} w_1-4\pi(1+\epsilon^2\frac{\sigma_a}{\sigma_s}) & w_2 & \dots & w_N \\ \vdots & & \ddots & \\ w_1 & w_2 & \dots & w_N--4\pi(1+\epsilon^2\frac{\sigma_a}{\sigma_s}) \end{pmatrix}, \tag{25}$$

and the source becomes simply $\epsilon\mathbf{Q}$. We will insert these scaled matrices into the two different time integration methods.

3.1.1 Predictor-Corrector Method

The scaled S_n equations for the predictor corrector method are

$$\frac{\epsilon}{v}\frac{\mathbf{u}^{n+1/2}-\mathbf{u}^n}{\Delta t/2}+\mathbf{A}_x\frac{\partial}{\partial x}\mathbf{u}^n+\mathbf{A}_z\frac{\partial}{\partial z}\mathbf{u}^n=\mathbf{C}_\epsilon\mathbf{u}^{n+1/2}+\epsilon\mathbf{Q}^{n+1/2}, \tag{26a}$$

$$\frac{\epsilon}{v}\frac{\mathbf{u}^{n+1}-\mathbf{u}^n}{\Delta t}+\mathbf{A}_x\frac{\partial}{\partial x}\mathbf{u}^{n+1/2}+\mathbf{A}_z\frac{\partial}{\partial z}\mathbf{u}^{n+1/2}=\mathbf{C}_\epsilon\mathbf{u}^{n+1}+\epsilon\mathbf{Q}^{n+1}. \tag{26b}$$

We now postulate that ψ and ϕ can be expanded as a power series of ϵ as

$$(\cdot)=\sum_{i=0}^{\infty}\epsilon^i(\cdot)^{(i)}\,, \tag{27}$$

where $(\cdot)$ is either ϕ or ψ. Using this expansion and equating like powers of ϵ, we get that the $O(\epsilon^{-1})$ terms of Eqs. (26) are

$$\psi_l^{(0),n+1/2}=\frac{1}{4\pi}\phi^{(0),n+1/2},\qquad \psi_l^{(0),n+1}=\frac{1}{4\pi}\phi^{(0),n+1}, \tag{28}$$

where $\psi^{(0)}$ is not yet determined. The $O(1)$ terms for each discrete ordinate are

$$\mu_l\frac{\partial}{\partial x}\phi^{(0),n}+\eta_l\frac{\partial}{\partial z}\phi^{(0),n}+4\pi\psi_l^{(1),n+1/2}=\sigma_t\phi^{(1),n+1/2}, \tag{29a}$$

$$\mu_l\frac{\partial}{\partial x}\phi^{(0),n+1/2}+\eta_l\frac{\partial}{\partial z}\phi^{(0),n+1/2}+4\pi\sigma_t\psi_l^{(1),n+1}=\sigma_t\phi^{(1),n+1}, \tag{29b}$$

where we have used Eq. (28) to replace $\psi^{(0)}$. Multiplying Eqs. (29) by $\mu_l w_l$ and summing over l gives after some rearrangement

$$4\pi\sum_l\mu_l w_l\psi^{(1),n+1/2}=\frac{1}{3\sigma_t}\frac{\partial}{\partial x}\phi^{(0),n}, \tag{30a}$$

$$4\pi\sum_l\mu_l w_l\psi^{(1),n+1}=\frac{1}{3\sigma_t}\frac{\partial}{\partial x}\phi^{(0),n+1/2}. \tag{30b}$$

Similarly, we get relations involving η_l:

$$4\pi\sum_l\eta_l w_l\psi^{(1),n+1/2}=\frac{1}{3\sigma_t}\frac{\partial}{\partial z}\phi^{(0),n}, \tag{31a}$$

$$4\pi\sum_l\eta_l w_l\psi^{(1),n+1}=\frac{1}{3\sigma_t}\frac{\partial}{\partial z}\phi^{(0),n+1/2}. \tag{31b}$$

This equations are versions of Fick's law; they relate the first moment of the angular flux to the derivative of the scalar flux.

