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Parallel Finite Element Electron-Photon Transport Analysis on 2-D Unstructured Mesh

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Parallel Finite Element Electron-Photon Transport Analysis on 2-D Unstructured Mesh

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Abstract

A computer code has been developed to solve the linear Boltzmann transport equation on an unstructured mesh of triangles, from a Pro/E model. An arbitrary arrangement of distinct material regions is allowed. Energy dependence is handled by solving over an arbitrary number of discrete energy groups. Angular dependence is treated by Legendre-polynomial expansion of the particle cross sections and a discrete ordinates treatment of the particle fluence. The resulting linear system is solved in parallel with a preconditioned conjugate-gradients method. The solution method is unique, in that the space-angle dependence is solved simultaneously, eliminating the need for the usual inner iterations. Electron cross sections are obtained from a Goudsmit-Saunderson modified version of the CEPXS code. A one-dimensional version of the code has also been developed, for testing and development purposes.

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1 Introduction

Radiation transport codes are needed to predict mechanical and electrical radiation effects from x- and γ -rays in hostile environments. In the absence of underground nuclear testing, such predictive capability is needed more than ever. Mechanical effects in materials result from shock waves that are generated by rapid and non-uniform energy deposition from x- and γ -rays incident on materials. Electrical effects are caused by the transport of photo-Compton electrons in structures, devices, and connecting cables. Computer codes are needed to predict energy- and charge-deposition distributions and electron emission.

Monte Carlo radiation transport is ideally suited for modeling complex geometries required for certification of weapons components, and Monte Carlo codes have proven very effective for predicting energy-deposition distributions and mechanical effects[1]. However, Monte Carlo methods are not as effective for predicting electrical effects, since electrical effects depend on the net motion of charge, which may be nearly zero, especially for hardened systems. For Monte Carlo to accurately model the charge deposition and transport needed to determine electrical effects on a complex geometry requires massive computer resources. Deterministic methods, such as the method described here, are much more efficient than Monte Carlo for computing charge depositions for hardened electrical systems.

This report describes analyses based on a two-dimensional spatial domain, meshed with triangles. A two-dimensional code is useful for applications where the solution is only weakly dependent on one of the spatial variables, such as for computing system-generated electromagnetic pulse (SGEMP) in cables. A two-dimensional code is also a useful intermediate step toward a general-geometry three-dimensional code.

This report describes the details of the mathematical foundation of the computer code, and a listing of the structs and function prototypes of the code is included in the Appendix. The Appendix also gives a high-level overview of the functioning of the code. This report includes the results of several benchmarks designed to test the methodology and coding, and a report that thoroughly benchmarks the complete photon-electron-positron transport capabilities of the code for general geometries will be released at a later date.

2 Background

The linear Boltzmann transport equation provides a mathematical description of physical processes involving the motion of microscopic particles through a host medium. There are many examples of such processes, including the diffusion of neutrons in a nuclear reactor, the radiative transfer of light in the atmosphere, the scattering of photons or neutrons in a radiation shield, and the motion of electrons in semiconductor devices.

The theory of particle transport is different from theories based on continuum mechanics, such as electromagnetism or fluid mechanics, in that the transport of particles through a host medium is a random process, instead of a deterministic process. Therefore, the result of a transport calculation is a probability density distribution, which is the expected number of particles in a given phase space: the number of particles per unit of volume, solid angle, energy, and time.

The balance relation describing the motion in space, angle, and energy of particles such as neutrons, photons, or electrons is the linear, steady-state Boltzmann transport equation[2],

$$\Omega \cdot \nabla \Phi + \sigma_t(\mathbf{r}, E) \Phi(\mathbf{r}, \Omega, E) = \iint \sigma_s(\mathbf{r}, \mu_0, E' \rightarrow E) \Phi(\mathbf{r}, \Omega', E') d\Omega' dE' + Q(\mathbf{r}, \Omega, E), \quad (1)$$

where $\sigma_t(\mathbf{r}, E)$ is the total cross section, $\Phi(\mathbf{r}, \Omega, E)$ is the particle fluence, $\sigma_s(\mathbf{r}, \mu_0, E' \rightarrow E)$ is the scattering cross section, which is the probability of scattering between different directions and energies, and $Q(\mathbf{r}, \Omega, E)$ is a specified external particle source distribution. The independent variables are: the spatial position $\mathbf{r}$, the particle direction Ω , and the particle energy E . μ_0 is the cosine between the pre- and post-scattered directions.

Figure 1: Typical Pro/E Mesh for a Coaxial Cable Cross Section.

This report is concerned with the method for discretizing Eq. (1) over the independent variables and with the numerical solution for the particle fluence over the resulting mesh. The energy dependence is handled with a standard multigroup treatment, integrating Eq. (1) over successive energy groups and solving the resulting equations iteratively from the highest energy group to the lowest. Multiple particle species (photons, electrons and positrons) are handled by concatenating the energy groups for all of the particle types, and then by solving over the source-particle energy groups and then successively over the remaining particle species. Problems with upscattering or full coupling between particle species require an additional outer iteration loop.

The angular dependence in Eq. (1) is handled by a standard discrete ordinates treatment, where the solution is specified at a discrete set of angles, and the angle integration is replaced by a quadrature sum. The angular dependence of the scattering cross sections is approximated by expanding the cross sections in a finite Legendre-polynomial approximation.

The spatial dependence is handled by a finite-elements method (FEM) treatment of a two-dimensional mesh of triangles. A typical Pro/E mesh of a coaxial cable cross section is shown in Fig. 1. The code is currently based on FEM applied to a mesh from a Pro/E model.

Because of the first-order spatial derivative term, the Boltzmann transport operator is neither symmetric nor positive definite. In order to develop a more efficient solution algorithm, Eq. (1) is modified by extracting the even- and odd-parity components of the particle fluence and then by solving for the two components separately. The advantage of the approach is that the FEM discretization then results in a symmetric positive-definite linear system, which can be efficiently solved with a parallel, preconditioned conjugate gradients algorithm.

Although Eq. (1) is quite adequate for modeling neutral particle transport, the equation, as it stands, is not very efficient for modeling charged particle transport. However, this form of the transport equation can be used to efficiently model charged-particle transport by using Goudsmit-Saunderson modified electron and positron cross sections[3], which enable modeling of charged particles without an explicit continuous slowing down (CSD) term for many problems of interest. The next phase of this work will involve including an explicit CSD term ($\frac{\partial}{\partial E}(S\Phi)$ where S is the stopping power) into Eq. (1).

3 Discretization of the Energy Dependence

The energy dependence is handled by integrating the Boltzmann equation over successive energy groups, and separating the known down-scattering source component from the unknown self-scattering source, resulting in the multigroup form of the equation,

$$\begin{aligned} \Omega \cdot \nabla \Phi_g + \sigma_t(\mathbf{r})\Phi_g(\mathbf{r}, \Omega) - \int \sigma_{s,g \rightarrow g}(\mathbf{r}, \mu_0)\Phi_g(\mathbf{r}, \Omega')d\Omega' \\ = \sum_{g' < g} \int \sigma_{s,g' \rightarrow g}(\mathbf{r}, \mu_0)\Phi_{g'}(\mathbf{r}, \Omega')d\Omega' + Q_g(\mathbf{r}, \Omega), \end{aligned} \quad (2)$$

where g is the energy group index. The unknown self-scatter portion of the source term has been moved to the left hand side, so that everything on the right hand side is known from the solutions at the previous energy groups. Eq. (2) is solved over successive energy groups from highest to lowest. For problems with multiple particle species, source particles are computed first, followed by the non-source particles. For problems with upscattering or full coupling between particle species, the equation is solved by iterating over all of the groups, until convergence. This is a standard and well-tested approach for handling particle energy dependence.

4 Derivation of the Even/Odd-Parity Transport Equations

4.1 Even-Parity Equation

Within a given energy group, the transport equation depends upon space and angle, with the angles coupled together by the scattering source integral. Because of the streaming term, $\Omega \cdot \nabla \Phi$, which is first order in space, the transport equation is non-symmetric and non-positive-definite. Applying FEM directly to the transport equation is ineffective, since the resulting linear system is also non-symmetric and non-positive-definite. The equation can be more conveniently solved by extracting the symmetric and antisymmetric components of the particle fluence, resulting in two coupled equations, which are partial differential equations (PDE's) that are second order in space. This is known as the even/odd parity formulation of the transport equation[4]. The advantage of the even/odd parity formulation is that the resulting linear system is symmetric and positive definite, so that very powerful solutions methods, such as conjugate-gradients, can be applied to their solution. Furthermore, powerful parallel linear-equation solvers, such as Aztec[5], can be directly applied to solving the linear system efficiently on massively parallel computers.

A further advantage of this approach is that, by taking advantage of symmetry in angle, only half of the directions need to be solved, reducing the size of the resulting linear system by half. Furthermore, the even/odd parity equations are self-adjoint in space and angle.

By including the (known) downscatter source into the external distributed source term and dropping the

group indices, Eq. (2) can be written,

$$\Omega \cdot \nabla \Phi(\mathbf{r}, \Omega) + \sigma_t(\mathbf{r})\Phi(\mathbf{r}, \Omega) - \int \sigma_s(\mathbf{r}, \Omega' \cdot \Omega)\Phi(\mathbf{r}, \Omega')d\Omega' = Q(\mathbf{r}, \Omega), \text{ for } \mathbf{r} \in V \quad (3)$$

where $\Phi(\mathbf{r}, \Omega)$ is the particle fluence, $\sigma_t(\mathbf{r})$ is the total cross section, which is the probability per unit path length of particle interaction, $\sigma_s(\mathbf{r}, \Omega' \cdot \Omega)$ is the scattering cross section, which is the probability per unit path length of scattering between different directions, and $Q(\mathbf{r}, \Omega)$ is a known particle source distribution. The independent variables are: $\mathbf{r}$, the spatial position and Ω , the particle direction. The boundary conditions specify the particle fluence for all incoming directions on the boundary,

$$\Phi(\mathbf{r}, \Omega) = \Phi_b(\mathbf{r}, \Omega), \text{ for } \Omega \cdot \mathbf{n} < 0, \text{ for } \mathbf{r} \in \partial V, \quad (4)$$

where $\mathbf{n}$ is the unit outward normal on the boundary, and $\Phi_b(\mathbf{r}, \Omega)$ is a specified function. The scattering and total cross sections are assumed to satisfy¹

$$\int \sigma_s(\mathbf{r}, \Omega' \cdot \Omega)d\Omega' < \sigma_t(\mathbf{r}). \quad (5)$$

This condition is needed to guarantee that the linear system is positive definite, as will be shown later in this report.

