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CONTINUOUS-SLOWING-DOWN OPERATOR

AUTHOR(S): Maximo S. Lazo, UNM
Jim E. Morel, X-6

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MASTER

A LINEAR-DISCONTINUOUS GALERKIN APPROXIMATION
FOR THE CONTINUOUS-SLOWING-DOWN-OPERATOR

Maximo S. Lazo
Dept. of Chem. and Nucl. Engr.
University of New Mexico
Albuquerque, NM 87131

J. E. Morel
Applied Theoretical Physics Division
Los Alamos National Laboratory
Los Alamos, NM 87545

Abstract

A linear-discontinuous Galerkin treatment is developed for the continuous-slowing-down operator. Multigroup Legendre coefficients are derived which allow this treatment to be implemented in standard S_n codes. A synthetic acceleration scheme is developed to accelerate the outer iterations required by this treatment. A computational comparison between a first-order multigroup treatment, the diamond-difference treatment, and the linear-discontinuous treatment is given.

INTRODUCTION

The continuous-slowing-down (CSD) operator is obtained by means of the Fokker-Planck approximation¹ to the Boltzmann scattering operator, and is generally used to model charged-particle energy losses due to small-angle scattering interactions in plasmas.^{2,3} However, this operator has also been recently used to model 14 MeV fusion neutron transport.⁴ Our main interest in the CSD operator stems from a desire to perform coupled electron-photon transport calculations with applications to space-radiation shielding and x-ray effects on electronics. Specifically, we intend to use the standard multigroup treatment to model the photon scattering and the large-angle electron scattering, while using a numerical treatment for the CSD operator to model the electron energy losses due to small-angle scattering. Ideally, one would like to develop numerical treatments for the CSD operator which can be expressed in terms of effective multigroup-Legendre coefficients, and thereby be implemented in standard S_n codes without modifying them. Because existing S_n codes can be used to perform the transport calculations, the advantage of such treatments is that one need only develop a code to generate appropriate multigroup-Legendre cross-section sets for coupled electron-photon transport rather than having to develop both a cross-section code and a specialized transport code. Morel has previously developed a first-order-accurate multigroup-Legendre treatment for the CSD operator,¹ and has recently derived multigroup-Legendre coefficients for the standard

diamond-difference treatment.⁵ The present work represents an extension of this previous work.

The purpose of our paper is five-fold:

- a) To describe a new linear-discontinuous Galerkin treatment for the continuous-slowing-down operator.
- b) To demonstrate that this treatment can be implemented in standard S_n codes by means of appropriate multigroup Legendre cross-section coefficients.
- c) To demonstrate that this treatment yields effective upscatter cross sections, and that the resulting spectral radius for the outer iterations approaches unity in optically-thick systems.
- d) To describe a synthetic acceleration scheme which reduces the outer-iteration spectral radius from unity to one-sixth.
- e) To compare the performance of a first-order multigroup treatment, the diamond-difference treatment, and the linear-discontinuous treatment for the CSD operator in electron transport problems.

I. DERIVATION OF THE BASIC EQUATIONS

The CSD operator is given by¹

$$C\psi(E) = \frac{\partial[S(E)\psi(E)]}{\partial E}, \quad (1)$$

where $S(E)$ is the stopping power and ψ is the angular flux. The derivation of our method is begun by considering the following simple equation:

$$\mu \frac{\partial \psi}{\partial x} = \frac{\partial S\psi}{\partial E}. \quad (2)$$

The energy domain is partitioned into contiguous cells with the high and low edge-energies for cell g respectively denoted by $E_{g-1/2}$ and $E_{g+1/2}$. The stopping power is assumed to be positive (i.e., it is assumed that on the average particles lose energy). This establishes a unique direction of flow for the particles in that they move from higher to lower energies due to the influence of the CSD operator. The energy dependence of the angular flux is assumed to be linear within each cell, with discontinuities allowed at the cell interfaces. In particular,

$$\psi(E) = \psi_{g,-}(E - E_{g+1/2})/\Delta E_g + \psi_{g,+}(E_{g-1/2} - E)/\Delta E_g, \quad (3)$$

