MULTIGROUP DISCRETE ORDINATES SOLUTION
OF BOLTZMANN-FOKKER-PLANCK EQUATIONS AND CROSS
SECTION LIBRARY DEVELOPMENT OF ION TRANSPORT

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1 Introduction

The objective of this study was to develop (i) a cross section library for energetic ion interactions with amorphous targets, focusing on classical Coulomb scattering, and (ii) a discrete ordinates transport code using a bilinear-discontinuous (BLD) basis in space and energy. Consistent with the linear basis in energy in the transport code, both multigroup and energy weighted cross sections are required in the library.

This report describes progress in the above two areas. In the next section, the methodology, implementation and results for scattering cross sections for arbitrary projectile target atom mass combinations is presented. In particular, the implementation of the Boltzmann Fokker-Planck decomposition of the singular differential cross section is delineated, and the status of implementing our library on a distributed memory parallel computer is briefly summarized. In Section 3, we present the bilinear discontinuous numerical solution of the time dependent transport equation. Time dependence was chosen as the simplest generalization of the linear-discontinuous scheme, which has enabled us to perform extensive accuracy and convergence testing of the code. As this discretization is motivated by the streaming operator, and noting that in the space-energy problem the operator is also first order, the analysis will carry over directly to the energy dependent problem. The scattering source is included in an iterative manner and, hence, once cross section data is available in the appropriate basis, extension to full space-energy implementation in our transport code will be straightforward. This transition will be undertaken in the next phase of this research.

2 Boltzmann Fokker-Planck Decomposition

Energetic ions moving through an amorphous medium interact via elastic and inelastic collisions with atomic nuclei and atomic electrons, mediated via long range Coulomb forces.¹ In view of the disparate masses, inelastic collisions with electrons are accurately approximated by a continuous slowing down process without angular deflections. Elastic interactions with nuclei, on the other hand, can result in large energy transfers and angular deflections and are therefore represented by a differential scattering cross section. The transport of ions can then be described by the linear transport equations for the angular flux, and established

numerical solution methods (e.g. multigroup, $S_n - P_n$, etc.) can be used in principle. However, ion cross sections are characteristically very forward peaked and tend to diverge as the scattering angle $\mu_0 \rightarrow 1$ but are relatively flat for $\mu_0 < 1$. This makes impractical an expansion of the scattering kernel in Legendre polynomials. The difficulty can be circumvented by first introducing a cut-off μ_c in the scattering angle range such that $\mu_c \sim 1$ and noting that the differential cross section is smooth over $\mu_{min} < \mu_0 \leq \mu_c$ (μ_{min} is defined below). The remaining (singular) component, defined over $\mu_c < \mu_0 \leq 1$ is then approximated as a continuous, Fokker-Planck process, resulting in a hybrid Boltzmann Fokker-Planck (BFP) equation.^{2,3} The large scattering angle encounters are now described by a well behaved function and can be represented by a low order Legendre expansion. However, the smooth cross section is only defined over the partial range $\mu_{min} < \mu_0 \leq \mu_c$ and must be extrapolated to the full range before implementation. One procedure for obtaining the full range Legendre moments is presented here.

We use the Partial Range Fit (PRF) method originally introduced by Landesman and Morel⁴ for single velocity electron transport. Consider two charged particles of masses m_1 and m_2 , where m_1 is the incident particle mass and m_2 is the mass of the target atom. The angular dependence of the differential scattering cross section is defined over the scattering angle cosine range $\mu_0 \in [\mu_{min}, 1]$, where kinematics gives $\mu_{min} = -1$ if $m_1 < m_2$, $\mu_{min} = 0$ if $m_1 = m_2$ while if $m_1 > m_2$, $\cos(\sin^{-1}(m_2/m_1))$. If this range is cutoff at some maximum scattering angle cosine μ_c , the cross section can be fit with a low-order Legendre expansion over the partial range $[\mu_{min}, \mu_c]$, and then the partial range fit expanded in terms of full range Legendre polynomials.

We proceed by first mapping the full range Legendre polynomials $P_l(\mu_0)$, orthogonal on $\mu_0 \in [-1, 1]$, to the partial range $\eta \in [\mu_{min}, \mu_c]$ as $\bar{P}_l(\eta) = P_l(\mu_0(\eta))$ with

$$\mu_0(\eta) = \frac{2\eta - \mu_c - \mu_{min}}{\mu_c - \mu_{min}}. \quad (1)$$

where the modified Legendre polynomials $\bar{P}_l(\eta)$ are orthogonal over the partial range. A least squares fit of the scattering cross section (with energy dependence suppressed) in a partial range expansion gives

$$\sigma_s^{partial}(\eta) = \sum_{l=0}^L \frac{2l+1}{2} \sigma_l^{partial} \bar{P}_l(\eta), \quad (2)$$

where

$$\sigma_l^{partial} = \frac{4\pi}{(\mu_c - \mu_{min})} \int_{\mu_{min}}^{\mu_c} \sigma_s(\mu_0(\eta)) \bar{P}_l(\eta) d\eta. \quad (3)$$

Now extrapolate the partial range fit onto the full range $[-1, 1]$ by defining the piecewise function

$$\sigma_s^B(\mu_0) = \begin{cases} 0, & -1 \leq \mu_0 < \mu_{min} \\ \sigma_s(\mu_0) = \sum_{l=0}^L \frac{2l+1}{2} \sigma_l^{partial} \bar{P}_l(\mu_0), & \mu_{min} < \mu_0 \leq 1. \end{cases} \quad (4)$$

Multiplying each side by the full range Legendre polynomials and integrating over $[-1, 1]$ maps the partial range fit cross section expansion coefficients onto the full range. After interchanging the order of integration and summation the result is

$$\begin{aligned} \sigma_j^B(\mu_0) &= \int_{-1}^1 \sigma_s^B(\mu_0) P_j(\mu_0) d\mu_0 \\ &= \sum_{l=0}^L \frac{2l+1}{2} \sigma_l^{partial} \int_{\mu_{min}}^1 \bar{P}_l(\mu_0) P_j(\mu_0) d\mu_0, \quad j = 0, L \end{aligned} \quad (5)$$

for the coefficients of the full range expansion to be used in numerical ion transport calculations.