By reversing the sign of the direction vector, Eq. (3) can be written equivalently as

$$-\Omega \cdot \nabla \Phi(\mathbf{r}, -\Omega) + \sigma_t(\mathbf{r})\Phi(\mathbf{r}, -\Omega) - \int \sigma_s(\mathbf{r}, -\Omega' \cdot \Omega)\Phi(\mathbf{r}, \Omega')d\Omega' = Q(\mathbf{r}, -\Omega). \quad (6)$$

Two new functions, Φ^+ and Φ^- are defined as follows, which extract the symmetric and anti-symmetric components of $\Phi(\mathbf{r}, \Omega)$,

$$\Phi^\pm(\mathbf{r}, \Omega) = \frac{\Phi(\mathbf{r}, \Omega) \pm \Phi(\mathbf{r}, -\Omega)}{2}. \quad (7)$$

Similarly, even and odd parity functions are defined for the scattering cross section and distributed source terms,

$$\sigma_s^\pm(\mathbf{r}, \Omega' \cdot \Omega) = \frac{\sigma_s(\mathbf{r}, \Omega' \cdot \Omega) \pm \sigma_s(\mathbf{r}, -\Omega' \cdot \Omega)}{2}, \quad (8)$$

and

$$Q^\pm(\mathbf{r}, \Omega) = \frac{Q(\mathbf{r}, \Omega) \pm Q(\mathbf{r}, -\Omega)}{2}. \quad (9)$$

Adding and subtracting the first-order transport equation in Ω and $-\Omega$, results in

$$\Omega \cdot \nabla \Phi^- + \sigma_t(\mathbf{r})\Phi^-(\mathbf{r}, \Omega) - \int \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega)\Phi^+(\mathbf{r}, \Omega')d\Omega' = Q^-(\mathbf{r}, \Omega), \quad (10)$$

and

$$\Omega \cdot \nabla \Phi^+ + \sigma_t(\mathbf{r})\Phi^+(\mathbf{r}, \Omega) - \int \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega)\Phi^-(\mathbf{r}, \Omega')d\Omega' = Q^+(\mathbf{r}, \Omega). \quad (11)$$

In order to derive an equation for the even-parity component, $\Phi^+(\mathbf{r}, \Omega)$, Eq. (11) is solved for $\Phi^-(\mathbf{r}, \Omega)$, which is then substituted into Eq. (10). At this point, it is useful to simplify the notation by defining two scattering operators,

$$\mathcal{G}_+ f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r})f(\mathbf{r}, \Omega) - \int \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega)f(\mathbf{r}, \Omega')d\Omega' \quad (12)$$

and

$$\mathcal{G}_- f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r})f(\mathbf{r}, \Omega) - \int \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega)f(\mathbf{r}, \Omega')d\Omega'. \quad (13)$$

With these scattering operators, Eqs. (10) and (11) can be rewritten

$$\Omega \cdot \nabla \Phi^- + \mathcal{G}_+ \Phi^+(\mathbf{r}, \Omega) = Q^-(\mathbf{r}, \Omega), \quad (14)$$

¹ There are cases where this assumption is not satisfied, e.g. fission and (n,2n) neutron interactions, but this condition is satisfied for many problems of interest.

and

$$\Omega \cdot \nabla \Phi^+ + \mathcal{G}_- \Phi^-(\mathbf{r}, \Omega) = Q^-(\mathbf{r}, \Omega). \quad (15)$$

Eq. (15) can be easily solved for $\Phi^-(\mathbf{r}, \Omega)$,

$$\Phi^-(\mathbf{r}, \Omega) = -\mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+ + \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega), \quad (16)$$

where the inverse of the odd-parity scattering operator, $\mathcal{G}_-^{-1}$, is assumed to exist. Some specific forms of the scattering operators and their inverses will be described later in this report. Eq.(16) is substituted into Eq. (14) resulting in the even-parity form of the transport equation,

$$-\Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+ + \mathcal{G}_+ \Phi^+(\mathbf{r}, \Omega) = -\Omega \cdot \nabla \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega) + Q^+(\mathbf{r}, \Omega), \text{ for } \mathbf{r} \in V. \quad (17)$$

4.2 Even-Parity Boundary Conditions

Boundary conditions for the even-parity equation are obtained from the boundary conditions for the first-order equation, Eq. (4). $\Phi_b(\mathbf{r}, \Omega)$ is the specified boundary condition for the first-order fluence, which is defined for all incoming directions. For incoming directions,

$$\Phi(\mathbf{r}, \Omega) = \Phi^+(\mathbf{r}, \Omega) + \Phi^-(\mathbf{r}, \Omega) = \Phi_b(\mathbf{r}, \Omega), \text{ for } \Omega \cdot \mathbf{n} < 0, \text{ for } \mathbf{r} \in \partial V, \quad (18)$$

and for outgoing directions, the boundary conditions are determined by replacing the direction vector by its inverse,

$$\Phi(\mathbf{r}, -\Omega) = \Phi^+(\mathbf{r}, \Omega) - \Phi^-(\mathbf{r}, \Omega) = \Phi_b(\mathbf{r}, -\Omega), \text{ for } \Omega \cdot \mathbf{n} > 0, \text{ for } \mathbf{r} \in \partial V. \quad (19)$$

Solving Eqs. (18) and (19) for $\Phi^-(\mathbf{r}, \Omega)$, and substituting the result into Eq. (16) yields the boundary conditions for $\Phi^+(\mathbf{r}, \Omega)$,

$$\pm \Phi^+(\mathbf{r}, \Omega) + \mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+ = \pm \Phi_b(\mathbf{r}, \mp \Omega) + \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega), \text{ for } \Omega \cdot \mathbf{n} \gtrless 0, \text{ for } \mathbf{r} \in \partial V. \quad (20)$$

Whereas the boundary conditions for the first-order form of the transport equation are specified only for incoming directions, the boundary conditions for the even-parity form of the equation are specified both for incoming and outgoing directions. This results in the proper number of boundary conditions for the even-parity transport equation, which is second order in space.

4.3 Odd-Parity Equation

The odd-parity equation can be derived analogously with the derivation of the even-parity equation, or may be obtained simply by interchanging +s and -s in the even-parity equation, Eq. (17),

$$-\Omega \cdot \nabla \mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^- + \mathcal{G}_- \Phi^-(\mathbf{r}, \Omega) = -\Omega \cdot \nabla \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega) + Q^-(\mathbf{r}, \Omega), \text{ for } \mathbf{r} \in V. \quad (21)$$

4.4 Odd-Parity Boundary Conditions

An expression for the even-parity fluence, $\Phi^+(\mathbf{r}, \Omega)$, in terms of the odd-parity fluence is obtained from Eq. (16), by interchanging +s and -s,

$$\Phi^+(\mathbf{r}, \Omega) = -\mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^- + \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega). \quad (22)$$

Solving Eqs. (18) and (19) for $\Phi^+(\mathbf{r}, \Omega)$, and substituting the result into Eq. (22) gives the boundary condition for the odd-parity equation,

$$\pm \Phi^-(\mathbf{r}, \Omega) + \mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^- = -\Phi_b(\mathbf{r}, \mp \Omega) + \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega), \text{ for } \Omega \cdot \mathbf{n} \gtrless 0, \text{ for } \mathbf{r} \in \partial V. \quad (23)$$

Note that the boundary conditions for the odd-parity equation cannot be obtained from those for the even-parity equation by interchanging +s and -s. This is because the even-parity fluence is symmetric in angle, while the odd-parity fluence is antisymmetric in angle, so the boundary term is slightly different for the odd-parity equation.

5 Symmetry and Positive Definiteness of the Even and Odd Parity Operators

To show that an operator, $\mathcal{L}$, is symmetric, it is necessary to show that

$$\langle f, \mathcal{L}g \rangle = \langle \mathcal{L}f, g \rangle, \quad (24)$$

for all f and g , where the inner product for real functions is defined as the integral over space and angle,

$$\langle f, \mathcal{L}g \rangle = \iiint f \mathcal{L}g d\mathbf{r} d\Omega. \quad (25)$$

To show positive definiteness, it is necessary to show that

$$\langle f, \mathcal{L}f \rangle > 0, \quad (26)$$

for all f .

5.1 Even-Parity Equation

From Eq. (17), the even parity transport operator, $\mathcal{L}_+$, is defined as

$$\mathcal{L}_+ f(\mathbf{r}, \Omega) = -\Omega \cdot \nabla \mathcal{G}_+^{-1} \Omega \cdot \nabla f(\mathbf{r}, \Omega) + \mathcal{G}_+ f(\mathbf{r}, \Omega). \quad (27)$$

It is first shown that the even-parity scattering operator, $\mathcal{G}_+$, is symmetric and positive definite, and then the symmetry and positive definiteness of the even parity transport operator, $\mathcal{L}_+$, follow directly.