for $E_{g-1/2} > E \geq E_{g+1/2}$, where $\Delta E_g = E_{g-1/2} - E_{g+1/2}$, $\psi_{g,-}$ represents $\psi(E_{g-1/2} - |\epsilon|)$ in the limit as $\epsilon \rightarrow 0$, and $\psi_{g,+}$ represents $\psi(E_{g+1/2})$. Note that the angular flux at each cell interface is continuous in the direction of particle flow. This is an essential property of the method. For simplicity, the dependence of the stopping power is assumed to be linear within each cell, with continuity at the cell interfaces. However, any type of continuous energy dependence can be assumed. Substituting Eq.(3) into Eq.(2) and integrating over the g'th energy cell, we obtain:

$$\mu \frac{\partial}{\partial x} \frac{(\psi_{g,-} + \psi_{g,+})}{2} = \frac{S_{g-1/2} \psi_{g-1,+}}{\Delta E_g} - \frac{S_{g+1/2} \psi_{g,+}}{\Delta E_g} \quad (4a)$$

Substituting Eq.(3) into Eq.(2), multiplying Eq.(2) by $(E - E_g)$, and integrating Eq.(2) over the g'th energy cell, we obtain:

$$\begin{aligned} \mu \frac{\partial}{\partial x} \frac{(\psi_{g,-} - \psi_{g,+})}{\Delta E_g} &= \frac{2(S_{g-1/2} - S_{g+1/2})}{\Delta E_g} (\psi_{g,-} - \psi_{g,+}) \\ &+ \frac{6S_{g-1/2}}{\Delta E_g} (\psi_{g-1,-} - \psi_{g,-}) \end{aligned} \quad (4b)$$

where $S_{g+1/2} = S(E_{g+1/2})$. Equation (4a) is an equation for the average

value of the solution over the g'th cell and is referred to as the zero'th moment equation. Equation (4b) is an equation for the slope of the solution over the g'th cell and is referred to as the first moment equation. From a physical viewpoint, Eqs. (4a) and (4b) express the conservation of both particle number and particle energy. Equations for $\psi_{g,-}$ and $\psi_{g,+}$ respectively can be obtained from Eqs. (4a) and (4b) by means of simple algebraic manipulation:

$$\begin{aligned} \mu \frac{\partial \psi_{g,-}}{\partial x} + \frac{(2S_{g-1/2} + S_{g+1/2})}{\Delta E_g} \psi_{g,-} &= \\ -\frac{S_{g-1/2}}{\Delta E_g} \psi_{g,+} + \frac{4S_{g-1/2}}{\Delta E_g} \psi_{g-1,+} \end{aligned} \quad (5a)$$

$$\begin{aligned} \mu \frac{\partial \psi_{g,+}}{\partial x} + \frac{(2S_{g+1/2} - S_{g-1/2})}{\Delta E_g} \psi_{g,+} &= \\ \frac{(2S_{g-1/2} + S_{g+1/2})}{\Delta E_g} \psi_{g,-} - \frac{2S_{g-1/2}}{\Delta E_g} \psi_{g-1,+} \end{aligned} \quad (5b)$$

Equations (5a) and (5b) have a form similar to that of the multigroup S_n equations. The left side of each equation can be interpreted as a streaming term plus a removal term, while the right side of each equation can be interpreted as a scattering source. However, whereas the standard multigroup equation for the g 'th energy cell has a single unknown which is the integral over the cell of the solution, these equations have two unknowns for the g 'th cell which are the upper and lower point values of the solution within the cell.

Although Eqs. (5a) and (5b) can be solved with a standard S_n code by means of appropriately defined cross-section data, these data do not satisfy an important property satisfied by standard multigroup cross-section data. In particular, the standard property not satisfied is:

$$\sigma_{r,k} = \sum_j \sigma_{k \rightarrow j} \quad (6)$$

where $\sigma_{r,k}$ denotes the removal cross section for group k and $\sigma_{k \rightarrow j}$ denotes the cross-section for a transfer from group k to group j . Because Eq.(6) is not satisfied, any acceleration scheme or edit routine relying upon this property will not function properly. This difficulty can be eliminated by transforming Eqs. (5a) and (5b) to what we call a generalized multigroup basis. A generalized multigroup basis is defined as any basis which satisfies:

$$\int_{E_{\min}}^{E_{\max}} \psi(E) dE = \sum_{k=1}^{NG} \psi_k \quad (7)$$

where $\psi(E)$ denotes the angular flux, $E_{\min}$ and $E_{\max}$ denote the minimum and maximum respective energies in the domain, ψ_k denotes the k 'th unknown for the discretized energy dependence, and NG is the number of unknowns or "groups". The generalized multigroup basis appropriate for the unknowns appearing in Eqs. (5a) and (5b) is defined by:

$$\psi_{2g-1} = \psi_{g,-\Delta E_g/2} \quad (8a)$$

$$\psi_{2g} = \psi_{g,+\Delta E_g/2} \quad (8b)$$

where ψ_k denotes the "multigroup flux" corresponding to "group" k . Note that there are two "groups" per cell rather than one group per cell as in the standard multigroup treatment. Also note that that these generalized multigroup unknowns do in fact satisfy Eq.(7). Transforming Eqs. (5a) and (5b) to the generalized multigroup basis by means of Eqs. (8a) and (8b), we obtain the desired multigroup equations:

$$\mu \frac{\partial \psi_{2g-1}}{\partial x} + \frac{(2S_{g-1/2} + S_{g+1/2})}{\Delta E_g} \psi_{2g-1} =$$

$$- \frac{S_{g-1/2}}{\Delta E_g} \Psi_{2g} + \frac{4S_{g-1/2}}{\Delta E_{g-1}} \Psi_{2g-2} \quad (9a)$$

$$\begin{aligned} \frac{\mu \partial \Psi_{2g}}{\partial x} + \frac{(2S_{g+1/2} - S_{g-1/2})}{\Delta E_g} \Psi_{2g} = \\ + \frac{(2S_{g-1/2} + S_{g+1/2})}{\Delta E_g} \Psi_{2g-1} - \frac{2S_{g-1/2}}{\Delta E_{g-1}} \Psi_{2g-2} \end{aligned} \quad (9b)$$

The multigroup transfer coefficients, $o_{k \rightarrow j}$, denoting the cross section for transferring from group k to group j without directional change, can be deduced from Eqs. (9a) and (9b) by writing these equations in the following generalized form:

$$\frac{\mu \partial \Psi_{2g-1}}{\partial x} + o_{r,2g-1} \Psi_{2g-1} = o_{2g+2g-1} \Psi_{2g} + o_{2g-2+2g-1} \Psi_{2g-2} \quad (10a)$$

$$\frac{\mu \partial \Psi_{2g}}{\partial x} + o_{r,2g} \Psi_{2g} = o_{2g-1+2g} \Psi_{2g-1} + o_{2g-2+2g} \Psi_{2g-2} \quad (10b)$$

where $o_{r,k}$ denotes the removal cross section for group k . Comparing Eqs. (9a), (10a), (9b), and (10b), one obtains the following definitions for the transfer coefficients:

$$o_{r,2g-1} = \frac{2S_{g-1/2} + S_{g+1/2}}{\Delta E_g} \quad (11a)$$

$$o_{2g-1+2g} = \frac{2S_{g-1/2} + S_{g+1/2}}{\Delta E_g} \quad (11b)$$

$$o_{r,2g} = \frac{2S_{g+1/2} - S_{g-1/2}}{\Delta E_g} \quad (12a)$$

$$o_{2g+2g-1} = - \frac{S_{g-1/2}}{\Delta E_g} \quad (12b)$$

$$o_{2g+2g+1} = \frac{4S_{g+1/2}}{\Delta E_g} \quad (12c)$$

$$o_{2g+2g+2} = - \frac{2S_{g+1/2}}{\Delta E_g} \quad (12d)$$

An absorption cross section is defined for the last group to account for the fact that particles which would normally down-scatter into the next group simply disappear from the system:

$$\sigma_{a,2NC} = \frac{2S_{NC+1/2}}{\Delta E_{NC}} \quad (13a)$$

$$\sigma_{r,2NC} = \frac{-S_{NC-1/2}}{\Delta E_{NC}} \quad (13b)$$

where NC denotes the number of energy cells. Note that these coefficients do in fact satisfy the standard multigroup property expressed by Eq.(6). The multigroup Legendre coefficients which we ultimately seek can be obtained from the multigroup transfer coefficients given in Eqs. (11) and (12) by noting that since the CSD operator changes the energy of a particle without changing its direction, the probability per unit pathlength per steradian for transferring from group k to group j is given by:

$$\sigma_{k \rightarrow j}(\mu_0) = \sigma_{k \rightarrow j} \frac{\delta(\mu_0 - 1)}{2\pi} \quad (14)$$

where μ_0 denotes the cosine of the scattering angle. The Legendre coefficients are simply given by the Legendre moments of Eq.(14). In particular, because

$$\int_{-1}^{+1} \delta(\mu_0 - 1) P_l(\mu_0) d\mu_0 = 1.0 \quad (15)$$

for all l where $P_l(\mu_0)$ denotes the l'th Legendre polynomial, it follows that:

$$\sigma_{k \rightarrow j}^l = \sigma_{k \rightarrow j} \quad , \quad l = 0, \infty \quad (16)$$

where $\sigma_{k \rightarrow j}^l$ denotes the l'th Legendre moment for a transfer from group k to group j. Since a truncated Legendre expansion must be used in an S_N code to represent the delta-function appearing in Eq.(14), it is natural to question the accuracy of such a gross approximation. In both References 1 and 5 it is shown that the truncated expansion for the delta-function will be exact in the sense that particles will indeed transfer between groups without any angular change if two simple rules are followed. First, only full-range Gauss or Galerkin⁶ quadrature sets may be used. Second, cross-section expansions of degree N-1 must be used in conjunction S_N quadrature sets.

It can be seen from Eqs. (11) and (12) that only downscatter occurs between cells, but upscatter occurs between the two groups within a cell. Thus outer iterations are required with the linear-discontinuous

approximation. Because outer iterations are not required with the first-order multigroup and diamond-difference approximations,^{1,5} the linear-discontinuous method is significantly more complicated than these other methods.

II. STABILITY OF THE INNER ITERATIONS

It can be seen from Eq.(12) that some of the transfer coefficients appearing in Eqs. (11) and (12) may be negative. It is important to assess the effect of these coefficients on the stability of the standard S_n iteration algorithms. In this section we consider the stability of the inner iteration process. Because there is no within-group scattering associated with the CSD operator, only one inner iteration per outer iteration need be performed to solve Eq.(2), but instabilities can nonetheless arise. Furthermore, in realistic calculations the CSD treatment will be combined with multigroup cross sections which include within-group scattering. Regardless of the presence of within-group scattering, the inner iteration process will be stable if the removal coefficients are positive. It can be seen from Eqs. (11a) and (12a) that the removal cross sections will be positive as long as the stopping power is positive and the stopping power does not change by more than a factor of two across a cell. Although particle stopping powers do become negative at thermal energies, the CSD approximation is only appropriate at suprathreshold energies because a higher-order Fokker-Planck approximation must be used to obtain the exact equilibrium spectrum. Thus when using the CSD approximation, one generally assumes a thermal cut-off energy such that particles slowing down below that energy are considered to be "absorbed" by the medium. Positive stopping powers can be ensured simply by choosing this thermal cut-off energy to be greater than the energy at which the stopping power becomes negative. The cell widths can always be chosen such that the stopping power does not change by more than a factor of two across the cell. This is not a restrictive requirement because the stopping power is generally a slowly-varying function of energy. Thus stability of the inner iteration process can be ensured without difficulty.

III. STABILITY AND EFFECTIVENESS OF THE OUTER ITERATIONS

In order to determine the stability and effectiveness of the outer iteration process, we have performed a Fourier analysis. In standard S_n codes, the outer iteration scheme is the Gauss-Seidel scheme. For the linear-discontinuous CSD equations, this scheme can be expressed as follows:

$$\mu \frac{\partial \psi_{2g-1}^{l+1}}{\partial x} + \sigma_{r,2g-1} \psi_{2g-1}^{l+1} = \sigma_{2g+2g-1} \psi_{2g}^l + QD_{2g-1}, \quad (17a)$$

$$\mu \frac{\partial \psi_{2g}^{l+1}}{\partial x} + \sigma_{r,2g} \psi_{2g}^{l+1} = \sigma_{2g-1+2g} \psi_{2g-1}^{l+1} + QD_{2g} , \quad (17b)$$

where l denotes the iteration index, and QD denotes the downscatter source from cell $g-1$. The downscatter source is assumed to be known. This means that the two multigroup fluxes within each cell must be converged before proceeding to the next cell. This is much more efficient than iterating on the downscatter sources as well as the upscatter sources by proceeding to the next cell after just one iteration as defined by Eqs. (17a) and (17b).