By implementing this method into our cross section computer model, we are able to investigate the implications of such a method for ion scattering cross sections. In Figure (1) we show the effect of the PRF cut-off angle cosine on the extrapolated partial range fit cross section extended to the full range for 100 keV Au ions incident on a Au target so that $\mu_{min} = 0$. Notice that as $\mu_{cut} \rightarrow 1$, the extrapolated cross section becomes increasingly peaked, however this cross section still allows an expansion in Legendre polynomials of modest order $L = 19$. We see in Figure (2) that the fit over the partial range is excellent; in fact it is indistinguishable from the exact cross section in the figure. So we expect that a full range expansion of this partial range, extrapolated, piecewise continuous function, (Eq. 4), of an order at least that of the partial range expansion should result in a reasonably accurate full range expansion. While this is true for $\mu_0 > \mu_{min}$ as can be seen in Figure (2), the full range expansion oscillates about $\sigma_s^B(\mu_0) = 0$ for $\mu_0 < \mu_{min}$ in view of the discontinuity at $\mu_0 = \mu_{min}$ (the absolute value of the cross section is shown here in order to plot the result on a log scale). the partial range fit is indistinguishable from the exact cross section. Note that this effect is not seen for incident electrons or for ions with $m_1 < m_2$ since then

$\mu_{min} = -1$ For $m_1 > m_2$ we can nevertheless obtain a reasonable fit over the full range with a relatively low order Legendre expansion as seen in Figure (3) for 1 MeV P ions on a Si target. We conclude that the PRF method is also viable for ion scattering cross sections. A similar procedure can be used for target recoil cross sections, if the transport problem is to include tracking of recoil ions.

We have cast the double differential cross section into a form suitable for use in energy dependent transport codes using appropriate energy domain discretization and energy dependent basis functions for the computational method. The resulting calculations have been implemented on a 400-node IBM SP2 distributed-memory parallel computer. A static load balance was used for each group-to-group full-range coefficient where each process calculates all requested Legendre orders. Preliminary results indicate that these calculations are too coarse-grained even for the powerful CPU's on each node of the SP2, and many processors remain idle at the end of the calculation. A dynamic load balance algorithm appears to be more suitable for this problem, where each Legendre order for each group-to-group full-range coefficient is calculated as each node becomes available. Optimization is currently under investigation, and these results will soon be tested in transport codes.

3 Bilinear-Discontinuous Space-Time Discretization of the Transport Equation

The time dependent transport equation has been solved in closed form only for a few simple model problems⁵⁻⁷ under fairly restrictive conditions, and in general numerical methods are necessary to obtain a solution. Various numerical methods for time dependent transport have been developed in the past,⁸⁻¹⁷ and have included different combinations of methods and discretizations for space, angle, energy and time dependent problems, but typically used only first order finite-differencing in time.

It has been shown that the linear-discontinuous discretization in space of the S_N equations in slab geometry is third order accurate,¹⁸⁻²⁰ and although the bilinear-discontinuous (BLD) method has been implemented in two spatial dimensions,^{17,21} there has not been any investigation into the numerical accuracy of the BLD algorithm in two dimensions.

We have implemented a two-dimensional BLD discretization in time and space, combined with a discrete ordinates angular approximation. The expected high-order accuracy of the method together with an inherent capability to better model discontinuous behavior could provide excellent solutions to problems involving pulsed sources and/or long simulation times.

In the next section, we derive the time and space dependent BLD equations and briefly discuss the implementation of the BLD scheme. We then compare results using the BLD method with analytical semi-infinite medium solutions as well as Monte Carlo results. We also contrast the BLD scheme with finite-difference methods, and then numerically investigate the order of the truncation error. The paper concludes with a few summary remarks.

We consider the one-dimensional, time dependent, slab geometry transport equation

$$\frac{1}{v} \frac{\partial \psi(x, \mu, t)}{\partial t} + \mu \frac{\partial \psi(x, \mu, t)}{\partial x} + \sigma_t(x) \psi(x, \mu, t) = 2\pi \int_{-1}^1 \sigma_s(x, \mu_0) \psi(x, \mu', t) d\mu' + Q(x, \mu, t) \quad (6)$$

for which we seek the solution $\psi(x, \mu, t)$, the angular flux of particles at position x and time t . The slab extends from $x = 0$ to $x = a$ and $Q(x, \mu, t)$ represents an external source of particles

To solve this equation numerically, we start with the S_N , or discrete ordinates, approximation²²⁻²⁴ to treat the angular dependence, including anisotropic scattering. With a quadrature set of N nodes and weights $\{\mu_m, w_m\}$ on the angular domain $\mu \in [-1, 1]$ the

iterative S_N scheme is written as

$$\begin{aligned} & \frac{1}{v} \frac{\partial \psi_m^k(x, t)}{\partial t} + \mu_m \frac{\partial \psi_m^k(x, t)}{\partial x} + \sigma_t(x) \psi_m^k(x, t) \\ &= \sum_{l=0}^L \frac{2l+1}{2} \sigma_l(x) P_l(\mu_m) \sum_{n=1}^N w_n P_l(\mu_n) \psi_n^{k-1}(x, t) + Q_m(x, t), \quad m = 1 \dots N. \end{aligned} \quad (7)$$

where, for the k^{th} iteration $\psi_m^k(x, t) = \psi^k(x, \mu_m, t)$, and $Q_m(x, t) = Q(x, \mu_m, t)$. The ordinates or direction cosines, μ_m , can be chosen in a variety of ways. Typically Gauss quadrature nodes are used, or Lobatto quadrature nodes are used with two points fixed at $\mu = \pm 1$ to more accurately model normally incident sources.