5.1.1 Even-Parity Scattering Operator

The even-parity scattering operator is

$$\mathcal{G}_+ f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r}) f(\mathbf{r}, \Omega) - \int \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\Omega', \quad (28)$$

with the restriction that the integral of the scattering cross section over angle is strictly less than the total cross section,

$$\int \sigma_s(\mathbf{r}, \Omega' \cdot \Omega) d\Omega' < \sigma_t(\mathbf{r}). \quad (29)$$

Symmetry Symmetry is shown by interchanging the angle-integration parameters and recognizing that the scattering and total cross sections are real.

$$\begin{aligned} \langle f, \mathcal{G}_+ g \rangle &= \langle f, \sigma_t(\mathbf{r}) g \rangle - \iiint f(\mathbf{r}, \Omega) \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) g(\mathbf{r}, \Omega') d\mathbf{r} d\Omega d\Omega' \\ &= \langle \sigma_t(\mathbf{r}) f, g \rangle - \iiint \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') g(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega' \\ &= \langle \sigma_t(\mathbf{r}) f, g \rangle - \left\langle \int \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\Omega', g(\mathbf{r}, \Omega) \right\rangle = \langle \mathcal{G}_+ f, g \rangle. \end{aligned} \quad (30)$$

Positive Definiteness Positive definiteness follows from an application of the Cauchy-Schwartz inequality, which is

$$\langle f, g \rangle \leq \sqrt{\langle f, f \rangle} \sqrt{\langle g, g \rangle}. \quad (31)$$

From the definition of the even-parity scattering operator,

$$\langle f, \mathcal{G}_+ f \rangle = \langle f, \sigma_t(\mathbf{r}) f \rangle - \iiint f(\mathbf{r}, \Omega) \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\mathbf{r} d\Omega d\Omega', \quad (32)$$

which can be written as

$$\langle f, \mathcal{G}_+ f \rangle = \langle f, \sigma_t(\mathbf{r}) f \rangle - \iiint \sqrt{\sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega)} f(\mathbf{r}, \Omega') \sqrt{\sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega)} f(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega'. \quad (33)$$

By the Cauchy-Schwartz inequality,

$$\langle f, \mathcal{G}_+ f \rangle \geq \langle f, \sigma_t(\mathbf{r}) f \rangle$$

$$- \sqrt{\iiint f(\mathbf{r}, \Omega') \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\mathbf{r} d\Omega d\Omega'} \sqrt{\iiint f(\mathbf{r}, \Omega) \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega'}. \quad (34)$$

Interchanging the angular integration variables in the first square root term results in

$$\langle f, \mathcal{G}_+ f \rangle \geq \langle f, \sigma_t(\mathbf{r}) f \rangle - \iiint f(\mathbf{r}, \Omega) \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega', \quad (35)$$

or

$$\langle f, \mathcal{G}_+ f \rangle \geq \left\langle f, \left(\sigma_t(\mathbf{r}) - \int \sigma_s(\mathbf{r}, \Omega' \cdot \Omega) d\Omega' \right) f \right\rangle > 0, \quad (36)$$

where the last inequality follows from the assumed relationship between the total and scattering cross sections, Eq. (29). Therefore, positive definiteness is guaranteed only for the strict inequality condition, Eq. (29).

5.1.2 Odd-Parity Scattering Operator

The odd-parity scattering operator is

$$\mathcal{G}_- f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r}) f(\mathbf{r}, \Omega) - \int \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\Omega'. \quad (37)$$

Symmetry Symmetry is shown by interchanging the angle-integration parameters and recognizing that the scattering and total cross sections are real.

$$\begin{aligned} \langle f, \mathcal{G}_- g \rangle &= \langle f, \sigma_t(\mathbf{r}) g \rangle - \iiint f(\mathbf{r}, \Omega) \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) g(\mathbf{r}, \Omega') d\mathbf{r} d\Omega d\Omega' \\ &= \langle \sigma_t(\mathbf{r}) f, g \rangle - \iiint \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') g(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega' \\ &= \langle \sigma_t(\mathbf{r}) f, g \rangle - \left\langle \int \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\Omega', g(\mathbf{r}, \Omega) \right\rangle = \langle \mathcal{G}_- f, g \rangle. \end{aligned} \quad (38)$$

Positive Definiteness Positive definiteness follows from an application of the Cauchy-Schwartz inequality. From the definition of the odd-parity scattering operator,

$$\langle f, \mathcal{G}_- f \rangle = \langle f, \sigma_t(\mathbf{r}) f \rangle - \iiint f(\mathbf{r}, \Omega) \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\mathbf{r} d\Omega d\Omega', \quad (39)$$

which can be written as

$$\langle f, \mathcal{G}_- f \rangle = \langle f, \sigma_t(\mathbf{r}) f \rangle - \iiint \sqrt{\sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega)} f(\mathbf{r}, \Omega') \sqrt{\sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega)} f(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega'. \quad (40)$$

By the Cauchy-Schwartz inequality,

$$\langle f, \mathcal{G}_+ f \rangle \geq \langle f, \sigma_t(\mathbf{r}) f \rangle$$

$$- \sqrt{\iiint f(\mathbf{r}, \Omega') \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega') d\mathbf{r} d\Omega d\Omega'} \sqrt{\iiint f(\mathbf{r}, \Omega) \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega'}. \quad (41)$$

Interchanging the angular integration variables in the first square root term results in

$$\langle f, \mathcal{G}_- f \rangle \geq \langle f, \sigma_t(\mathbf{r}) f \rangle - \iiint f(\mathbf{r}, \Omega) \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) f(\mathbf{r}, \Omega) d\mathbf{r} d\Omega d\Omega', \quad (42)$$

or

$$\langle f, \mathcal{G}_- f \rangle \geq \left\langle f, \left(\sigma_t(\mathbf{r}) - \int \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) d\Omega' \right) f \right\rangle = \langle f, \sigma_t(\mathbf{r}) f \rangle > 0, \quad (43)$$

where the integral of the odd-parity scattering cross section over angle is zero because it is antisymmetric in angle,

$$\int \sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) d\Omega' = \frac{\int \sigma_s(\mathbf{r}, \Omega' \cdot \Omega) d\Omega' - \int \sigma_s(\mathbf{r}, -\Omega' \cdot \Omega) d\Omega'}{2} = 0. \quad (44)$$

5.1.3 Even Parity Transport Operator

The even parity transport operator is

$$\mathcal{L}_+ f(\mathbf{r}, \Omega) = -\Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla f(\mathbf{r}, \Omega) + \mathcal{G}_+ f(\mathbf{r}, \Omega), \quad (45)$$

with vacuum boundary conditions

$$\pm f(\mathbf{r}, \Omega) + \mathcal{G}_-^{-1} \Omega \cdot \nabla f = 0, \text{ for } \Omega \cdot \mathbf{n} \gtrless 0. \quad (46)$$

Symmetry Symmetry is shown by two applications of the divergence theorem and including the vacuum boundary conditions,

$$\langle f, \mathcal{L}_+ g \rangle = -\langle f, \Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla g \rangle + \langle f, \mathcal{G}_+ g \rangle. \quad (47)$$

One application of the divergence theorem results in

$$\langle f, \mathcal{L}_+ g \rangle = \langle \Omega \cdot \nabla f, \mathcal{G}_-^{-1} \Omega \cdot \nabla g \rangle - \int \oint f \mathcal{G}_-^{-1} \Omega \cdot \nabla g \Omega \cdot \mathbf{n} ds d\Omega + \langle f, \mathcal{G}_+ g \rangle. \quad (48)$$

Applying vacuum boundary conditions for g in the surface integral term results in

$$\langle f, \mathcal{L}_+ g \rangle = \langle \Omega \cdot \nabla f, \mathcal{G}_-^{-1} \Omega \cdot \nabla g \rangle + \int \oint f g |\Omega \cdot \mathbf{n}| ds d\Omega + \langle f, \mathcal{G}_+ g \rangle. \quad (49)$$

A second application of the divergence theorem results in

$$\langle f, \mathcal{L}_+ g \rangle = -\langle \Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla f, g \rangle + \int \oint \mathcal{G}_-^{-1} \Omega \cdot \nabla f g \Omega \cdot \mathbf{n} ds d\Omega + \int \oint f g |\Omega \cdot \mathbf{n}| ds d\Omega + \langle f, \mathcal{G}_+ g \rangle. \quad (50)$$

Applying vacuum boundary conditions for f in the first surface integral term results in

$$\langle f, \mathcal{L}_+ g \rangle = -\langle \Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla f, g \rangle - \int \oint f g |\Omega \cdot \mathbf{n}| ds d\Omega + \int \oint f g |\Omega \cdot \mathbf{n}| ds d\Omega + \langle \mathcal{G}_+ f, g \rangle = \langle \mathcal{L}_+ f, g \rangle. \quad (51)$$

Positive Definiteness Applying the divergence theorem and vacuum boundary conditions results in

$$\begin{aligned} \langle f, \mathcal{L}_+ f \rangle &= -\langle f, \Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla f \rangle + \langle f, \mathcal{G}_+ f \rangle \\ &= \langle \Omega \cdot \nabla f, \mathcal{G}_-^{-1} \Omega \cdot \nabla f \rangle + \int \oint f^2 |\Omega \cdot \mathbf{n}| ds d\Omega + \langle f, \mathcal{G}_+ f \rangle > 0. \end{aligned} \quad (52)$$

Since the scattering operators, $\mathcal{G}_+$ and $\mathcal{G}_-$, are positive definite, their inverses are also positive definite. Therefore, $\mathcal{L}_+$ is also positive definite.

5.2 Odd-Parity Equation

From Eq. (21), the odd-parity transport operator, $\mathcal{L}_-$, is defined as

$$\mathcal{L}_- f(\mathbf{r}, \Omega) = -\Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla f(\mathbf{r}, \Omega) + \mathcal{G}_- f(\mathbf{r}, \Omega). \quad (53)$$

Symmetry and positive definiteness of the odd-parity transport operator follow from the positive definiteness of the scattering operators, $\mathcal{G}_+$ and $\mathcal{G}_-$, analogously with the even-parity operator.

6 Derivation of the Weak Form of the Even/Odd-Parity Equations

As a first step in developing the FEM equations, the weak forms of the equations are derived. This is done by multiplying by a weight function, $u(\mathbf{r})$, integrating over the spatial domain, applying the divergence theorem, and then applying the boundary conditions.