The error associated with the l 'th iterate for the k 'th group is defined as:

$$\epsilon_k^l = \psi_k - \psi_k^l , \quad (18)$$

where ψ_k denotes the exact angular flux solution for group k . It is not difficult to show that the error satisfies:

$$\mu \frac{\partial \epsilon_{2g-1}^{l+1}}{\partial x} + \sigma_{r,2g-1} \epsilon_{2g-1}^{l+1} = \sigma_{2g+2g-1} \epsilon_{2g}^l , \quad (19a)$$

$$\mu \frac{\partial \epsilon_{2g}^{l+1}}{\partial x} + \sigma_{r,2g} \epsilon_{2g}^{l+1} = \sigma_{2g-1+2g} \epsilon_{2g-1}^{l+1} . \quad (19b)$$

The basic idea of the Fourier analysis is to convert Eqs. (19a) and (19b) from a system of coupled differential equations to an algebraic system of equations by assuming the following spatial dependence for the error vector:

$$\underline{\epsilon}(x, \mu) = \underline{\epsilon}(\lambda, \mu) e^{i\lambda x} , \quad -\infty < x < +\infty , \quad -\infty < \lambda < +\infty , \quad i = \sqrt{-1} , \quad (20)$$

where

$$\underline{\epsilon} = (\epsilon_{2g-1} , \epsilon_{2g}) . \quad (20a)$$

The resulting equations are:

$$(\mu i \lambda + \sigma_{r,2g-1}) \epsilon_{2g-1}^{l+1} = \sigma_{2g+2g-1} \epsilon_{2g}^l , \quad (21a)$$

$$(\mu i \lambda + \sigma_{r,2g}) \epsilon_{2g}^{l+1} = \sigma_{2g-1+2g} \epsilon_{2g-1}^{l+1} . \quad (21b)$$

Equations (21a) and (21b) can be expressed in matrix form as follows:

$$\underline{\epsilon}^{l+1} = A^{-1} B \underline{\epsilon}^l , \quad (22)$$

where

$$A_{1,1} = (\mu_1 \lambda + \sigma_{r,2g-1}), \quad A_{1,2} = 0, \quad A_{2,1} = \sigma_{2g-1+2g},$$

$$A_{2,2} = (\mu_1 \lambda + \sigma_{r,2g}). \quad (22a)$$

$$B_{1,1} = 0, \quad B_{1,2} = \sigma_{2g+2g-1}, \quad B_{2,1} = 0, \quad B_{2,2} = 0. \quad (22b)$$

The matrix $A^{-1}B$ is called the iteration matrix. The eigenvalues of this matrix determine the asymptotic convergence rate for the iteration scheme. In particular, after "many" iterations, successive error vectors satisfy:

$$|\underline{\varepsilon}|^{k+1} = \omega |\underline{\varepsilon}|^k, \quad (23)$$

where ω is the spectral radius of the iteration matrix. The spectral radius of a matrix is defined as the maximum of the absolute values of its eigenvalues. From Eq.(23) it follows that a spectral radius near unity results in slow convergence while a spectral radius near zero results in rapid convergence.

The elements of the 2×2 matrix $A^{-1}B$ depend upon several parameters. Thus two eigenvalues, denoted by ω_1 and ω_2 , are obtained for each set of parameter values. However, if the stopping power is assumed to be constant, the eigenvalues can be expressed as a function of a single parameter, $p = \lambda \mu \Delta E_g / S$. In Fig. 1 a plot is given of $\omega = \max(|\omega_1|, |\omega_2|)$ as a function of p . Values are plotted only for positive p because ω is an even function of p . From Fig. 1 it can be seen that ω has a maximum value of unity at $p = 0$. Thus the spectral radius for the outer iteration operator is unity. Our model analysis is based upon the assumption of an infinite medium and therefore does not include boundary effects. In any real calculation, particle leakage will cause the spectral radius to be less than unity, but in the limit as the thickness of the system is increased, the spectral radius will approach unity. Thus arbitrarily slow convergence rates are possible in realistic calculations. Computational testing has shown that extremely slow convergence rates are indeed obtained in almost any realistic calculation. Thus the outer iterations must be accelerated for the linear-discontinuous method to be practical. Although the first-order multigroup and diamond-difference CSD methods can be efficiently implemented in unmodified S_n codes, the linear-discontinuous CSD treatment cannot be so implemented due to the need for convergence acceleration. However, our ability to express the unaccelerated method in standard S_n form is not wasted because fewer modifications are required to implement the accelerated scheme than would otherwise be required.

IV. ACCELERATION OF THE OUTER ITERATIONS

We have developed a synthetic scheme to accelerate the outer iterations required by the linear-discontinuous treatment for the CSD operator. Synthetic acceleration is a very general form of convergence acceleration which can be applied to any type of equation. Most methods developed to date have been used to accelerate the inner iterations in S_n codes.^{7,8,9} The basic idea of our synthetic acceleration scheme is fairly easy to explain. We begin by expressing the outer iteration scheme in operator form:

$$T\underline{\psi}^{l+1} = B\underline{\psi}^l + \underline{QD} , \quad (24)$$

where T is obtained from the matrix A , defined by Eq.(22a), by replacing the term " μ_0 " by " $\mu \frac{\partial}{\partial x}$ ", B is defined by Eq.(22b), and $\underline{QD}$ is the downscatter source.