In more compact notation this is written

$$\hat{H}_m \psi_m^k(x, t) = \hat{S}_m \psi_m^{k-1} + Q_m(x, t), \quad m = 1 \dots N. \quad (8a)$$

where

$$\hat{H}_m = \frac{1}{v} \frac{\partial}{\partial t} + \mu_m \frac{\partial}{\partial x} + \sigma_t(x), \quad (8b)$$

and

$$\hat{S}_m = \sum_{l=0}^L \frac{2l+1}{2} \sigma_l(x) P_l(\mu_m) \sum_{n=1}^N w_n P_l(\mu_n). \quad (8c)$$

The right hand side of Eq. 8a is a scattering source from the previous iteration in addition to the external distributed source.

A pulsed beam initial condition

$$\psi_m(x, 0) = \begin{cases} \frac{2}{w_m} \delta(x), & \text{for } m \text{ where } \mu_m = 1, \\ 0, & \text{otherwise,} \end{cases} \quad (9a)$$

or an isotropic initial condition

$$\psi_m(x, 0) = 2\delta(x), \quad \text{for all } m. \quad (9b)$$

may be specified.

Zero incident flux boundary conditions

$$\left. \begin{aligned} \psi_m(0, t) &= 0, \quad \text{for all } m \text{ where } \mu_m > 0 \\ \psi_m(a, t) &= 0, \quad \text{for all } m \text{ where } \mu_m < 0 \end{aligned} \right\} \quad \text{for } t > 0, \quad (9c)$$

or a reflective condition on one side of the slab

$$\left. \begin{aligned} \psi_m(0, t) &= 0, \text{ for all } m \text{ where } \mu_m > 0 \\ \psi_m(a, t) &= \psi_{m'}(a, t), \text{ for all } m \text{ where } \mu_m = -\mu_{m'} \end{aligned} \right\} \text{ for } t > 0. \quad (9d)$$

must also be specified.

We now can discretize the S_N equations in space and time. Dividing the spatial domain into N_x intervals, the i^{th} cell is defined on $[x_{i-1/2}, x_{i+1/2}]$, the point x_i being the midpoint of the interval and Δx_i the width of the interval. The time domain is divided into N_t intervals where the time t_s is the midpoint of the s^{th} interval defined over $[t_{s-1/2}, t_{s+1/2}]$, and Δt_s the interval width. With this discretization we define the cell-center average flux

$$\psi_{s,i,m} = \frac{1}{\Delta t_s} \frac{1}{\Delta x_i} \int_{t_{s-1/2}}^{t_{s+1/2}} dt \int_{x_{i-1/2}}^{x_{i+1/2}} dx \psi_m(x, t) \quad (10)$$

We assume that the cross sections are piecewise spatially constant on $x \in [x_{i-1/2}, x_{i+1/2}]$, so that for this interval $\sigma_l(x) = \sigma_{l,i}$ and $\sigma_t(x) = \sigma_{t,i}$. Further, we assume that the material properties do not change with time.

Although several equivalent formulations are possible^{17,25} we outline an approach using the Galerkin method, since it can be used to derive an entire family of schemes suitable for numerical implementation, including finite-difference methods described earlier, as well as the BLD method.

We begin by forming the residual, given here by

$$R_m(x, t) = \hat{H}_m \tilde{\psi}_m^k(x, t) - (\hat{S}_m \tilde{\psi}_m^{k-1} + Q_m(x, t)), \quad m = 1 \dots N. \quad (11)$$

where $\tilde{\psi}_m^k$ represents an approximate expansion of the flux. Then expand the flux in a linear basis in space

$$\tilde{\psi}_m(x, t) = \sum_{i=1}^N \{ \psi_{i,m}^L(t) B_i^L(x) + \psi_{i,m}^R(t) B_i^R(x) \} \quad (12a)$$

where

$$B_i^L(x) = \begin{cases} (x_{i+1/2} - x)/\Delta x_i, & x \in [x_{i-1/2}, x_{i+1/2}] \\ 0, & \text{otherwise,} \end{cases} \quad (12b)$$

and

$$B_i^R(x) = \begin{cases} (x - x_{i-1/2})/\Delta x_i, & x \in [x_{i-1/2}, x_{i+1/2}] \\ 0, & \text{otherwise.} \end{cases} \quad (12c)$$

This form for the basis functions is chosen to more easily introduce a discontinuity in our approximation when deriving the LD equations.

To apply the Galerkin procedure we form inner products of the residual with the basis functions used in the expansion of the flux and equate the result to zero. We note that this can be viewed as minimizing the residual in a weighted least squares sense.²⁶⁻²⁸ Geometrically this is a projection of the actual solution onto a finite-dimensional approximate solution space, which represents a minimum "distance" between the approximate and actual solution, resulting in a "best approximation".²⁷

To continue, we insert the expansion for the flux in the transport equation Eq. 8a, multiply by each basis function in Eqs. 12, and integrate over the cell. Noting the compact support of the the basis functions, we obtain for cell i

$$\hat{H}_m < B_i^R(x), \tilde{\psi}_m(x, t) > = \hat{S}_m < B_i^R(x), \tilde{\psi}_m(x, t) > + < B_i^R(x), Q_m(x, t) >, \quad (13a)$$

and

$$\hat{H}_m < B_i^L(x), \tilde{\psi}_m(x, t) > = \hat{S}_m < B_i^L(x), \tilde{\psi}_m(x, t) > + < B_i^L(x), Q_m(x, t) >. \quad (13b)$$