The $O(\epsilon)$ equations for each discrete ordinate are

$$\frac{1}{4\pi v}\frac{\phi^{(0),n+1/2}-\phi^{(0),n}}{\Delta t/2}+\mu_l\frac{\partial}{\partial x}\psi_l^{(1),n}+\eta_l\frac{\partial}{\partial z}\psi_l^{(1),n}+\sigma_t\psi_l^{(2),n+1/2}=\frac{\sigma_t}{4\pi}\phi^{(2),n+1/2}-\frac{\sigma_a}{4\pi}\phi^{(0),n+1/2}+\frac{Q}{4\pi}, \tag{32a}$$

$$\frac{1}{4\pi v}\frac{\phi^{(0),n+1}-\phi^{(0),n}}{\Delta t}+\mu_l\frac{\partial}{\partial x}\psi_l^{(1),n+1/2}+\eta_l\frac{\partial}{\partial z}\psi_l^{(1),n+1/2}+\sigma_t\psi_l^{(2),n+1}=\frac{\sigma_t}{4\pi}\phi^{(2),n+1}-\frac{\sigma_a}{4\pi}\phi^{(0),n+1}+\frac{Q}{4\pi}. \tag{32b}$$

Multiplying these equations by w_l and summing over l and using Eqs. (30)- (31b) gives the diffusion equations

$$\frac{1}{v}\frac{\phi^{(0),n+1/2}-\phi^{(0),n}}{\Delta t/2}+\frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial}{\partial x}\phi^{(0),n-1/2}+\frac{\partial}{\partial z}\frac{1}{3\sigma_t}\frac{\partial}{\partial z}\phi^{(0),n-1/2}+\sigma_a\phi^{(0),n+1/2}=Q, \tag{33a}$$

$$\frac{1}{v}\frac{\phi^{(0),n+1}-\phi^{(0),n}}{\Delta t}+\frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial}{\partial x}\phi^{(0),n}+\frac{\partial}{\partial z}\frac{1}{3\sigma_t}\frac{\partial}{\partial z}\phi^{(0),n}+\sigma_a\phi^{(0),n+1}=Q. \tag{33b}$$

Equation (32b) is a semi-implicit discretization of the diffusion equation, Eq. (23), using forward Euler for the diffusive term and backward Euler for the absorption term. This discretization was shown by McClarren, *et al.* to be a stable discretization for the equilibrium diffusion limit of thermal radiative transfer [9].

3.1.2 IMEX BDF-2

For the IMEX BDF-2 method given in Eq. (20), the $O(\epsilon^{-1})$ equations give that the leading order angular flux is isotropic as in the predictor-corrector method (c.f. the value of $\psi_l^{(0),n+1}$ in Eq. (28)). For the IMEX BDF-2 method the $O(1)$ equations are

$$\mu_l\frac{\partial}{\partial x}(2\phi^{(0),n}-\phi^{(0),n-1})+\eta_l\frac{\partial}{\partial z}(2\phi^{(0),n}-\phi^{(0),n-1})+4\pi\psi_l^{(1),n+1}=\sigma_t\phi^{(1),n+1}. \tag{34}$$

Multiplying these equations by $\mu_l w_l$ and summing over l as before gives

$$4\pi\sum_l \mu_l w_l\psi_l^{(1),n+1}=-\frac{1}{3\sigma_t}\frac{\partial}{\partial x}(2\phi^{(0),n}-\phi^{(0),n-1}), \tag{35}$$

in the z direction we get

$$4\pi\sum_l \eta_l w_l\psi_l^{(1),n+1}=-\frac{1}{3\sigma_t}\frac{\partial}{\partial z}(2\phi^{(0),n}-\phi^{(0),n-1}). \tag{36}$$

The $O(\epsilon)$ equations for the IMEX BDF-2 method are

$$\frac{1}{4\pi v\Delta t}\left(\frac{3}{2}\phi^{(0),n+1}-2\phi^{(0),n}+\frac{1}{2}\phi^{(0),n-1}\right)+\mu_l\frac{\partial}{\partial x}(2\psi_l^{(1),n}-\psi_l^{(1),n-1})+\eta_l\frac{\partial}{\partial z}(2\psi_l^{(1),n}-\psi_l^{(1),n-1})+\sigma_t\psi_l^{(2),n+1}$$
$$=\frac{\sigma_t}{4\pi}\phi^{(2),n+1}-\frac{\sigma_a}{4\pi}\phi^{(0),n+1}+\frac{Q}{4\pi}. \tag{37}$$