6.1 Even-Parity Equation

The even-parity equation, Eq. (17), multiplied by a weight function and integrated over the spatial domain is

$$\begin{aligned} & - \int u(\mathbf{r}) \Omega \cdot \nabla \mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+ d\mathbf{r} + \int u(\mathbf{r}) \mathcal{G}_+ \Phi^+(\mathbf{r}, \Omega) d\mathbf{r} \\ & = - \int u(\mathbf{r}) \Omega \cdot \nabla \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega) d\mathbf{r} + \int u(\mathbf{r}) Q^+(\mathbf{r}, \Omega) d\mathbf{r}. \end{aligned} \quad (54)$$

After applying the divergence theorem to the $\Omega \cdot \nabla$ terms,

$$\begin{aligned} & \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+ d\mathbf{r} + \int u(\mathbf{r}) \mathcal{G}_+ \Phi^+(\mathbf{r}, \Omega) d\mathbf{r} - \oint u(\mathbf{r}) \mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+(\mathbf{r}, \Omega) \Omega \cdot \mathbf{n} ds \\ & = \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega) d\mathbf{r} + \int u(\mathbf{r}) Q^+(\mathbf{r}, \Omega) d\mathbf{r} - \oint u(\mathbf{r}) \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega) \Omega \cdot \mathbf{n} ds, \end{aligned} \quad (55)$$

where the surface integrals are integrated over the problem boundary. After including the boundary conditions, the weak form of the even-parity transport equation is,

$$\begin{aligned} & \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_-^{-1} \Omega \cdot \nabla \Phi^+ d\mathbf{r} + \int u(\mathbf{r}) \mathcal{G}_+ \Phi^+(\mathbf{r}, \Omega) d\mathbf{r} + \oint u(\mathbf{r}) \Phi^+(\mathbf{r}, \Omega) |\Omega \cdot \mathbf{n}| ds \\ & = \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_-^{-1} Q^-(\mathbf{r}, \Omega) d\mathbf{r} + \int u(\mathbf{r}) Q^+(\mathbf{r}, \Omega) d\mathbf{r} + \oint u(\mathbf{r}) \Phi_b(\mathbf{r}, \mp \Omega) |\Omega \cdot \mathbf{n}| ds, \quad \Omega \cdot \mathbf{n} \geq 0. \end{aligned} \quad (56)$$

6.2 Odd-Parity Equation

Following a similar procedure for the odd-parity equation,

$$\begin{aligned} & - \int u(\mathbf{r}) \Omega \cdot \nabla \mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^- d\mathbf{r} + \int u(\mathbf{r}) \mathcal{G}_- \Phi^-(\mathbf{r}, \Omega) d\mathbf{r} \\ & = - \int u(\mathbf{r}) \Omega \cdot \nabla \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega) d\mathbf{r} + \int u(\mathbf{r}) Q^-(\mathbf{r}, \Omega) d\mathbf{r}. \end{aligned} \quad (57)$$

After applying the divergence theorem to the $\Omega \cdot \nabla$ terms,

$$\begin{aligned} & \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^- d\mathbf{r} + \int u(\mathbf{r}) \mathcal{G}_- \Phi^-(\mathbf{r}, \Omega) d\mathbf{r} - \oint u(\mathbf{r}) \mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^-(\mathbf{r}, \Omega) \Omega \cdot \mathbf{n} ds \\ & = \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega) d\mathbf{r} + \int u(\mathbf{r}) Q^-(\mathbf{r}, \Omega) d\mathbf{r} - \oint u(\mathbf{r}) \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega) \Omega \cdot \mathbf{n} ds. \end{aligned} \quad (58)$$

Include boundary conditions,

$$\begin{aligned} & \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_+^{-1} \Omega \cdot \nabla \Phi^- d\mathbf{r} + \int u(\mathbf{r}) \mathcal{G}_- \Phi^-(\mathbf{r}, \Omega) d\mathbf{r} + \oint u(\mathbf{r}) \Phi^-(\mathbf{r}, \Omega) |\Omega \cdot \mathbf{n}| ds \\ & = \int \Omega \cdot \nabla u(\mathbf{r}) \mathcal{G}_+^{-1} Q^+(\mathbf{r}, \Omega) d\mathbf{r} + \int u(\mathbf{r}) Q^-(\mathbf{r}, \Omega) d\mathbf{r} \mp \oint u(\mathbf{r}) \Phi_b(\mathbf{r}, \mp \Omega) |\Omega \cdot \mathbf{n}| ds, \quad \Omega \cdot \mathbf{n} \geq 0. \end{aligned} \quad (59)$$

Note that the boundary source term of the odd-parity equation is slightly different from that of the even-parity

equation.

The computer code is based on solving Eq. (56) and (59), which are the weak forms of the even- and odd-parity equations, respectively. The computational procedure is to specify a form for the scattering operators and to specify interpolation functions, and then to discretize the weak form over the FEM mesh of the spatial domain and the angular quadrature set. This procedure results in a large, symmetric, positive-definite linear system that is solved in parallel with the Aztec software. The following sections of the report contain detailed information on how this procedure is carried out.

7 Specific Forms of the Scattering Cross Section

At this point it is convenient to introduce explicit forms for the scattering cross section. With these explicit expressions, we will be ready to develop the discrete ordinates finite-elements solution of the even- and odd-parity equations.

7.1 General Anisotropic Scattering

The angular dependence of the scattering cross sections are generally handled by a truncated Legendre polynomial expansion. The scattering cross section can be exactly represented by an infinite-order Legendre polynomial expansion,

$$\sigma_s(\mathbf{r}, \mu_0) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}) P_l(\mu_0). \quad (60)$$

The even and odd components of the scattering cross section extract the even and odd Legendre components,

$$\sigma_s^+(\mathbf{r}, \mu_0) = \sum_{l \text{ even}}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}) P_l(\mu_0), \quad (61)$$

and

$$\sigma_s^-(\mathbf{r}, \mu_0) = \sum_{l \text{ odd}}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}) P_l(\mu_0). \quad (62)$$

The scattering operators are, therefore,

$$\mathcal{G}_+ f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r}) f(\mathbf{r}, \Omega) - \sum_{l \text{ even}}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}) \int P_l(\mu_0) f(\mathbf{r}, \Omega') d\Omega', \quad (63)$$

and

$$\mathcal{G}_- f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r}) f(\mathbf{r}, \Omega) - \sum_{l \text{ odd}}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}) \int P_l(\mu_0) f(\mathbf{r}, \Omega') d\Omega'. \quad (64)$$

The inverse operators are[6]

$$\mathcal{G}_+^{-1} f(\mathbf{r}, \Omega) = \frac{1}{\sigma_t(\mathbf{r})} \left[f(\mathbf{r}, \Omega) + \sum_{l \text{ even}}^{\infty} \frac{2l+1}{4\pi} \frac{\sigma_{sl}(\mathbf{r})}{\sigma_t(\mathbf{r}) - \sigma_{sl}(\mathbf{r})} \int P_l(\mu_0) f(\mathbf{r}, \Omega') d\Omega' \right], \quad (65)$$

and

$$\mathcal{G}_-^{-1} f(\mathbf{r}, \Omega) = \frac{1}{\sigma_t(\mathbf{r})} \left[f(\mathbf{r}, \Omega) + \sum_{l \text{ odd}}^{\infty} \frac{2l+1}{4\pi} \frac{\sigma_{sl}(\mathbf{r})}{\sigma_t(\mathbf{r}) - \sigma_{sl}(\mathbf{r})} \int P_l(\mu_0) f(\mathbf{r}, \Omega') d\Omega' \right]. \quad (66)$$

7.2 Isotropic Scattering

For scattering that is equally probable in all directions, the scattering cross section can be written as

$$\sigma_s(\mathbf{r}, \Omega' \cdot \Omega) = \sigma_s^+(\mathbf{r}, \Omega' \cdot \Omega) = c \frac{\sigma_t(\mathbf{r})}{4\pi}, \quad 0 \leq c < 1, \quad (67)$$

where c is the scattering ratio, which is the ratio of scattering interactions to total interactions. Integrating Eq. (67) over angle results in an expression for the scattering ratio,

$$c = \frac{\int \sigma_s(\mathbf{r}, \Omega' \cdot \Omega) d\Omega}{\sigma_t(\mathbf{r})}. \quad (68)$$

For isotropic scattering, the odd-parity scattering cross section is zero, since the odd-parity scattering cross section is antisymmetric,

$$\sigma_s^-(\mathbf{r}, \Omega' \cdot \Omega) = 0. \quad (69)$$

With these simplified forms of the scattering cross sections, the scattering operators are

$$\mathcal{G}_+ f(\mathbf{r}, \Omega) = \sigma_t(\mathbf{r}) \left[f(\mathbf{r}, \Omega) - \frac{c}{4\pi} \int f(\mathbf{r}, \Omega') d\Omega' \right] \quad (70)$$

and

$$\mathcal{G}_- = \sigma_t(\mathbf{r}). \quad (71)$$

The inverses of the operators are

$$\mathcal{G}_+^{-1} f(\mathbf{r}, \Omega) = \frac{1}{\sigma_t(\mathbf{r})} \left[f(\mathbf{r}, \Omega) + \frac{c}{1-c} \frac{1}{4\pi} \int f(\mathbf{r}, \Omega') d\Omega' \right], \quad \text{for } 0 \leq c < 1, \quad (72)$$

and

$$\mathcal{G}_-^{-1} = \frac{1}{\sigma_t(\mathbf{r})}. \quad (73)$$

These simplified forms of the scattering operators will be useful for benchmarking studies.

8 Discrete Ordinates FEM Analyses

In a discrete-ordinates formulation, the angular variable is replaced by a finite set of discrete directions, and the angular integrals are replaced by quadrature sums. The one-dimensional version of the code has built-in Gauss and Lobatto quadrature sets, of orders from 2 to 32. Gauss quadrature is more accurate than Lobatto, while Lobatto quadrature has a direction that is normal to the boundary, which is useful for simulating normally-incident sources. The two-dimensional version of the code has built in quadrature sets of orders from 2 to 16, which were taken from TWODANT.

The spatial domain is approximated by the FEM, where the domain is partitioned into finite elements, and a set of interpolation functions, $\psi_n(\mathbf{r})$, is defined for approximating the dependent variable within each finite element. Using a Galerkin FEM treatment, the weight functions, $u(\mathbf{r})$, are the same as the interpolation functions,

$$u(\mathbf{r}) = \psi_n(\mathbf{r}), \quad n = 1 : N, \quad (74)$$

where N is the number of interpolation functions per element.