For each angular index $m = 1 \dots N$, these two equations represent a system of $2N_x$ equations for the expansion coefficients $\psi_{i,m}^R(t)$ and $\psi_{i,m}^L(t)$. These coefficients are themselves dependent on time and are expanded in the linear form

$$\tilde{\psi}_{i,m}^R(t) = \sum_{s=1}^T \left\{ \psi_{s,i,m}^{R-} B_s^-(t) + \psi_{s,i,m}^{R+} B_s^+(t) \right\}, \quad (14a)$$

$$\tilde{\psi}_{i,m}^L(t) = \sum_{s=1}^T \left\{ \psi_{s,i,m}^{L-} B_s^-(t) + \psi_{s,i,m}^{L+} B_s^+(t) \right\}, \quad (14b)$$

where

$$B_s^-(t) = \begin{cases} (t_{s+1/2} - t)/\Delta t_s, & t \in [t_{s-1/2}, t_{s+1/2}] \\ 0, & \text{otherwise,} \end{cases} \quad (14c)$$

and

$$B_s^+(t) = \begin{cases} (t - t_{s-1/2})/\Delta t_s, & t \in [t_{s-1/2}, t_{s+1/2}] \\ 0, & \text{otherwise.} \end{cases} \quad (14d)$$

Again we apply the Galerkin method, this time forming inner products of the time dependent basis functions with Eqs. 13. The result is

$$\begin{aligned} \hat{H}_m < B_s^+(t), < B_i^R(x), \tilde{\psi}'_m(x, t) > > = \hat{S}_m < B_s^+(t), < B_i^R(x), \tilde{\psi}'_m(x, t) > > \\ & + < B_s^+(t), < B_i^R(x), Q_m(x, t) > >, \end{aligned} \quad (15a)$$

$$\begin{aligned} \hat{H}_m < B_s^-(t) | < B_i^R(x), \tilde{\psi}'_m(x, t) > > = \hat{S}_m < B_s^-(t) | < B_i^R(x), \tilde{\psi}'_m(x, t) > > \\ & + < B_s^-(t) | < B_i^R(x), Q_m(x, t) > >, \end{aligned} \quad (15b)$$

and

$$\begin{aligned} \hat{H}_m < B_s^+(t) | < B_i^L(x), \tilde{\psi}'_m(x, t) > > = \hat{S}_m < B_s^+(t) | < B_i^L(x), \tilde{\psi}'_m(x, t) > > \\ & + < B_s^+(t) | < B_i^L(x), Q_m(x, t) > >, \end{aligned} \quad (15c)$$

$$\begin{aligned} \hat{H}_m < B_s^-(t) | < B_i^L(x), \tilde{\psi}'_m(x, t) > > = \hat{S}_m < B_s^-(t) | < B_i^L(x), \tilde{\psi}'_m(x, t) > > \\ & + < B_s^-(t) | < B_i^L(x), Q_m(x, t) > >. \end{aligned} \quad (15d)$$

Here, for notational purposes, we have written $\tilde{\psi}'_m(x, t)$ for the complete expansion of $\psi_m(x, t)$ although in practice it is never used because the inner products are evaluated sequentially. The result is $2N_t$ sets of $2N_x$ equations for the four BLD expansion coefficients, $\psi_{s,i,m}^{R+}$, $\psi_{s,i,m}^{R-}$, $\psi_{s,i,m}^{L+}$, and $\psi_{s,i,m}^{L-}$, for each quadrature node index $m = 1 \dots N$. With the chosen basis functions the cell-center average flux given in Eq. 10 is just the arithmetic average of the expansion coefficients.

Allowing discontinuities at cell edges in the BLD expansion results in higher order accuracy. The discontinuities are introduced when we apply Green's Theorem (integration by parts) to the inner product of the streaming terms of the transport equation, and requires only that appropriate angular flux cell-edge values be specified. This is the point at which cell-to-cell and step-to-step coupling takes place, noting also that the spatial coupling is different for the directions $\mu_m < 0$ than for $\mu_m > 0$.

The final form for the BLD equations in matrix notation are for $\mu_m > 0$

$$\mathbf{A}_{s,i,m}^{(+)} \Psi_{s,i,m}^k = \mathbf{B}_{s,i,m}^{(+)} \Psi_{s,i-1,m}^k + \hat{S}_m \mathbf{C} \Psi_{s,i,m}^{k-1} + \mathbf{D} \Psi_{s-1,i,m} + \frac{18}{\Delta x_i} \mathbf{Q}_{s,i,m}, \quad (16a)$$

and for $\mu_m < 0$

$$\mathbf{A}_{s,i,m}^{(-)} \Psi_{s,i,m}^k = \mathbf{B}_{s,i,m}^{(-)} \Psi_{s,i+1,m}^k + \hat{S}_m \mathbf{C} \Psi_{s,i,m}^{k-1} + \mathbf{D} \Psi_{s-1,i,m} + \frac{18}{\Delta x_i} \mathbf{Q}_{s,i,m}. \quad (16b)$$

Here the solution vector for the k th iteration is

$$\Psi_{s,i,m}^k = \begin{bmatrix} \psi^{R+} \\ \psi^{R-} \\ \psi^{L+} \\ \psi^{L-} \end{bmatrix}_{s,i,m}^k \quad (17)$$

The matrices in the above equations are given below, where the superscripts (+) and (-) indicate separate expressions for $\mu_m > 0$ and $\mu_m < 0$, respectively.