Multiplying these equations by w_l and summing over the index l we get

$$\frac{1}{v\Delta t}\left(\frac{3}{2}\phi^{(0),n+1}-2\phi^{(0),n}+\frac{1}{2}\phi^{(0),n-1}\right)-\frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial}{\partial x}(4\phi^{(0),n-1}-4\phi^{(0),n-2}+\phi^{(0),n-3})$$
$$-\frac{\partial}{\partial z}\frac{1}{3\sigma_t}\frac{\partial}{\partial z}(4\phi^{(0),n-1}-4\phi^{(0),n-2}+\phi^{(0),n-3})+\sigma_a\phi^{(0),n+1}=Q. \tag{38}$$

Equation (38) is a second-order in time discretization of the diffusion equation. Nevertheless, the stencil is *outré* for it uses no information from the nth time step and depends on data as far back in time as the $n-3$ time step.

3.2 P_n Equations

We now turn to the diffusion limit of the P_n equations. Under the ϵ scaling used above, the collision matrix for the P_n equations becomes

$$\mathbf{C}_\epsilon=\mathsf{diag}(\epsilon\sigma_a,\sigma_t/\epsilon,\ldots,\sigma_t\epsilon), \tag{39}$$

and the source term becomes $\epsilon\mathbf{Q}$.

3.2.1 Predictor-Corrector Method

The thermal radiative transfer equilibrium diffusion limit for the predictor-corrector method with the 1-D P_n equations was investigated by McClarren, *et al.* [9]. In that work it was shown that the in the diffusion limit the P_n equations limit to a forward Euler discretization of the diffusion equation (similar to what we saw above for the S_n predictor-corrector equations). In this subsection we will show that this analysis applies for linear transport in 2-D.

The scaled P_n equations are identical in form to Eqs. (26). The $O(\epsilon^{-1})$ terms of Eqs. (26) for the P_n system give the following relation

$$\psi_l^{(0),m,n} = \psi_l^{(0),m,n+1/2} = 0 \qquad l,m \neq 0. \tag{40}$$

This relation is equivalent to the leading order terms for the S_n equations in Eq. (28): the leading order angular flux is isotropic.

The $O(1)$ equations give the following relations

$$\psi_1^{(1),0,n+1/2} = -\frac{1}{\sqrt{3}\sigma_t}\frac{\partial \psi_0^{(0),0,n}}{\partial z}, \qquad \psi_1^{(1),1,n+1/2} = \frac{1}{\sqrt{6}\sigma_t}\frac{\partial \psi_0^{(0),0,n}}{\partial x}, \tag{41a}$$

$$\psi_1^{(1),0,n+1} = -\frac{1}{\sqrt{3}\sigma_t}\frac{\partial \psi_0^{(0),0,n+1/2}}{\partial z}, \qquad \psi_1^{(1),1,n+1} = \frac{1}{\sqrt{6}\sigma_t}\frac{\partial \psi_0^{(0),0,n+1/2}}{\partial x}, \tag{41b}$$

$$\psi_l^{(1),m,n} = \psi_l^{(1),m,n+1/2} = 0 \qquad l,m > 1. \tag{41c}$$

Continuing on to the $O(\epsilon)$ equations yields

$$\frac{\psi_0^{(0),0,n+1/2} - \psi_0^{(0),0,n}}{v\Delta t/2} - \sqrt{\frac{2}{3}}\frac{\partial}{\partial x}\psi_1^{(1),1,n} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\psi_1^{(1),0,n} + \sigma_a \psi_0^{(0),0,n+1/2} = \frac{Q}{2\sqrt{\pi}}\,, \tag{42a}$$

$$\frac{\psi_0^{(0),0,n+1} - \psi_0^{(0),0,n}}{v\Delta t} - \sqrt{\frac{2}{3}}\frac{\partial}{\partial x}\psi_1^{(1),1,n+1/2} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\psi_1^{(1),0,n+1/2} + \sigma_a \psi_0^{(0),0,n+1} = \frac{Q}{2\sqrt{\pi}}\,. \tag{42b}$$