The fluences, sources, and boundary conditions are approximated by expansions in the interpolation functions. The even- and odd-parity fluences within an element, e , at discrete direction Ω_m are approximated by

$$\Phi^\pm(\mathbf{r}, \Omega_m) = \sum_{n'=1}^N \phi_{e,m,n'}^\pm \psi_{n'}(\mathbf{r}), \quad \text{for } m = 1 : M, \quad e = 1 : NE, \quad \mathbf{r} \in V_e, \quad (75)$$

and the even- and odd-parity distributed sources within an element, e , are approximated by

$$Q^\pm(\mathbf{r}, \Omega_m) = \sum_{n'=1}^N q_{e,m,n'}^\pm \psi_{n'}(\mathbf{r}), \text{ for } m = 1 : M, e = 1 : NE, \mathbf{r} \in V_e, \quad (76)$$

where M is the number of discrete directions, and NE is the number of finite elements. $\phi_{e,m,n'}^\pm$ are the coefficients for the even- and odd-parity fluences, and $q_{e,m,n'}^\pm$ are the coefficients for the even- and odd-parity distributed sources. These coefficients correspond to the values of the functions at the nodes of the finite elements. The source coefficients, $q_{e,m,n'}^\pm$, are known values, which contribute to the right hand side of the linear system, and the fluence coefficients, $\phi_{e,m,n'}^\pm$, are the unknowns in the linear system.

The boundary conditions are also specified as expansions in the interpolation functions,

$$\Phi_b(\mathbf{r}, \Omega_m) = \sum_{n'=1}^N \phi_{e,m,n'}^b \psi_{n'}(\mathbf{r}), \text{ for } m = 1 : M, e = 1 : NE, \mathbf{r} \in \partial V_e. \quad (77)$$

The boundary values, $\phi_{e,m,n'}^b$, are the specified values of the boundary conditions at the FEM nodes on the external boundary, and also contribute to the right hand side of the linear system.

The strategy is to substitute these expressions, Eqs. (75-77), for the even- and odd-parity fluences, distributed sources, and boundary values, into the weak forms of the even- and odd-parity equations and to solve for the coefficients, $\phi_{e,m,n}^\pm$. The result of this process is a large, symmetric, positive-definite linear system, the size of which is the number of directions, M , in the quadrature set multiplied by the number of nodes in the FEM mesh. The resulting linear system is solved in parallel by using the Aztec software.

In order to do this, discrete forms of the scattering operators, $\mathcal{G}_+$ and $\mathcal{G}_-$, are needed. Since material data are constant within an element, the spatial dependence of the scattering operators is dropped. The discrete-ordinates form of the scattering operators are

$$\mathcal{G}_+ f_m = \sigma_t f_m - \sum_{l \text{ even}}^L \frac{2l+1}{4\pi} \sigma_{sl} \sum_{m'=1}^M w_{m'} P_l(\Omega_{m'} \cdot \Omega_m) f_{m'}, \quad (78)$$

and

$$\mathcal{G}_- f_m = \sigma_t f_m - \sum_{l \text{ odd}}^L \frac{2l+1}{4\pi} \sigma_{sl} \sum_{m'=1}^M w_{m'} P_l(\Omega_{m'} \cdot \Omega_m) f_{m'}, \quad (79)$$

where L is the order of the Legendre expansion of the scattering cross section, and f_m is the value of the function at the m -th discrete direction. The inverse operators are

$$\mathcal{G}_+^{-1} f_m = \frac{1}{\sigma_t} \left[f_m + \sum_{l \text{ even}}^L \frac{2l+1}{4\pi} \frac{\sigma_{sl}}{\sigma_t - \sigma_{sl}} \sum_{m'=1}^M w_{m'} P_l(\Omega_{m'} \cdot \Omega_m) f_{m'} \right], \quad (80)$$

and

$$\mathcal{G}_-^{-1} f_m = \frac{1}{\sigma_t} \left[f_m + \sum_{l \text{ odd}}^L \frac{2l+1}{4\pi} \frac{\sigma_{sl}}{\sigma_t - \sigma_{sl}} \sum_{m'=1}^M w_{m'} P_l(\Omega_{m'} \cdot \Omega_m) f_{m'} \right]. \quad (81)$$

8.1 Even-Parity FEM Weak Form

Substituting these expressions for the fluence and distributed source into the weak form of the even-parity equation results in

$$\begin{aligned} \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \mathcal{G}_+^{-1} \phi_{e,m,n'}^+ \Omega_m \cdot \nabla \psi_{n'}(\mathbf{r}) d\mathbf{r} + \int_{V_e} \psi_n(\mathbf{r}) \mathcal{G}_+ \phi_{e,m,n'}^+ \psi_{n'}(\mathbf{r}) d\mathbf{r} \right. \\ \left. + \phi_{e,m,n'}^+ \oint_{\partial V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) |\Omega_m \cdot \mathbf{n}| ds \right\} \end{aligned}$$

$$\begin{aligned}
&= \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \mathcal{G}_+^{-1} q_{e,m,n'}^- \psi_{n'}(\mathbf{r}) d\mathbf{r} + q_{e,m,n'}^+ \int_{V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) d\mathbf{r} \right\} \\
&+ \phi_{e,\mp m,n'}^b \oint_{\partial V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) |\Omega_m \cdot \mathbf{n}| ds, \text{ for } \Omega_m \cdot \mathbf{n} \geq 0, m = 1 : M, n = 1 : N. \quad (82)
\end{aligned}$$

The volume integrals are carried out over the element volumes. Specifying the range of the surface integrals is a little more complicated. An element boundary is either a part of the external boundary of the spatial domain, or else an internal boundary. The surface integrals are carried out only over those element boundaries that are a part of the external boundary of the problem and not over the internal boundaries. This is because the surface integrals in the weak forms of the equations are carried out only over the external boundary of the spatial domain.

8.2 Odd-Parity FEM Weak Form

Substituting these expressions for the fluence and distributed source into the weak form of the odd-parity equation results in

$$\begin{aligned}
&\sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \mathcal{G}_+^{-1} \phi_{e,m,n'}^- \Omega_m \cdot \nabla \psi_{n'}(\mathbf{r}) d\mathbf{r} + \int_{V_e} \psi_n(\mathbf{r}) \mathcal{G}_- \phi_{e,m,n'}^- \psi_{n'}(\mathbf{r}) d\mathbf{r} \right. \\
&\quad \left. + \phi_{e,m,n'}^- \oint_{\partial V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) |\Omega_m \cdot \mathbf{n}| ds \right\} \\
&= \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \mathcal{G}_+^{-1} q_{e,m,n'}^+ \psi_{n'}(\mathbf{r}) d\mathbf{r} + q_{e,m,n'}^- \int_{V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) d\mathbf{r} \right\} \\
&+ \phi_{e,\mp m,n'}^b \oint_{\partial V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) |\Omega_m \cdot \mathbf{n}| ds, \text{ for } \Omega_m \cdot \mathbf{n} \geq 0, m = 1 : M, n = 1 : N. \quad (83)
\end{aligned}$$

8.3 Element Base Matrices

From the foregoing analysis, it is evident that forming the element matrices, whose coefficients are computed from Eqs. (82) and (83), and assembling over all of the elements is quite complicated. However, the element matrices are based upon a smaller number of base matrices, which are easier to analyze. From Eq. (82) and Eq. (83), four base matrices contain the spatial information, three involving integrals over the spatial elements,

$$\begin{aligned}
\mathcal{I}_1 &= \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \Omega_{m'} \cdot \nabla \psi_{n'}(\mathbf{r}) d\mathbf{r}, \\
\mathcal{I}_2 &= \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) d\mathbf{r}, \\
\mathcal{I}_3 &= \int_{V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) d\mathbf{r}, \quad (84)
\end{aligned}$$

and one involving a surface integral over the external boundary of the spatial domain,

$$\mathcal{I}_4 = \oint_{\partial V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) |\Omega_m \cdot \mathbf{n}| ds. \quad (85)$$

Again, it is important to emphasize that the surface integral in Eq. (85) is carried out only over the portion of the element boundary that is also a part of the external boundary of the spatial domain, so that for internal elements that do not share a portion of the external boundary the surface integral component will be zero.

9 FEM Analyses for Specific Interpolation Functions

It is these equations, Eq. (82) and Eq. (83), that are solved to determine the coefficients of the even- and odd-parity fluences, $\phi_{e,m,n}^+$ and $\phi_{e,m,n}^-$. Once these coefficients are known, the even- and odd-parity fluences are known over the entire spatial domain, at the discrete directions that are included in the discrete-ordinates quadrature set. At this point, it is useful to consider some specific sets of interpolation functions, beginning with one-dimensional linear and quadratic interpolation functions, and then considering two-dimensional linear triangular interpolation functions.

9.1 Coordinate Transformations

Rather than carrying out the integrals over the actual spatial elements, it is more convenient to perform the integrals over a master element, which is defined in a specific coordinate system, and then perform a coordinate transformation to relate the integral over the master element to that over the actual element. The transformations involve the Jacobian matrix, J , and the determinant of the Jacobian matrix, $|J|$. Two relations between the integrals in the two coordinate systems are particularly useful[7],

$$\int f(\mathbf{r}) d\mathbf{r} = \int \hat{f}(\hat{\mathbf{r}}) |J| d\hat{\mathbf{r}}, \quad (86)$$

and

$$\int \nabla f(\mathbf{r}) d\mathbf{r} = \int J^{-1} \nabla \hat{f}(\hat{\mathbf{r}}) |J| d\hat{\mathbf{r}}, \quad (87)$$

where $\mathbf{r}$ are the spatial coordinates in the FEM system, and $\hat{\mathbf{r}}$ are the coordinates in the master system. These relationships will be used later.