$$\mathbf{A}_{s,i,m}^{(+)} = \begin{bmatrix} (6+6f+4g) & (-6+3f+2g) & (3-6f+2g) & (-3-3f+g) \\ (6+3f+2g) & (6+6f+4g) & (3-3f+g) & (3-6f+2g) \\ (3+6f+2g) & (-3+3f+g) & (6+6f+4g) & (-6+3f+2g) \\ (3+3f+g) & (6+6f+2g) & (6+3f+2g) & (6+6f+4g) \end{bmatrix}_{s,i,m} \quad (18a)$$

$$\mathbf{A}_{s,i,m}^{(-)} = \begin{bmatrix} (6-6f+4g) & (-6-3f+2g) & (3-6f+2g) & (-3-3f+g) \\ (6-3f+2g) & (6-6f+4g) & (3-3f+g) & (3-6f+2g) \\ (3+6f+2g) & (-3+3f+g) & (6-6f+4g) & (-6-3f+2g) \\ (3+3f+g) & (6+6f+2g) & (6-3f+2g) & (6-6f+4g) \end{bmatrix}_{s,i,m} \quad (18b)$$

where

$$f_{s,i,m} = \frac{\mu_m \Delta t_s}{\Delta x_i} \text{ and } g_{s,i} = \sigma_{t,i} \Delta t_s.$$

Similarly,

$$\mathbf{B}_{s,i,m}^{(+)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 12f & 6f & 0 & 0 \\ 6f & 12f & 0 & 0 \end{bmatrix}_{s,i,m} \quad (19a)$$

$$\mathbf{B}_{s,i,m}^{(-)} = \begin{bmatrix} 0 & 0 & -12f & -6f \\ 0 & 0 & -6f & -12f \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}_{s,i,m} \quad (19b)$$

Also, we have

$$\mathbf{C} = \begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & 4 & 1 & 2 \\ 2 & 1 & 4 & 2 \\ 1 & 2 & 2 & 4 \end{bmatrix} \quad (20)$$

and

$$\mathbf{D} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 12 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 \\ 6 & 0 & 12 & 0 \end{bmatrix} \quad (21)$$

The source vector in the above equations, $\mathbf{Q}_{s,i,m}$, is the inner product of the basis functions with the source term $Q_m(x, t)$ which we treat as a material property that is piecewise constant in space and time, although the BLD formalism is not restricted to any particular form for the source.

The BLD equations are solved sequentially from one time step to the next, at each step s performing the usual S_N angular sweeps by marching back and forth across the slab, applying boundary conditions where appropriate, for each discrete ordinate and iterating until converged. Convergence is determined by a user-specified tolerance on the absolute errors of the zeroth scalar flux moment. Note that the term $\mathbf{D}\Psi_{s-1,i,m}$ on the right hand sides of Eqs. 16 contains the converged angular flux vector from the previous $(s - 1)$ time step. Also note that the spatial cell coupling in the first term on the right of each of Eqs. 16 depends on the direction cosine μ_m .

The BLD equations may also be solved directly with some matrix inversion method, but it has been found that direct inversion can be computationally prohibitive in higher dimensions.^{16,29} For this reason, we chose the spatial march scheme outlined above, solving a 4x4 matrix equation for the BLD flux vector at each spatial mesh cell and for every angle during each iteration.

The initial slab boundary angular fluxes for the spatial march at each time step are determined by the initial boundary and source conditions, Eqs. 9. The initial source conditions and distributed sources are either normalized to some total number of particles entering the

system during some user-specified number of time steps, or to a specified source rate. This is done separately for both incident and distributed sources. Alternatively, a First-Scattered Distributed Source ¹⁰ may be specified to model the pulsed incident source conditions.

Results

The BLD equations derived in the previous section were implemented in a computer program along with first (step) and second order (diamond) finite-difference discretizations^{25,30,31} in either space or time. We will now present the results of this implementation and examine the performance of the BLD method. We start by describing an analytical solution which can be used to compare against numerical results. Results using the BLD scheme are contrasted with results from second order diamond-differencing in space and time (DD). We then estimate the order of accuracy of the BLD method as a function of discretization interval widths. This is carried out for the space and time dimension separately, the discretization being fixed in the other dimension in each case. The analytical solution can be found by solving the time dependent transport equation Eq. 7 with $N = 2$. With Lobatto quadrature this is simply the rod model.^{25,32} The result is most easily obtained for a semi-infinite medium such that the boundary conditions in Eqs. 9 at the slab boundary $x = a$ must be replaced by the regularity condition on the angular flux

$$\lim_{x \rightarrow \infty} \psi(x, t) < \infty, \text{ for } t \geq 0.$$

The resulting two coupled equations for the two angular fluxes (one for $\mu = +1$ and one for $\mu = -1$) were solved by Laplace transforms for the case of isotropic scattering, no distributed sources, $v = 1$, and $\sigma_t = 1.0$. We also use the definition for the scattering ratio, $c \equiv \frac{\sigma_s}{\sigma_t}$. The result for the positively-directed angular flux as a function of space and time is

$$\psi_{\infty}^{+}(x, t) = e^{-t(1-c/2)} \left[\delta(t - x) + \frac{cx}{2(t^2 - x^2)^{1/2}} I_1\left(\frac{c}{2}[t^2 - x^2]^{1/2}\right) \Theta(t - x) \right]. \quad (22)$$

We have also derived an expression for the reflected current at $x = 0$ that is in general defined by

$$J^{-}(t) = \int_0^1 \mu \psi(0, -\mu, t) d\mu,$$

and which in this case is simply the negatively-directed angular flux evaluated at $x = 0$ or

$$J_{\infty}^{-}(t) = \psi_{\infty}^{-}(0, t) = \frac{1}{t} e^{-t(1-c/2)} I_1\left(\frac{ct}{2}\right). \quad (23)$$

In the preceding expressions δ and Θ are the delta and step distributions, respectively, and I_1 is the modified Bessel function of first order. The subscripts ∞ denote that the expressions are for a semi-infinite medium.

These analytical results can be used to validate the numerical method so long as any comparisons are made before the effects of leakage from the far side of the slab influence the numerical solution.³² This corresponds to any time t in mean free times less than the slab width a given in mean free paths. However, we note that discrepancies will arise which are due to the attendant truncation errors and dispersion and dissipation effects of the numerical algorithm.