Substituting the relations from Eqs. (41) into Eqs. (42) and using the definition of the scalar flux in terms of the spherical harmonics moments, we get the diffusion equations

$$\frac{\phi^{(0),n+1/2} - \phi^{(0),n}}{v\Delta t/2} - \frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial}{\partial x}\phi^{(0),n-1/2} - \frac{\partial}{\partial z}\frac{1}{3\sigma_t}\frac{\partial}{\partial z}\phi^{(0),n-1/2} + \sigma_a \psi^{(0),n+1/2} = Q\,, \tag{43a}$$

$$\frac{\phi^{(0),n+1} - \phi^{(0),n}}{v\Delta t} - \frac{\partial}{\partial x}\frac{1}{3\sigma}\frac{\partial}{\partial x}\phi^{(0),n} - \frac{\partial}{\partial z}\frac{1}{3\sigma_t}\frac{\partial}{\partial z}\phi^{(0),n} + \sigma_a \phi^{(0),n+1} = Q\,. \tag{43b}$$

This diffusion discretization is identical to the forward Euler discretization that the S_n predictor-corrector system limits to.

3.2.2 IMEX BDF-2

Omitting the straightforward details we simply state that the diffusion equation of the IMEX BDF-2 method applied to the P_n equations is

$$\begin{aligned}\frac{1}{v\Delta t}\left(\frac{3}{2}\phi^{(0),n+1} - 2\phi^{(0),n} + \frac{1}{2}\phi^{(0),n-1}\right) &- \frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial}{\partial x}(4\phi^{(0),n-1} - 4\phi^{(0),n-2} + \phi^{(0),n-3}) \\ &- \frac{\partial}{\partial z}\frac{1}{3\sigma_t}\frac{\partial}{\partial z}(4\phi^{(0),n-1} - 4\phi^{(0),n-2} + \phi^{(0),n-3}) + \sigma_a \phi^{(0),n+1} = Q,\end{aligned} \tag{44}$$

which is identical to Eq. (38), the leading order diffusion for S_n with the IMEX BDF-2 discretization.

3.3 Summary of Asymptotics

In this section we have shown that both the predictor-corrector and IMEX BDF-2 methods limit to a valid time discretization of the diffusion equation for either P_n or S_n . The predictor-corrector limits to a forward Euler discretization of the diffusion equation. This is a first-order discretization. On the other hand, the IMEX BDF-2 method limits to a second-order time discretization of diffusion equation. Unfortunately, though the IMEX BDF-2 method has a favorable convergence rate, its stencil in the diffusion limit for updating the $n+1$ time step relies on data from the $n-3$ time step.

4 BLD Finite Element Discretization

The spatial discretization that we will use is the bilinear discontinuous Galerkin (BLD) finite element method on rectangular cells. The derivation below will treat the continuous-in-time equations, and then at the end of the section we will discuss the CFL limits of the combined schemes. The BLD discretization (for unlumped, mass-lumped, and fully-lumped treatments) has been shown to have the diffusion limit on rectangular cells in two-dimensions with the fully-lumped treatment the most robust. [10].

To derive the BLD method, we expand the solution vector in terms of spatial basis functions:

$$\mathbf{u} = \sum_k \sum_{j=1}^{4} B_{k,j}(x,z)\mathbf{u}_{k,j}(t), \tag{45}$$

where the cells that make up of the computational domain are indicated by the subscript k. Also, we expand the source Q in this form. The basis functions B_j are defined for a generic cell k as

$$B_{k,1}(x,z) = \frac{x_R - x}{\Delta x}\frac{z_T - z}{\Delta z}, \tag{46a}$$

$$B_{k,2}(x,z) = \frac{x - x_L}{\Delta x}\frac{z_T - z}{\Delta z}, \tag{46b}$$

$$B_{k,3}(x,z) = \frac{x - x_L}{\Delta x}\frac{z - z_B}{\Delta z}, \tag{46c}$$

$$B_{k,4}(x,z) = \frac{x_R - x}{\Delta x}\frac{z - z_B}{\Delta z}. \tag{46d}$$

In the definition of the basis functions, $\Delta x = x_R - x_L$ and $\Delta z = z_T - z_B$ are the width of the cell in the x and z directions, the left and right edges of the cell are denoted by x_L and x_L, and the bottom and top of the cell are denoted by z_B and z_T. These basis functions are cardinal in the sense that each function is 1 at one corner of the cell and vanishes at the other corners.