9.2 One-Dimensional Analyses

In a one-dimensional domain, there is a single spatial variable, z , and a single directional variable, μ , which is the direction cosine relative to the positive z axis. The range of μ is $-1 < \mu < 1$. The even-parity fluence is symmetric in angle and the odd-parity fluence is anti-symmetric in angle, so that only half of the angular range needs to be modeled, for example, $-1 < \mu < 0$, which is the angular range considered here. In one spatial dimension, the Legendre polynomial of the scattering cosine takes a particularly simple form, the product of the Legendre polynomials of the two direction cosines separately. The one-dimensional discrete-ordinates form of the scattering operators are

$$\mathcal{G}_+ f_m = \sigma_t f_m - \sum_{l \text{ even}}^L \frac{2l+1}{4\pi} \sigma_{sl} \sum_{m'=1}^M w_{m'} P_l(\mu_{m'}) P_l(\mu_m) f_{m'}, \quad (88)$$

and

$$\mathcal{G}_- f_m = \sigma_t f_m - \sum_{l \text{ odd}}^L \frac{2l+1}{4\pi} \sigma_{sl} \sum_{m'=1}^M w_{m'} P_l(\mu_{m'}) P_l(\mu_m) f_{m'}, \quad (89)$$

where L is the order of the Legendre expansion of the scattering cross section. The inverse operators are

$$\mathcal{G}_+^{-1} f_m = \frac{1}{\sigma_t} \left[f_m + \sum_{l \text{ even}}^L \frac{2l+1}{4\pi} \frac{\sigma_{sl}}{\sigma_t - \sigma_{sl}} \sum_{m'=1}^M w_{m'} P_l(\mu_{m'}) P_l(\mu_m) f_{m'} \right], \quad (90)$$

and

$$\mathcal{G}_-^{-1} f_m = \frac{1}{\sigma_t} \left[f_m + \sum_{l \text{ odd}}^L \frac{2l+1}{4\pi} \frac{\sigma_{sl}}{\sigma_t - \sigma_{sl}} \sum_{m'=1}^M w_{m'} P_l(\mu_{m'}) P_l(\mu_m) f_{m'} \right]. \quad (91)$$

9.2.1 Even-Parity Weak Form

The one-dimensional version of the even-parity weak form is

$$\begin{aligned}
& \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \mu_m \mathcal{G}_-^{-1} \mu_m \phi_{e,m,n'}^+ \int_{z_e} \frac{d\psi_n}{dz} \frac{d\psi_{n'}}{dz} dz + \mathcal{G}_+ \phi_{e,m,n'}^+ \int_{z_e} \psi_n(z) \psi_{n'}(z) dz \right. \\
& \quad \left. + \phi_{e,m,n'}^+ [\psi_n(z_u) \psi_{n'}(z_u) + \psi_n(z_l) \psi_{n'}(z_l)] |\mu_m| \right\} \\
& = \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \mu_m \mathcal{G}_-^{-1} q_{e,m,n'}^- \int_{z_e} \frac{d\psi_n}{dz} \psi_{n'}(z) dz + q_{e,m,n'}^+ \int_{z_e} \psi_n(z) \psi_{n'}(z) dz \right. \\
& \quad \left. + [\phi_{e,-m,n'}^b(z_l) \psi_n(z_l) \psi_{n'}(z_l) + \phi_{e,m,n'}^b(z_u) \psi_n(z_u) \psi_{n'}(z_u)] |\mu_m| \right\}, \text{ for } m = 1 : M, n = 1 : N, \quad (92)
\end{aligned}$$

where z_u is the upper bound of the spatial domain, z_l is the lower bound, and z_e is the range of the e -th element.

9.2.2 Odd-Parity Weak Form

Substituting these expressions for the fluence and distributed source into the element weak form of the odd-parity equation results in

$$\begin{aligned}
& \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \mu_m \mathcal{G}_+^{-1} \mu_m \phi_{e,m,n'}^- \int_{z_e} \frac{d\psi_n}{dz} \frac{d\psi_{n'}}{dz} dz + \mathcal{G}_- \phi_{e,m,n'}^- \int_{z_e} \psi_n(z) \psi_{n'}(z) dz \right. \\
& \quad \left. + \phi_{e,m,n'}^- [\psi_n(z_u) \psi_{n'}(z_u) + \psi_n(z_l) \psi_{n'}(z_l)] |\mu_m| \right\} \\
& = \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \mathcal{G}_+^{-1} \mu_m q_{e,m,n'}^+ \int_{z_e} \frac{d\psi_n}{dz} \psi_{n'}(z) dz + q_{e,m,n'}^- \int_{z_e} \psi_n(z) \psi_{n'}(z) dz \right\} \\
& \quad + [-\phi_{e,-m,n'}^b(z_l) \psi_n(z_l) \psi_{n'}(z_l) + \phi_{e,m,n'}^b(z_u) \psi_n(z_u) \psi_{n'}(z_u)] |\mu_m|, \text{ for } m = 1 : M, n = 1 : N. \quad (93)
\end{aligned}$$

9.2.3 Linear Interpolation Functions

For a master element ($0 \leq s \leq 1$) the two linear interpolation functions are

$$\psi_1(s) = 1 - s,$$

and

$$\psi_2(s) = s. \quad (94)$$

A general function is approximated by

$$f(s) = f_1 \psi_1(s) + f_2 \psi_2(s). \quad (95)$$

The equations relating the element coordinates to the master coordinates are

$$x = x_1 + hs,$$

where h is the element width. The Jacobian of the coordinate transformation from the master element to a general element is [7]

$$J = \frac{\partial x}{\partial s} = h. \quad (96)$$

The base matrices are

$$\begin{aligned}
\mathcal{I}_1 &= \int_{z_e} \mu_m \frac{d\psi_n}{dz} \mu_{m'} \frac{d\psi_{n'}}{dz} dz = \frac{1}{h} \int_0^1 \mu_m \frac{d\psi_n}{ds} \mu_{m'} \frac{d\psi_{n'}}{ds} ds = \frac{\mu_m \mu_{m'}}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \\
\mathcal{I}_2 &= \int_{z_e} \mu_m \frac{d\psi_n}{dz} \psi_{n'}(z) dz = \int_0^1 \mu_m \frac{d\psi_n}{ds} \psi_{n'}(s) ds = \frac{\mu_m}{2} \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix},
\end{aligned}$$

and

$$\mathcal{I}_3 = \int_{z_e} \psi_n(z) \psi_{n'}(z) dz = h \int_0^1 \psi_n(s) \psi_{n'}(s) ds = \frac{h}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}. \quad (97)$$

9.2.4 Quadratic Interpolation Functions

Quadratic interpolation functions for the master one-dimensional element are

$$\psi_1(s) = (1-s)(1-2s),$$

$$\psi_2(s) = 4s(1-s),$$

and

$$\psi_3(s) = -s(1-2s). \quad (98)$$

A general function is approximated by

$$f(s) = f_1 \psi_1(s) + f_2 \psi_2(s) + f_3 \psi_3(s). \quad (99)$$

The base matrices are

$$\mathcal{I}_1 = \int_{z_e} \mu_m \frac{d\psi_n}{dz} \mu_{m'} \frac{d\psi_{n'}}{dz} dz = \frac{1}{h} \int_0^1 \mu_m \frac{d\psi_n}{ds} \mu_{m'} \frac{d\psi_{n'}}{ds} ds = \frac{\mu_m \mu_{m'}}{3h} \begin{bmatrix} 7 & -8 & 1 \\ -8 & 16 & -8 \\ 1 & -8 & 7 \end{bmatrix}, \quad (100)$$

$$\mathcal{I}_2 = \int_{z_e} \mu_m \frac{d\psi_n}{dz} \psi_{n'}(z) dz = \int_0^1 \mu_m \frac{d\psi_n}{ds} \psi_{n'}(s) ds = \frac{\mu_m}{6} \begin{bmatrix} -3 & -4 & 1 \\ 4 & 0 & -4 \\ -1 & 4 & 3 \end{bmatrix}, \quad (101)$$

and

$$\mathcal{I}_3 = \int_{z_e} \psi_n(z) \psi_{n'}(z) dz = h \int_0^1 \psi_n(s) \psi_{n'}(s) ds = \frac{h}{30} \begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}. \quad (102)$$

9.3 Two-Dimensional Analyses

In a two-dimensional domain there are two spatial variables, x and y , and it is assumed that the functions are independent of z . The angular domain is specified by the three direction cosines along each of the unit axes, μ_x , μ_y , and μ_z . Because the even-parity fluence is symmetric in angle and the odd-parity fluence is anti-symmetric in angle, only one quadrant of the angular domain needs to be modeled, for example,

$$-1 < \mu_x < 1,$$

$$-1 < \mu_y < 0,$$

and

$$0 < \mu_z < 1. \quad (103)$$

Identities relating the even- and odd-parity fluences in the four quadrants are,

$$\Phi^+(\mu'_x, \mu'_y, \mu'_z) = \Phi^+(\mu'_x, \mu'_y, -\mu'_z) = \Phi^+(-\mu'_x, -\mu'_y, \mu'_z) = \Phi^+(-\mu'_x, -\mu'_y, -\mu'_z),$$

and

$$\Phi^-(\mu'_x, \mu'_y, \mu'_z) = \Phi^-(\mu'_x, \mu'_y, -\mu'_z) = -\Phi^-(-\mu'_x, -\mu'_y, \mu'_z) = -\Phi^-(-\mu'_x, -\mu'_y, -\mu'_z). \quad (104)$$

9.3.1 Two-Dimensional Identities

The scattering operators and their inverses are given by Eqs. (63)-(66). It is convenient at this point to introduce some identities, which are useful for computing the Legendre expansion coefficients of the scattering operators. The addition theorem relates the Legendre polynomial of the cosine of the angle between the two

directions to the associated Legendre polynomials of the two directions [2],

$$P_l(\mu_0) = P_l(\mu_z)P_l(\mu'_z) + 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu_z)P_l^m(\mu'_z) \cos[m(\varphi - \varphi')], \quad (105)$$

where m refers to the order of the associated Legendre (not to be confused with m , which refers to the direction in the discrete ordinates formulation). φ is the azimuthal angle from the positive x axis.