In the numerical solutions, we take $v = 1$ and $\sigma_t = 1.0$ for convenience and such that points in time t and space x are equivalently given in unitless mean free times and mean free paths, respectively, or in cgs units. At each time step, the S_N angular iterations are converged when a maximum pointwise change in absolute value between successive angular flux iterates is less than 10^{-9} (all computations are in double precision FORTRAN). The incident pulsed source condition is modeled with a first-scattered distributed source.

We first examine the spatial discretization. For a slab of width $a = 32$ with scattering ratio $c = 1$, we computed S_2 solutions for $N_x = 2^n, n = 6 \dots 11$, using a fixed number of time intervals $N_t = 2^9$ from $t = 0$ to $t_{max} = 32$. Physically the solutions track the movement and degradation (through scattering and absorption interactions) in space and time of a wave front of particles due to the pulsed source on the left slab face incident. Note that the wave moves a distance x in time t such that at $t = 32$ the wave front is located at the right slab edge $x = 32$. Fig. 4 compares the BLD and DD numerical results for the positively-directed angular flux against the evaluation of Eq. 22 at time $t = t_{max}$ for $N_x = 2^8$. Both the BLD and DD solutions are in excellent agreement with the analytical solution. This spatial discretization was chosen since the DD scheme can be unstable if the Courant (or Courant-Freidrichs-Lewy) limit¹⁰

$$r \equiv \frac{v\Delta t}{\Delta x} = 1, \quad (24)$$

is exceeded. Oscillations near strong gradients can be induced when $r > 1$ and may lead to instabilities and undesirable negative fluxes. The oscillations can be very severe in the presence of discontinuities and the attendant errors can propagate throughout the mesh, as

in this case where we model an incident pulsed source. An example is shown in Fig. 5 where the DD S_2 spatial flux profile is shown for $n = 9, 10, 11$. If $n = 9$ then $r = 1$, and even though the Courant limit is not exceeded severe oscillations occur near the slab edge which coincides with the arrival of the wave front and which the method simply cannot resolve. For the cases $n = 10, 11$ similar instabilities occur, though earlier in time and hence at smaller values of x ; the associated errors are then propagated in time. The BLD method on the other hand does not appear to be limited by the Courant condition although it still has some difficulty in capturing the discontinuous nature of the wave front. However the solution outside of a small neighborhood of the wave front remains unaffected and any associated high-frequency errors are apparently quickly damped.

Thus the BLD method is superior to the DD scheme in one respect in that it avoids oscillations and instabilities and is also therefore less likely to result in negative fluxes. We can use results for similar problems to determine whether the method shows third order truncation error in the discretization interval width in space and time independently, as opposed to the second order accuracy of the DD method.

We first define the truncation error as

$$\| \psi^{(n)} - \psi_{exact} \| = \vartheta(\Delta_n)^k \quad (25)$$

where the order of a method is determined by the power k and the norm is some appropriate norm in the dimension under consideration. In this expression $\psi^{(n)}$ represents the numerical solution along that dimension at some point in the other dimension; the discretization width Δ_n represents the space or time interval width. The superscript (n) denotes the numerical solution for some discretization "level" n in a sequence of increasing interval widths. Also ψ_{exact} is an exact solution that is presumed to be known and which we take to be the S_2 analytical solution.

Now, suppose that successive discretization levels are taken to be $\Delta_{n+1} = \Delta_n/2$ and we plot the absolute error

$$| \psi^{(n)} - \psi_{exact} | ,$$

or the relative error

$$\left| \frac{\psi^{(n)} - \psi_{exact}}{\psi_{exact}} \right|$$

for various values of n along the dimension of interest. Using Eq. 25 it is easy to show that the ratios of these errors for successive values of n should be equal to 2^k . Thus for the DD method this ratio should be four (second order) and while for the BLD scheme it should be eight (third order).

For the present case $\psi^{(n)}$ is the ψ^{R+} component of the converged BLD solution vector $\Psi_{N_t, i, 1}$ and $\psi_{exact} = \psi_{\infty}^{+}(x_i, t_{max})$ for $i = 1 \dots N_x$. The relative errors for the BLD method are shown in Fig. 6 while the relative errors for the DD scheme are shown in Fig. 7. In these figures the spatial interval width sequence is given by $\Delta x_n = 2^{5-n}$ ($N_x = 2^n$) for $n = 6 \dots 9$. Except for a neighborhood near the wave front at the right edge of the slab, the ratio of successive errors are as anticipated, eight for BLD and four for DD. This can be seen more clearly in Fig. 8 where we plot the absolute error between the S_2 BLD numerical solution and analytical solution and confirm that the ratio is indeed eight. Note that the relative errors for the BLD case $N_x = 2^6$ are about the same or slightly smaller than the DD case where $N_x = 2^9$, which is expected since the BLD method is third order while DD is second order accurate.

We note that the pulsed initial conditions for this problem do represent a very stringent test for any numerical scheme and in the neighborhood of the wave front the errors for both numerical schemes can be quite large as seen in the figures. However, further evidence that the BLD method is better-suited than the DD scheme for treating such discontinuities is provided by the fact that maximum errors over the cases $n = 6 \dots 9$ of the BLD method were $2.704 \cdot 10^{-5}$ (absolute) and 0.2451 (relative), whereas for the DD scheme the maximum errors were 1.672 (absolute) and $2.593 \cdot 10^6$ (relative).