We now introduce the weak form of (12) by multiplying by a basis function and integrating over cell k,

$$\begin{aligned}\frac{1}{v}\frac{d}{dt}\int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, B_{k,i}\mathbf{u} + \mathbf{A}_x\left(\int_{z_B}^{z_T} dz\, [B_{k,i}\mathbf{u}]_x - \int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, \mathbf{u}\frac{dB_{i,k}}{dx}\right) \\ + \mathbf{A}_z\left(\int_{x_R}^{x_L} dx\, [B_{k,i}\mathbf{u}]_z - \int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, \mathbf{u}\frac{dB_{i,k}}{dz}\right) = \\ \mathbf{C}\int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, B_{k,i}\mathbf{u} + \int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, B_{k,i}\mathbf{Q}_{k,i}.\end{aligned} \tag{47}$$

Here, $[\cdot]_\xi$ is a function evaluated at the endpoints of the cell in the ξ direction. Upon substituting our finite element expansion, (45), into (47) and dropping the k subscript where it is not necessary, we arrive at

$$\mathbf{M}\frac{1}{v}\frac{d\mathbf{U}}{dt} + \mathbf{A}_x\left((\mathbf{LU})^{x,surf} + \mathbf{L}_x\mathbf{U}_k\right) + \mathbf{A}_z\left((\mathbf{LU})^{z,surf} + \mathbf{L}_z\mathbf{U}_k\right) = \mathbf{CMU} + \mathbf{MS}, \tag{48}$$

for $\mathbf{U} = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4)^T$ and $\mathbf{S} = (\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \mathbf{Q}_4)^T$ The mass matrix M is defined by

$$M_{i,j} = \int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, B_i B_j, \tag{49}$$

$\mathbf{L}_\xi$ is given by

$$L_{\xi,i,j} = \int_{z_B}^{z_T} dz \int_{x_L}^{x_R} dx\, B_j \frac{dB_i}{d\xi}, \tag{50}$$

and we have defined the vectors

$$(\mathbf{LU})^{x,surf} = \int_{z_B}^{z_T} dz\, [B_i B_j \mathbf{u}_j]_x, \tag{51}$$

$$(\mathbf{LU})^{z,surf} = \int_{x_L}^{x_R} dx\, [B_i B_j \mathbf{u}_j]_z. \tag{52}$$

Using our definitions of the basis functions we get that

$$\mathbf{M} = \frac{\Delta x \Delta z}{36} \begin{pmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{pmatrix}, \tag{53}$$

$$\mathbf{L}_x = \frac{\Delta z}{12} \begin{pmatrix} -2 & -2 & -1 & -1 \\ 2 & 2 & 1 & 1 \\ 1 & 1 & 2 & 2 \\ -1 & -1 & -2 & -2 \end{pmatrix}, \tag{54}$$

$$\mathbf{L}_z = \frac{\Delta x}{12} \begin{pmatrix} -2 & -1 & -1 & -2 \\ -1 & -2 & -2 & -1 \\ 1 & 2 & 2 & 1 \\ 2 & 1 & 1 & 2 \end{pmatrix}, \tag{55}$$

$$(\mathbf{LU})^{x,surf} = \frac{\Delta z}{6} \begin{pmatrix} -2\mathbf{u}_1^{x-} - \mathbf{u}_4^{x-} \\ 2\mathbf{u}_2^{x+} + \mathbf{u}_3^{x+} \\ \mathbf{u}_2^{x+} + 2\mathbf{u}_3^{x+} \\ -\mathbf{u}_1^{x-} - 2\mathbf{u}_4^{x-} \end{pmatrix}, \tag{56}$$

$$(\mathbf{LU})^{z,surf} = \frac{\Delta x}{6} \begin{pmatrix} -2\mathbf{u}_1^{z-} - \mathbf{u}_2^{z-} \\ -\mathbf{u}_1^{z-} + 2\mathbf{u}_2^{z-} \\ 2\mathbf{u}_3^{z+} + \mathbf{u}_4^{z+} \\ \mathbf{u}_3^{z+} + 2\mathbf{u}_4^{z+} \end{pmatrix}. \tag{57}$$

Here the superscipts on $\mathbf{u}_j$ denote a value evaluated on the cell edge, for instance $\mathbf{u}_1^{x-}$ is value on the edge just to the left of (x_L, z_B).