Because of symmetry, only one quadrant of the angular domain is modeled, so the following identities are needed to complete the integrals over 4π solid angle,

$$P_l^m(-\mu'_z) = P_l^m(\mu'_z), \text{ for } l+m \text{ even},$$

and

$$P_l^m(-\mu'_z) = -P_l^m(\mu'_z), \text{ for } l+m \text{ odd}. \quad (106)$$

Identities related to the azimuthal angle are as follows,

$$\begin{aligned} \varphi(\mu'_y) &= \arctan(\mu'_y/\mu'_x), \\ \varphi(-\mu'_y) &= -\varphi(\mu'_y), \\ \cos[m(\varphi - (\varphi' + \pi))] &= \cos[m(\varphi - \varphi')], \text{ for } m \text{ even}, \end{aligned} \quad (107)$$

and

$$\cos[m(\varphi - (\varphi' + \pi))] = -\cos[m(\varphi - \varphi')], \text{ for } m \text{ odd}. \quad (108)$$

9.3.2 Scattering Operators

With these identities, the scattering operators are

$$\begin{aligned} \mathcal{G}_+ f(\mathbf{r}, \Omega) &= \sigma_t(\mathbf{r}) f(\mathbf{r}, \Omega) - \sum_{l \text{ even}}^{\infty} \frac{2l+1}{\pi} \sigma_{sl}(\mathbf{r}) \\ &\int \left\{ P_l(\mu_z)P_l(\mu'_z) + 2 \sum_{m \text{ even}}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu_z)P_l^m(\mu'_z) \cos[m(\varphi - \varphi')] \right\} f(\mathbf{r}, \Omega') d\Omega', \end{aligned} \quad (109)$$

and

$$\begin{aligned} \mathcal{G}_- f(\mathbf{r}, \Omega) &= \sigma_t(\mathbf{r}) f(\mathbf{r}, \Omega) - \sum_{l \text{ odd}}^{\infty} \frac{2l+1}{\pi} \sigma_{sl}(\mathbf{r}) \\ &\int \left\{ 2 \sum_{m \text{ odd}}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu_z)P_l^m(\mu'_z) \cos[m(\varphi - \varphi')] \right\} f(\mathbf{r}, \Omega') d\Omega', \end{aligned} \quad (110)$$

where the angular integrations are carried out over one quadrant, where the angular ranges are given by Eqs. (103). The inverse operators are

$$\begin{aligned} \mathcal{G}_+^{-1} f(\mathbf{r}, \Omega) &= \frac{1}{\sigma_t(\mathbf{r})} \left[f(\mathbf{r}, \Omega) + \sum_{l \text{ even}}^{\infty} \frac{2l+1}{\pi} \frac{\sigma_{sl}(\mathbf{r})}{\sigma_t(\mathbf{r}) - \sigma_{sl}(\mathbf{r})} \right. \\ &\left. \int \left\{ P_l(\mu_z)P_l(\mu'_z) + 2 \sum_{m \text{ even}}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu_z)P_l^m(\mu'_z) \cos[m(\varphi - \varphi')] \right\} f(\mathbf{r}, \Omega') d\Omega' \right], \end{aligned} \quad (111)$$

and

$$\begin{aligned} \mathcal{G}_-^{-1} f(\mathbf{r}, \Omega) &= \frac{1}{\sigma_t(\mathbf{r})} \left[f(\mathbf{r}, \Omega) + \sum_{l \text{ odd}}^{\infty} \frac{2l+1}{\pi} \frac{\sigma_{sl}(\mathbf{r})}{\sigma_t(\mathbf{r}) - \sigma_{sl}(\mathbf{r})} \right. \\ &\left. \int \left\{ 2 \sum_{m \text{ odd}}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu_z)P_l^m(\mu'_z) \cos[m(\varphi - \varphi')] \right\} f(\mathbf{r}, \Omega') d\Omega' \right], \end{aligned} \quad (112)$$

where the angular integrals are also carried out over one quadrant of the angular domain.

9.3.3 Even-Parity FEM Weak Form

Substituting these expressions for the fluence and distributed source into the weak form of the even-parity equation results in

$$\begin{aligned}
& \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{A_e} \left(\mu_x^m \frac{\partial \psi_n}{\partial x} + \mu_y^m \frac{\partial \psi_n}{\partial y} \right) \mathcal{G}_{-1}^{-1} \phi_{e,m,n'}^+ \left(\mu_x^m \frac{\partial \psi_{n'}}{\partial x} + \mu_y^m \frac{\partial \psi_{n'}}{\partial y} \right) dx dy \right. \\
& \quad \left. + \int_{A_e} \psi_n(x, y) \mathcal{G}_{+} \phi_{e,m,n'}^+ \psi_{n'}(x, y) dx dy + \phi_{e,m,n'}^+ \oint \psi_n(x, y) \psi_{n'}(x, y) |\Omega_m \cdot \mathbf{n}| ds \right\} \\
& = \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \left(\mu_x^m \frac{\partial \psi_n}{\partial x} + \mu_y^m \frac{\partial \psi_n}{\partial y} \right) \mathcal{G}_{-1}^{-1} q_{e,m,n'}^- \psi_{n'}(x, y) dx dy + q_{e,m,n'}^+ \int_{A_e} \psi_n(x, y) \psi_{n'}(x, y) dx dy \right\} \\
& \quad + \oint \psi_n(x, y) \Phi_{b,\mp m}(x, y) |\Omega_m \cdot \mathbf{n}| ds, \text{ for } \Omega_m \cdot \mathbf{n} \gtrless 0, m = 1 : M, n = 1 : N, \quad (113)
\end{aligned}$$

where the surface integrals are carried out over the external boundary of the spatial domain.

9.3.4 Odd-Parity FEM Weak Form

Substituting these expressions for the fluence and distributed source into the weak form of the odd-parity equation results in

$$\begin{aligned}
& \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{A_e} \left(\mu_x^m \frac{\partial \psi_n}{\partial x} + \mu_y^m \frac{\partial \psi_n}{\partial y} \right) \mathcal{G}_{+1}^{-1} \phi_{e,m,n'}^- \left(\mu_x^m \frac{\partial \psi_{n'}}{\partial x} + \mu_y^m \frac{\partial \psi_{n'}}{\partial y} \right) dx dy \right. \\
& \quad \left. + \int_{A_e} \psi_n(x, y) \mathcal{G}_{-} \phi_{e,m,n'}^- \psi_{n'}(x, y) dx dy + \phi_{e,m,n'}^- \oint \psi_n(x, y) \psi_{n'}(x, y) |\Omega_m \cdot \mathbf{n}| ds \right\} \\
& = \sum_{e=1}^{NE} \sum_{n'=1}^N \left\{ \int_{A_e} \left(\mu_x^m \frac{\partial \psi_n}{\partial x} + \mu_y^m \frac{\partial \psi_n}{\partial y} \right) \mathcal{G}_{+1}^{-1} q_{e,m,n'}^+ \psi_{n'}(x, y) dx dy + q_{e,m,n'}^- \int_{A_e} \psi_n(x, y) \psi_{n'}(x, y) dx dy \right\} \\
& \quad \mp \oint \psi_n(x, y) \Phi_{b,\mp m}(x, y) |\Omega_m \cdot \mathbf{n}| ds, \text{ for } \Omega_m \cdot \mathbf{n} \gtrless 0, m = 1 : M, n = 1 : N. \quad (114)
\end{aligned}$$

9.3.5 Linear Interpolation Functions

A triangular element includes three nodes and, therefore, three linear interpolation functions. The n th interpolation function, $\varphi_n(\mathbf{r})$, is 1 at node n and 0 at the other two nodes. Fig. 2 shows a typical triangular element, with the coordinates of the three nodes shown.

The area of the element and the interpolation functions can be conveniently developed as the determinants of simple 3x3 matrices. The area, A , of an element can be computed from

$$A = \frac{1}{2} \begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} = \frac{x_1 y_2 + x_2 y_3 + x_3 y_1 - x_2 y_1 - x_3 y_2 - x_1 y_3}{2}. \quad (115)$$

The interpolation functions are,

$$\psi_1(x, y) = \frac{1}{2A} \begin{vmatrix} 1 & x & y \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} = \frac{x_2 y_3 - x_3 y_2 + (y_2 - y_3)x + (x_3 - x_2)y}{2A}, \quad (116)$$

$$\psi_2(x, y) = \frac{1}{2A} \begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x & y \\ 1 & x_3 & y_3 \end{vmatrix} = \frac{x_3 y_1 - x_1 y_3 + (y_3 - y_1)x + (x_1 - x_3)y}{2A}, \quad (117)$$

and

$$\psi_3(x, y) = \frac{1}{2A} \begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x & y \end{vmatrix} = \frac{x_1 y_2 - x_2 y_1 + (y_1 - y_2)x + (x_2 - x_1)y}{2A} \quad (118)$$

Figure 2: Typical FEM triangular element.

9.3.6 Master Triangular Element

The elemental integrations can be more conveniently carried out based on a master triangular element[7]. The integrations are then transformed to integrations over the actual elements by including the Jacobian matrix of the transformation. Fig. 3 shows a master triangular element, where s and t are the independent variables,

Figure 3: Master triangular element.