It is not difficult to show that the error corresponding to $\underline{\psi}^{l+1}$ can be expressed as follows:

$$\underline{\epsilon}^{l+1} = (T - B)^{-1} B(\underline{\psi}^{l+1} - \underline{\psi}^l) . \quad (25)$$

Thus the exact solution could be obtained by solving Eq.(25) and adding $\underline{\epsilon}^{l+1}$ to $\underline{\psi}^{l+1}$. However, if one could afford to invert $T - B$, one would not be iterating in the first place because, as can be seen from Eq.(24),

$$\underline{\psi} = (T - B)^{-1} \underline{QD} . \quad (26)$$

Nonetheless, Eq.(25) implies that if an easily invertible operator, W , could be found which approximates $T - B$, a good approximation for the error might be efficiently obtained by substituting W^{-1} for $(T - B)^{-1}$ in Eq.(25):

$$\underline{\epsilon}^{l+1} \approx W^{-1} B(\underline{\psi}^{l+1} - \underline{\psi}^l) . \quad (27)$$

If the "improved" iterate obtained by adding the approximate error to $\underline{\psi}^{l+1}$ is more accurate than the iterate which would be obtained with another standard iteration, convergence acceleration results. This is the basic idea upon which all synthetic acceleration schemes are based. As Eqs. (18), (24) and (27) suggest, the accelerated iteration scheme is a two-step scheme which can be expressed as follows:

$$T\underline{\psi}^{l+1/2} = B\underline{\psi}^l + \underline{QD} , \quad (28a)$$

$$\underline{\epsilon}^{l+1/2} = W^{-1} B(\underline{\psi}^{l+1/2} - \underline{\psi}^l) , \quad (28b)$$

$$\underline{\psi}^{l+1} = \underline{\psi}^{l+1/2} + \underline{\epsilon}^{l+1/2} . \quad (28c)$$

The operator W is called the low-order operator, and its properties completely determine the effectiveness of the scheme. As one would suspect, the main difficulty in developing a synthetic acceleration scheme is finding a suitable low-order operator.

The low-order operator which we use was chosen on the basis of the following observation. From Fig. 1 it can be seen that the unaccelerated iteration operator strongly attenuates those Fourier error modes corresponding to large values of λ , but completely fails to attenuate the error modes in the limit as λ approaches zero. This suggests that the low-order operator should closely approximate T - B in the limit as λ approaches zero, and thereby compensate for the poor performance in this limit of the unaccelerated iteration operator. To begin the derivation of our low-order operator, note that the zero'th moment equation defined by Eq.(4a) is simply the balance equation which is satisfied by all standard differencing schemes (such as the step and diamond schemes) for the CSD operator. The standard schemes differ only in the "auxiliary" equation which relates the cell-edge and cell-average fluxes. The first-moment equation defined by Eq.(4b) is really just an auxiliary equation which is particularly complicated due to the presence of a spatial derivative term. Specifically, Eq.(4b) can be expressed as follows:

$$\begin{aligned} \frac{\mu \partial}{\partial x} \frac{2(\psi_g - \psi_{g,+})}{\Delta E_g} &= \frac{2(S_{g-1/2} - S_{g+1/2})}{\Delta E_g} \frac{2(\psi_g - \psi_{g,+})}{\Delta E_g} \\ &+ \frac{6S_{g-1/2}}{\Delta E_g} (\psi_{g-1,+} - 2\psi_g + \psi_{g,+}), \end{aligned} \quad (29)$$

where $\psi_{g-1,+}$ is the upper cell-edge flux, $\psi_{g,+}$ is the lower cell-edge flux, and the cell-average flux, ψ_g , is defined by:

$$\psi_g = \frac{\psi_{g,-} + \psi_{g,+}}{2}. \quad (29a)$$

Setting the spatial derivative term in Eq.(29) to zero results in an auxiliary relationship corresponding to a weighted-diamond scheme:

$$\psi_g = \tau \psi_{g,+} + (1-\tau) \psi_{g-1,+}, \quad (30a)$$

where

$$\tau = \frac{2S_{g+1/2} + S_{g-1/2}}{2S_{g+1/2} + 4S_{g-1/2}}. \quad (30b)$$

The important point to be made is that the spatial derivative term in Eq.(4b) approaches zero in the limit as λ approaches zero. Therefore this weighted-diamond scheme becomes equivalent to the linear-discontinuous scheme in the limit as λ approaches zero. Furthermore, a weighted-diamond

scheme does not require outer iterations, so the weighted-diamond solution can be efficiently obtained. Because this weighted-diamond scheme has all of the desired properties, we use it as the low-order operator in our synthetic acceleration scheme. The solution of the weighted-diamond equations for the iterative error estimate is equivalent to doing one outer iteration for the linear-discontinuous equations with half the energy groups. Thus the computational cost of the accelerated scheme is approximately 1.5 times larger than that of the unaccelerated scheme.

We have performed a Fourier analysis for the synthetically accelerated outer iteration process. An eigenvalue plot for the accelerated scheme is given in Fig. 2, which is analogous to that given in Fig. 1 for the unaccelerated scheme. It can be seen from Fig. 2 that w goes to zero in the limit as p goes to zero. This follows directly from the fact that the low-order operator becomes equivalent to the linear-discontinuous operator in the same limit. Furthermore, w asymptotically approaches a maximum value of one-sixth in the limit as p approaches infinity. Thus the spectral radius for the accelerated scheme is one-sixth. This represents a tremendous improvement over the unaccelerated scheme.

It is important to note that when within-group scattering is added to Eq.(2), the low-order operator no longer becomes equivalent to the linear-discontinuous operator in the limit as λ goes to zero. This suggests that our acceleration scheme might not be effective in this case. However, we have performed a Fourier analysis, based upon the S_2 -Gauss equations with P_1 within-group scattering, which shows that even though the dependence of w upon p changes dramatically as a function of the within-group scattering cross-sections, the spectral radius remains at one-sixth. Details of this analysis are given in Reference 10.

V. COMPUTATIONAL RESULTS

We have performed a series of electron transport calculations to compare our linear-discontinuous treatment for the CSD operator with a first-order-accurate multigroup treatment and the diamond-difference treatment. The transport equation solved is the standard Fokker-Planck equation for charged particles:

$$\mu \frac{\partial \psi}{\partial x} = 0.5 \sigma_{tr} \frac{\partial [(1 - \mu^2) \psi]}{\partial \mu} + \frac{\partial [S\psi]}{\partial E}, \quad (31)$$

where σ_{tr} is the transport-corrected scattering cross section (also known as the momentum transfer). In Reference 1 it is shown that the angular redistribution operator appearing in Eq.(31) can be represented in terms of a set of within-group Legendre scattering coefficients. Because the momentum transfer is energy dependent, an appropriate value must be chosen for each group. The average value of the energy for group k is given by:

$$\langle E \rangle_k = E_{g-1/2} - LE_g/3, \text{ if } k = 2g-1 \quad (32a)$$

$$= E_{g+1/2} + \Delta E_g / 3, \text{ if } k = 2g. \quad (32b)$$

The momentum transfer for each group k is simply chosen to be $\sigma_{tr}(\langle E \rangle_k)$. Although it may not be obvious, this is equivalent to a collocation treatment for the energy-dependence of the angular redistribution operator which is consistent with the linear-discontinuous trial space.

The results which we present in this section include energy and charge deposition profiles. For our linear discontinuous approximation, the energy deposition is given by:

$$ED(x) = \sum_{k=1}^{NG} \langle S \rangle_k \phi_k, \quad (33)$$

where ϕ_k is the scalar flux for group k and:

$$\langle S \rangle_k = \sum_{j=1}^{NG} \sigma_{k \rightarrow j} [\langle E \rangle_k - \langle E \rangle_j], \quad (33a)$$

Because only the last group has an absorption cross-section, the charge deposition profile is simply given by:

$$CD(x) = \sigma_{a,NG} \phi_{NG}. \quad (34)$$

All calculations with the linear-discontinuous treatment were performed using a version of the ONETRAN¹¹ code. Which was modified to implement our outer-iteration acceleration scheme. The first-order multigroup and diamond-difference calculations were performed using the standard version of ONETRAN. To obtain "exact" solutions, calculations were performed using a version of the coupled electron-photon Monte Carlo code, TIGER¹², which was modified to solve Eq.(31).