Equation (48) can be simplified by multiplying by $\mathbf{M}$ to get

$$\frac{1}{v}\frac{d}{dt}\mathbf{U} + \frac{\mathbf{A}_x}{\Delta x} \begin{pmatrix} -4u_1^{x-} - 2u_2^{x+} \\ 2u_1^{x-} + 4u_2^{x+} \\ 4u_3^{x+} + 2u_4^{x-} \\ -2u_3^{x+} - 4u_4^{x-} \end{pmatrix} + \frac{\mathbf{A}_x}{\Delta x} \begin{pmatrix} 3 & 3 & 0 & 0 \\ -3 & -3 & 0 & 0 \\ 0 & 0 & -3 & -3 \\ 0 & 0 & 3 & 3 \end{pmatrix} \mathbf{U}$$
$$+ \frac{\mathbf{A}_z}{\Delta z} \begin{pmatrix} -4u_1^{z-} - 2u_4^{z+} \\ -4u_2^{z-} - 2u_3^{z+} \\ 2u_2^{z-} + 4u_3^{z+} \\ 2u_1^{z-} + 4u_4^{z+} \end{pmatrix} + \frac{\mathbf{A}_z}{\Delta z} \begin{pmatrix} 3 & 0 & 0 & 3 \\ 0 & 3 & 3 & 0 \\ 0 & -3 & -3 & 0 \\ -3 & 0 & 0 & -3 \end{pmatrix} \mathbf{U} = \mathbf{CU} + \mathbf{S}. \tag{58}$$

We performed the integration to evaluate the mass matrix, $\mathbf{M}^L$, exactly. It is also possible to evaluate the mass matrix using the trapezoidal rule. This process, called mass matrix lumping, leads to a diagonal mass matrix [10]. The lumped mass matrix, $\mathbf{M}^L$, is

$$\mathbf{M}^L = \frac{\Delta x \Delta z}{4}\mathbf{I}\,, \tag{59}$$

for $\mathbf{I}$ the 4×4 identity matrix. In this case (58) becomes

$$\begin{aligned}\frac{1}{v}\frac{d}{dt}\mathbf{U} + \frac{\mathbf{A}_x}{3\Delta x}\begin{pmatrix}-4u_1^{x-} - 2u_4^{x-}\\ 4u_2^{x+} + 2u_3^{x+}\\ 2u_2^{x+} + 4u_3^{x+}\\ -2u_1^{x-} - 4u_4^{x-}\end{pmatrix} + \frac{\mathbf{A}_x}{3\Delta x}\begin{pmatrix}2 & 2 & 1 & 1\\ -2 & -2 & -1 & -1\\ -1 & -1 & -2 & -2\\ 1 & 1 & 2 & 2\end{pmatrix}\mathbf{U}&\\ + \frac{\mathbf{A}_z}{3\Delta z}\begin{pmatrix}-4u_1^{z-} - 2u_2^{z-}\\ -2u_1^{z-} - 4u_2^{z-}\\ 4u_3^{z+} + 2u_4^{z+}\\ 2u_3^{z+} + 4u_4^{z+}\end{pmatrix} + \frac{\mathbf{A}_z}{3\Delta z}\begin{pmatrix}2 & 1 & 1 & 2\\ 1 & 2 & 2 & 1\\ -1 & -2 & -2 & -1\\ -2 & -1 & -1 & -2\end{pmatrix}\mathbf{U} &= \mathbf{C}\mathbf{U} + \mathbf{S}.\end{aligned} \tag{60}$$