The numerical analysis presented is for a finite, though extremely thick slab, yet we used the exact solution for a semi-infinite medium to estimate the error. In order to more accurately model the semi-infinite case numerically, we included some absorption in the problems described above. An example showing the errors between the S_2 BLD numerical results and the analytical solution for $c = 0.9$ is shown in Fig. 9 for $n = 6 \dots 9$. These results are almost identical with those for the case $c = 1$ and support the previous conclusion that BLD is third order accurate in the spatial discretization interval width. The results presented so far have not concerned scalar fluxes, but have implicitly included

the angular coupling through scattering, albeit in only two directions. We also had the opportunity to use an analytical solution to estimate the truncation error in Eq. 25. It is possible in principle to similarly solve the S_N equations for $N > 2$ for a semi-infinite medium as in the S_2 case presented above, though it would be very complicated and a closed-form solution would not necessarily be possible. But using Eq. 25 it is easy to see that the error can be estimated by taking difference of successive discretization levels n and $n + 1$

$$\| \phi^{(n)} - \phi^{(n+1)} \| = \vartheta(\Delta_n)^k \left[1 + \left(\frac{\Delta_{n+1}}{\Delta_n} \right)^k \right], \quad (26)$$

where the norm is now estimated by subtracting the scalar fluxes at the same points along the dimension of interest, at some fixed point in the other dimension. Of course, this is an estimate of the actual error only if one assumes that the derivatives and constants implicit in Eqs. 25 and 26 do not change much in any given interval. Note that this assumption was also applied to the previous analysis. In both cases the derivatives are not really constant, and so there may be some structure in the error curves along the dimension of interest as in the previous figures. This also explains why the ratio of successive errors may not be exactly equal to 2^k .

If successive discretization levels are again taken to be $\Delta_{n+1} = \Delta_n/2$, then it can be seen from Eq. 26 that the ratio of the errors between the cases $n, n + 1$ and $n + 1, n + 2$ will be 2^k as before. Together with the numerical BLD results for the point scalar fluxes, this fact can be used to see both that the truncation error analysis is not dependent on the S_N approximation and that the scalar fluxes show the same third order accuracy as the angular fluxes.¹⁹

In Figs. 10 and 11 we show results for S_8 and S_{32} , respectively, using the BLD method. In this case again, $\Delta x_n = 2^{5-n}$ for a slab of width $a = 32$ and $c = 1$. The error estimate in the point scalar fluxes

$$| \phi^{(n)} - \phi^{(n+1)} |$$

at the spatial locations $x_i = i\Delta x_n$, $i = 1 \dots 2^n$, for successive discretization levels $n, n + 1$ are shown at time $t_{max} = 32$ ($N_t = 2^9$) for various values of n . The ratio between each case is again eight, indicating third order accuracy for the scalar fluxes, independent of number discrete ordinates N . Note again that the features in the error curves are due to the

variation of the derivatives or constants in the truncation error expression.

We will now consider the performance of the BLD method as a function of the discretization of the time dimension. First, we validate the results in time by showing in Fig. 12 the reflected current $J^-(t)$ exiting the left face of the slab as a function of time. The results shown are for a slab of width $a = 64$ and $N_x = 2^8$ with scattering ratio $c = 1$, and for a pulsed incident source condition modelled with the FSDS method. The DD and BLD results for $t_{max} = 64$ and $N_t = 2^9$ are compared to the analytical semi-infinite medium solution given by Eq. 23. Again the agreement is very good, especially at later times where the asymptotic solution is preserved by the numerical schemes. The early time oscillations of the results are shown in the inset of Fig. 12, making it clear that the BLD results show oscillations that are far less severe than the DD method. Although these errors are damped by both schemes, it has been our experience that for some discretizations the DD method will not damp these high-frequency errors and catastrophic instabilities can often result, leading to unphysical solutions, even with a first-scattered distributed source. This has not been the case with the BLD scheme.

The results for similar problems were used to determine the order of accuracy in the time dimension for the BLD method, by successively halving the discretization interval width $\Delta t_{n+1} = \Delta t_n/2$. The relative errors

$$\left| \frac{J^{(n)} - J_\infty}{J_\infty} \right|,$$

where $J^{(n)}$ is the BLD numerical result and J_∞ is the analytical solution for the S_2 reflected current, are plotted in Fig. 13. The slab width is $a = 64$, $N_x = 2^{11}$, for $c = 1$ and $\Delta t = 2^{6-n}$ ($N_t = 2^n$). For the cases $n = 4 \dots 8$ shown in the figure, it can be seen that, at least at long times after any oscillations due to the discontinuous incident pulse die out, the method shows third order accuracy since the ratio of two successive error curves n and $n + 1$ is eight.

As in the case of the spatial discretization we can determine the effect, if any, on the error analysis due to the S_N approximation by taking the difference between the numerical results for the reflected current at successive discretization levels as an error estimate for $N > 2$. This is shown in Fig. 14 for the same parameters as in the previous figure. The

error estimate in the S_8 reflected currents

$$| J^{(n)} - J^{(n+1)} |$$

at the points $t_s = s\Delta t_n$, $s = 1 \dots 2^n$, for each pair of successive discretization levels $n, n+1$ are shown for $n = 4 \dots 9$. The ratio between cases $n, n+1$ and $n+1, n+2$ is eight, and since the current is an angle-integrated quantity this verifies that the third order accuracy of the BLD scheme in the time dimension is independent of the angular discretization.

In the last figure, Fig. 15, we show the relative computational effort of the BLD discretization method compared to the diamond-difference scheme. Shown is the CPU time ratio of the two methods (normalized to DD execution times) on an IBM RISC 6000 Model 370 for an S_{32} incident beam calculation with the FSDS option. It can be seen that the BLD method is about four to six times slower than the diamond-difference scheme. It is our experience that this is an asymptotic result, independent of space, angle or time discretization as seen in the figure.