Although we have performed calculations for several different problems, we show results here only for a single problem consisting of a slab of cold aluminum with 1 MeV electrons isotropically incident upon the left face, and a vacuum boundary on the right face. The slab has a thickness of .0635 cm (25 mils). The expressions used for the electron stopping power and momentum transfer are identical to those used in Reference 1. The transmitted current spectrum is plotted in Fig. 3 for the four methods: Monte Carlo (MC), first-order-accurate multigroup (MG), diamond-difference (DD), and linear-discontinuous (LD). Fifty groups (25 cells) were used in the linear-discontinuous calculation, while 25 groups (25 cells) were used in the multigroup and diamond-difference calculations. It can be seen from Fig. 3 that the MG spectrum is far too broad due to numerical straggling. The DD and LD solutions are much more accurate than the MG spectrum, but the DD spectrum shows significant oscillations whereas the LD spectrum is quite smooth and in better overall agreement with the MC spectrum. Unfortunately, the LD spectrum shows a slight negative dip, but this dip affords a better approximation to the rapid rise in the spectrum which occurs near 0.75 MeV.

Energy deposition profiles for the slab are compared in Fig. 4. All of the profiles are in good agreement, but the DD profile shows very slight oscillations. In Fig. 5 the charge profiles are compared. The MG profile is not as accurate as the LD profile, but it is still fairly good. Conversely, the DD profile is almost worthless due to extremely severe oscillations. Considering the oscillations in the spectrum, this type of behavior is not surprising since, as shown in Eq.(34), the charge deposition is proportional to the flux in a single group.

Although the DD scheme performs rather poorly when 25 groups are used, the oscillatory behavior in the energy deposition profile is completely eliminated with 50 groups, and the oscillatory behavior in the charge deposition profile is nearly eliminated. For instance, the MC, 25-Cell LD, 50-group DD, and 50-group MG charge deposition profiles are plotted in Fig. 6. The improvement in the 50-group DD profile relative to the 25-group DD profile is dramatic.

Numerical estimates of the effective spectral radius for the outer iteration process were made in the 25-cell LD calculation, and these estimates agreed well with the theoretical value of 0.16. A pointwise relative convergence criterion on the scalar flux was used for both the outer and inner iterations. As indicated in Section III, optimal efficiency is obtained by performing independent outer iterations for each cell. The outer iterations were terminated when the pointwise relative change in the group-dependent scalar fluxes was less than 10^{-3} . The average number of outer iterations required per cell was 4.3. If the number of inner iterations performed per group is fixed and a similar number of energy cells is used, the accelerated LD scheme will cost about three times more per outer iteration than the DD scheme. Measuring computational cost in terms of the total number of inner iterations performed, the 25-cell LD calculation costs only about 4.6 rather than 12.9 times more than the 25-group DD calculation. This occurred because the number of inner iterations performed per group was not fixed, but rather strongly varied for this problem to the advantage of the LD treatment. Thus the cost of the LD scheme relative to that of the DD scheme is not necessarily proportional to the number of outer iterations required in the LD calculation.

Our overall results indicate that with the same number of energy cells, the LD solution is always superior in a general sense to the DD solution, but it is not always superior in all respects. For instance, although the diamond-difference spectrum shown in Fig. 3 oscillates badly, it is nonetheless everywhere positive whereas the linear-discontinuous spectrum has a negative dip. The accuracy of the LD method relative to that of the DD method can be expected to be strongly dependent upon both the problem being modeled and the particular transport quantities (spectra, profiles, bulk deposition, etc.) of interest.

VI. CONCLUSIONS

Our study clearly shows that the linear-discontinuous treatment for the CSD operator is a valuable alternative to other schemes. This method shows considerable promise and should be further investigated. In particular, alternatives to our method for solving the S_n -CSD equation should be investigated. Because of the need for outer-iteration acceleration, most of the advantages associated with making the LD scheme compatible with standard S_n codes are lost. Better efficiency can probably be obtained by using a direct method rather than an iterative method to solve for the two fluxes within an energy cell. For instance, W. F. Walters has proposed a space-energy linear-discontinuous treatment for Eq.(2) which is analogous to the spatial linear-discontinuous treatment for the standard S_n equation in X-Y geometry, and can be similarly solved using a direct method.¹³

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Figure 1: Eigenvalues for Unaccelerated Scheme.

Figure 2: Eigenvalues for Accelerated Scheme.

Figure 3: Spectral Comparison.

Figure 4: Energy Deposition Comparison.

Figure 5: Charge Deposition Comparison.

Figure 6: Charge Deposition Comparison - More Groups.