The process of lumping can be extended further to the within-cell gradient, $\mathbf{L}_j$, and surface, $(\mathbf{LU})^{x,surf}$, matrices. The resulting equations are the fully-lumped bilinear discontinuous equations [10], and are also called the simple corner balance method [11]. The fully-lumped equations are

$$\begin{aligned}\frac{1}{v}\frac{d}{dt}\mathbf{U} + 2\frac{\mathbf{A}_x}{\Delta x}\begin{pmatrix}-u_1^{x-}\\ u_2^{x+}\\ u_3^{x+}\\ u_4^{x-}\end{pmatrix} + \frac{\mathbf{A}_x}{\Delta x}\begin{pmatrix}1 & 1 & 0 & 0\\ -1 & -1 & 0 & 0\\ 0 & 0 & -1 & -1\\ 0 & 0 & 1 & 1\end{pmatrix}\mathbf{U}&\\ + 2\frac{\mathbf{A}_z}{\Delta z}\begin{pmatrix}-u_1^{z-}\\ -u_2^{z-}\\ u_3^{z+}\\ u_4^{z+}\end{pmatrix} + \frac{\mathbf{A}_z}{\Delta z}\begin{pmatrix}1 & 0 & 0 & 1\\ 0 & 1 & 1 & 0\\ 0 & -1 & -1 & 0\\ -1 & 0 & 0 & -1\end{pmatrix}\mathbf{U} &= \mathbf{C}\mathbf{U} + \mathbf{S}.\end{aligned} \tag{61}$$

To this point we have note specified how the surface terms, such as u_1^{x-}, are evaluated. These terms are easily determined for the S_n equations in an upwind fashion based on the sign of μ_l or η_l. For the x surface terms, when μ_l is positive the value to the left of the interface is used; negative μ_l makes the interfacial value the unknown just to the right of the interface.

The upwind interfacial values for the P_n equations are more difficult to determine. The values are determined by solving a Riemann problem at the interface (see, for example, Ref. [12]). With this procedure the value at an interface is given by

$$\mathbf{A}_i\mathbf{u}|_{surf} = \frac{1}{2}\mathbf{A}_i(\mathbf{u}_L + \mathbf{u}_R) - \frac{1}{2}|\mathbf{A}|_i(\mathbf{u}_R - \mathbf{u}_R)\,, \tag{62}$$

for $i = x, z$, and L and R denoting the value to the left and right of the interface respectively. We have also used the definition

$$|\mathbf{A}|_i = \sum_k \mathbf{r}_k|\lambda_k|\mathbf{l_k}, \tag{63}$$

with $\mathbf{r}_k$ and $\mathbf{l}_k$ are the kth right and left eigenvectors of $\mathbf{A}_i$ with corresponding eigenvalue λ_k. Equations (62) are upwind in the sense that the characteristic variable to the left or right of the interface is used depending on the sign of λ_k.

The above upwind surface terms will be used to utilize a ghost cell boundary condition for P_n . This boundary condition places a cell outside the physical region of interest with a prescribed value of $\mathbf{u}$ based on the value of $\Gamma(\mathbf{x}, \hat{\Omega})$. The upwinding then moves the proper information into the problem. This approach has been shown to work well for isotropic, vacuum, and reflecting boundaries [3,5], though how to uniquely specify $\mathbf{u}$ in the ghost cells for a general value of $\Gamma(\mathbf{x}, \hat{\Omega})$ remains an open question.

Table 1: Upper bound of ν for various combinations of time and spatial discretization.

	Predictor-Corrector	IMEX BDF-2
Unlumped	1/3	0.20
Lumped	1/2	0.44

4.1 CFL Limit for Fully Discretized Equations

Combining the two methods for treating the time variable in section 2, with the BLD discretization we now state the CFL limits for the fully discrete equations. Defining the CFL number as

$$\nu \equiv \frac{v\Delta t}{x}, \tag{64}$$

the time step limits are given in Table 4.1.

These timestep restrictions could be relaxed in the diffusion limit, as noted by McClarren, *et al.* [9] and Klar [13, 14]. However, since in general we are interested in problems with both diffusive and optically thin regions, such cases where the more restrictive limit on ν of Table 4.1 applies in the thin regions, we do not explore diffusive timestep restrictions here.

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