The poorer run-time performance of the BLD method is primarily due to the 4x4 matrix inversion required to calculate the angular flux vector for each mesh cell during a spatial march, despite our attempt to optimize the BLD algorithm by developing code for the 4x4 solution at each spatial mesh cell using the symbolic algebra system MAPLE.³³ With MAPLE the matrix equations, Eqs. 16, were solved symbolically for a given space-time mesh cell. This solution was then translated into optimized FORTRAN by MAPLE for each of the cases $\mu_m > 0$ and $\mu_m < 0$. Taking advantage of the specific structure of the matrix equation in this way resulted in as much as a 40% reduction in computing time, compared to a solution using a general LU factorization and back substitution at every mesh cell. Still, in contrast to the BLD algorithm, only the cell-average angular flux is evaluated for each cell during the spatial march in a finite-difference calculation. The remaining cell-edge angular flux value is then found by assignment (step-differencing) or by a simple evaluation (diamond-differencing). On the other hand, the four components of the BLD flux vector must be computed at each spatial march step, the arithmetic average of which is the cell-centered average angular flux, accounting for the increased CPU execution times.

4 Summary

We have developed and successfully implemented a two-dimensional bilinear discontinuous discretization in space and time, used in conjunction with the S_N angular approximation, to numerically solve the time dependent, one-dimensional, one-speed, slab geometry, transport equation.

Numerical results and comparison with analytical solutions have shown that the BLD scheme is third-order accurate in the space and time dimensions independently.

Comparison of the BLD results with diamond-difference methods indicate that the BLD method is both quantitatively and qualitatively superior to the DD scheme. We note that the form of the transport operator is such that these conclusions carry over to energy dependent problems that include the constant-slowness-approximation term, and to multiple space dimensions or combinations thereof.

An optimized marching or inversion scheme or a parallel algorithm should be investigated to determine if the increased accuracy can compensate for the extra overhead required for a BLD solution, and then could be compared to other discretization methods such as nodal or characteristic schemes.

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Figure 1: Dependence of the microscopic scattering cross section on μ_{cut} for 100 KeV Au ions incident on a Au target.

Figure 2: Comparison of full and partial range fits with the exact microscopic scattering cross section for 100 keV Au ions incident on a Au target.

Figure 3: Dependence of the full range fits on Legendre order for 1 MeV P ions incident on a Si target.

Figure 4: Comparison of BLD and DD S_2 results with the S_2 analytical solution. The positively directed angular flux is shown at $t = 32$ mean free times in a slab 32 mean free paths thick. Results are for a scattering ratio $c = 1$ and a mesh with $N_t = 2^9$ and $N_x = 2^8$.

Figure 5: DD oscillations about the S_2 analytical solution for various spatial discretizations that equal or exceed the Courant limit. The positively directed angular flux is shown at $t = 32$ mean free times ($N_t = 2^9$) in a 32 mean free path thick slab with scattering ratio $c = 1$.

Figure 6: Relative error between the S_2 numerical BLD results for the positively directed angular flux and the analytical solution at $t = 32$ mean free times ($N_t = 2^9$). The slab is 32 mean free paths thick, $c = 1$, and $\Delta x_n = 2^{5-n}$ for $n = 6 \dots 9$. The ratio of errors for successive values of n is eight, indicating the BLD method is third order accurate.

Figure 7: Relative error between the numerical DD S_2 results for the positively directed angular flux and the analytical solution at $t = 32$ mean free times ($N_t = 2^9$) in a 32 mean free path thick slab, $c = 1$, with $\Delta x_n = 2^{5-n}$ for $n = 6 \dots 9$. The ratio of errors for successive values of n is four, indicating the DD method is second order accurate.

Figure 8: Error between the numerical S_2 BLD results for the positively directed angular flux and the analytical solution at $t = 32$ mean free times ($N_t = 2^9$) in a 32 mean free path thick slab, $c = 1$, with $\Delta x_n = 2^{5-n}$ for $n = 6 \dots 9$. The ratio of errors for successive values of n is clearly eight. (The $n = 9$ curve cannot be seen on this scale.)

Figure 9: For a scattering ratio $c = 0.9$, the relative errors of the numerical S_2 BLD results between the positively directed angular flux and the analytical solution are shown at $t = 32$ ($N_t = 2^9$) in a slab 32 mean free paths thick with $\Delta x_n = 2^{5-n}$ for $n = 6 \dots 9$.

Figure 10: Error estimate for the BLD S_8 scalar fluxes showing the difference in absolute value of the scalar fluxes at successive discretization levels $\Delta x_n = 2^{5-n}$ for several values of n . The error is estimated at $t = 32$ mean free times ($N_t = 2^9$) in a 32 mean free path thick slab with $c = 1$.

Figure 11: Error estimate for the BLD S_{32} scalar fluxes showing the difference in absolute value of the scalar fluxes at successive discretization levels $\Delta x_n = 2^{5-n}$ for several values of n . The error is estimated at $t = t_{max} = 32$ mean free times ($N_t = 2^9$) in a 32 mean free path thick slab with $c = 1$.

Figure 12: Reflected current exiting the left face of a slab 64 mean free paths thick with $N_x = 2^8$ and $c = 1$. The maximum time is $t_{max} = 64$ and $N_t = 2^9$. The results of the DD and BLD S_2 numerical calculations are compared with the S_2 analytical solution. The inset shows the reflected current at early times.

Figure 13: Relative error between the S_2 numerical BLD results and the analytical solution for the reflected current exiting a 64 mean free path thick slab with $c = 1$ and $N_x = 2^{11}$. The errors are shown for $\Delta t_n = 2^{6-n}$ ($t_{max} = 64$) for the cases $n = 4 \dots 8$. The ratio of the errors between successive values of n is eight.

Figure 14: Error estimate for the BLD S_8 numerical results for the reflected current exiting from a 64 mean free path thick slab, $c = 1$, and $N_x = 2^{11}$. The difference in absolute value of the current for successive discretization levels $\Delta t_n = 2^{6-n}$ is shown for several values of n .

Figure 15: Ratio of the CPU execution time for the BLD method to that for the DD finite-difference scheme. The comparison is shown as a function of the number of spatial mesh cells for various time meshes. Timings were performed on an IBM RS6000/370. Absolute times for a 1024x1204 mesh were about 5300 seconds for the BLD method and 1030 seconds for the DD scheme.