The nodes are numbered as listed in Table 1,

Table 1: Nodal coordinates of the master triangular element.

node	x coordinate	y coordinate
1	0	0
2	1	0
3	0	1

For the master triangular element, the linear interpolation functions are quite simple,

$$\psi_1(s, t) = 1 - s - t,$$

$$\psi_2(s, t) = s,$$

and

$$\psi_3(s, t) = t. \quad (119)$$

A general function is approximated by

$$f(s, t) = f_1\psi_1(s, t) + f_2\psi_2(s, t) + f_3\psi_3(s, t). \quad (120)$$

The equations relating the element coordinates to the master coordinates are

$$x = x_1 + (x_2 - x_1)s + (x_3 - x_1)t,$$

and

$$y = y_1 + (y_2 - y_1)s + (y_3 - y_1)t. \quad (121)$$

The Jacobian matrix of the coordinate transformation from the master triangular element to a general triangular element is [7]

$$J = \begin{bmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \end{bmatrix} = \begin{bmatrix} x_2 - x_1 & y_2 - y_1 \\ x_3 - x_1 & y_3 - y_1 \end{bmatrix}, \quad (122)$$

and the inverse Jacobian matrix is,

$$J^{-1} = \frac{1}{2A} \begin{bmatrix} y_3 - y_1 & y_1 - y_2 \\ x_1 - x_3 & x_2 - x_1 \end{bmatrix}, \quad (123)$$

and the determinant of J is

$$|J| = 2A, \quad (124)$$

where A is the area of the element. There are four base matrices that need to be computed, with elements computed from,

$$\begin{aligned} \mathcal{I}_1 &= \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \Omega_{m'} \cdot \nabla \psi_{n'}(\mathbf{r}) d\mathbf{r}, \\ \mathcal{I}_2 &= \int_{V_e} \Omega_m \cdot \nabla \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) d\mathbf{r}, \\ \mathcal{I}_3 &= \int_{V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) d\mathbf{r}, \end{aligned} \quad (125)$$

and

$$\mathcal{I}_4 = \oint_{\partial V_e} \psi_n(\mathbf{r}) \psi_{n'}(\mathbf{r}) |\Omega_m \cdot \mathbf{n}| ds. \quad (126)$$

With these identities, the integral terms can be determined fairly easily as outer products of terms involving the interpolation functions. The outer product of two vectors, ψ and φ , is defined as

$$\psi \otimes \varphi = \begin{bmatrix} \psi_1 \varphi_1 & \psi_1 \varphi_2 & \psi_1 \varphi_3 \\ \psi_2 \varphi_1 & \psi_2 \varphi_2 & \psi_2 \varphi_3 \\ \psi_3 \varphi_1 & \psi_3 \varphi_2 & \psi_3 \varphi_3 \end{bmatrix}.$$

The vector of linear interpolation functions for the master triangular element is

$$\hat{\psi}(s, t) = \begin{bmatrix} \hat{\psi}_1(s, t) \\ \hat{\psi}_2(s, t) \\ \hat{\psi}_3(s, t) \end{bmatrix} = \begin{bmatrix} 1 - s - t \\ s \\ t \end{bmatrix}.$$

The derivatives of $\hat{\psi}(s, t)$ are particularly simple,

$$\frac{\partial \hat{\psi}}{\partial s} = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix},$$

and

$$\frac{\partial \hat{\psi}}{\partial t} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}.$$

The following identity is useful for completing the derivation of the base matrices,

$$\Omega \cdot J^{-1} \cdot \nabla \hat{\psi} = \frac{1}{2A} \left[\mu_x \begin{pmatrix} y_2 - y_3 \\ y_3 - y_1 \\ y_1 - y_2 \end{pmatrix} + \mu_y \begin{pmatrix} x_3 - x_2 \\ x_1 - x_3 \\ x_2 - x_1 \end{pmatrix} \right]. \quad (127)$$

Using these identities, the base matrix, $\mathcal{I}_1$, for linear interpolation functions is

$$\begin{aligned} \mathcal{I}_1 &= \int \int_A \left(\mu_x \frac{\partial \psi}{\partial x} + \mu_y \frac{\partial \psi}{\partial y} \right) \otimes \left(\mu'_x \frac{\partial \psi}{\partial x} + \mu'_y \frac{\partial \psi}{\partial y} \right) dx dy \\ &= \frac{1}{4A} \left[\mu_x \begin{pmatrix} y_2 - y_3 \\ y_3 - y_1 \\ y_1 - y_2 \end{pmatrix} + \mu_y \begin{pmatrix} x_3 - x_2 \\ x_1 - x_3 \\ x_2 - x_1 \end{pmatrix} \right] \otimes \left[\mu'_x \begin{pmatrix} y_2 - y_3 \\ y_3 - y_1 \\ y_1 - y_2 \end{pmatrix} + \mu'_y \begin{pmatrix} x_3 - x_2 \\ x_1 - x_3 \\ x_2 - x_1 \end{pmatrix} \right], \end{aligned} \quad (128)$$

where A is the area of the real element, and the area of the master triangular element is $\frac{1}{2}$.

The base matrix, $\mathcal{I}_2$, is

$$\begin{aligned} \mathcal{I}_2 &= \int \int_A \left(\mu_x \frac{\partial \psi}{\partial x} + \mu_y \frac{\partial \psi}{\partial y} \right) \otimes \psi(x, y) dx dy \\ &= \frac{1}{6} \left[\mu_x \begin{pmatrix} y_2 - y_3 \\ y_3 - y_1 \\ y_1 - y_2 \end{pmatrix} + \mu_y \begin{pmatrix} x_3 - x_2 \\ x_1 - x_3 \\ x_2 - x_1 \end{pmatrix} \right] \otimes \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \end{aligned} \quad (129)$$

and the base matrix, $\mathcal{I}_3$, is

$$\mathcal{I}_3 = \int \int_A \psi(x, y) \otimes \psi(x, y) dx dy = \int \int_{A_m} \psi(s, t) \otimes \psi(s, t) |J| ds dt = \frac{A}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}. \quad (130)$$

9.3.7 Boundary Terms

The components of the base matrices, $\mathcal{I}_4$, resulting from the boundary integrals are computed as follows. The numbering convention used here is that side i is opposite node i . The length of side i is given by

$$l_i = \sqrt{(y_{i+1} - y_{i-1})^2 + (x_{i+1} - x_{i-1})^2}, \quad (131)$$

where the indices are computed from

$$i + 1 \Leftarrow 1 + \text{mod}(i, 3),$$

and

$$i - 1 \Leftarrow 1 + \text{mod}(i + 1, 3), \quad (132)$$

where mod is the modulus operator.

The unit outward normal of side i is given by

$$\mathbf{n}_i = \frac{(y_{i-1} - y_{i+1}, x_{i+1} - x_{i-1})}{l_i} \quad (133)$$

Defining an integration parameter, l , the spatial variables x and y are

$$x = x_{i+1} - n_y l,$$

and

$$y = y_{i+1} + n_x l. \quad (134)$$

The base matrices are closely related to those for the one-dimensional linear interpolation functions. Elements of the base matrices for side i containing $\varphi_i(\mathbf{r})$ are zero, since the interpolation functions are zero along that side. The other entries are the same as those for the one-dimensional linear interpolation functions, Eq. (97), with the mesh width, h , replace by the side length, l_i . The base matrix integrated along side 1 is

$$\mathcal{I}_4 = |\mu_x n_x + \mu_y n_y| \int_0^{l_1} \psi(x, y) \otimes \psi(x, y) dl = \frac{|\mu_x n_x + \mu_y n_y| l_1}{6} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}, \quad (135)$$

and integrated along side 2 is

$$\mathcal{I}_4 = |\mu_x n_x + \mu_y n_y| \int_0^{l_2} \psi(x, y) \otimes \psi(x, y) dl = \frac{|\mu_x n_x + \mu_y n_y| l_2}{6} \begin{bmatrix} 2 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 2 \end{bmatrix}, \quad (136)$$

and integrated along side 3 is

$$\mathcal{I}_4 = |\mu_x n_x + \mu_y n_y| \int_0^{l_3} \psi(x, y) \otimes \psi(x, y) dl = \frac{|\mu_x n_x + \mu_y n_y| l_3}{6} \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (137)$$

9.4 Vacuum Regions

For vacuum regions interior to the problem geometry, $\sigma_t = 0$, so the inverses of the scattering operators do not exist. The development of the even- and odd-parity equations breaks down in this situation. Internal vacuum regions have not yet been incorporated into the code.

10 Benchmarking

In this section the convergence rate of the error due to the spatial and angular approximations of the code will be investigated by analyzing several simple test problems, where analytic solutions are available. In this section, the spatial error will be investigated, and in the succeeding section, the error due to the angular approximation will be investigated, and finally, a comparison will be given with a measured electron energy-deposition profile. The L^2 norm of the spatial error is

$$\epsilon = \sqrt{\int |f(\mathbf{r}) - \tilde{f}(\mathbf{r})|^2 d\mathbf{r}}, \quad (138)$$

where $f(\mathbf{r})$ is the exact solution, and $\tilde{f}(\mathbf{r})$ is an approximate solution.

As a check on the computational method and the coding, the convergence rate of the computational result is compared with the theoretical convergence rate. The theoretical error obeys the relation,

$$\epsilon \leq ch^r, \quad (139)$$

where r is the convergence rate, h is the maximum element size, which is a parameter Pro/E uses to determine

the triangularization of the spatial domain, and c is a positive constant. The theoretical convergence rate for FEM with linear interpolation functions is 2, and that for quadratic interpolation functions is 3.

Unless otherwise noted, the Aztec tolerance is set to 10^{-8} ,

$$\frac{\|\mathbf{r}^{(k)}\|_2}{\|\mathbf{r}^{(0)}\|_2} < 10^{-8}, \quad (140)$$

where $\mathbf{r}^{(k)}$ is the residual at the k^{th} conjugate gradient iteration. For some of the comparisons presented below, the error norm is small enough that the Aztec tolerance had to be reduced below 10^{-8} .

10.1 One-Dimensional Spatial Domain

The spatial domain considered is a uniform, unit cell,

$$0 < z < 1, \quad (141)$$

with unit total cross section,

$$\sigma_t = 1. \quad (142)$$

Two directions are considered, particles traveling to the left and to the right,

$$\mu = \pm 1. \quad (143)$$

10.1.1 No scattering, No Distributed Source, Unit Left Boundary Source

With zero scattering cross section,

$$\sigma_s = 0, \quad (144)$$

zero distributed sources,

$$Q^\pm(z, \mu) = 0, \quad (145)$$

and unit normal left boundary condition,

$$\Phi_b(0, 1) = 1, \quad (146)$$

the even- and odd-parity equations, boundary conditions, and solutions are listed in the following tables,

μ	Equations	
+1	$-\frac{d^2\Phi^+}{dz^2} + \Phi^+ = 0$	$-\frac{d^2\Phi^-}{dz^2} + \Phi^- = 0$
-1	$-\frac{d^2\Phi^+}{dz^2} + \Phi^+ = 0$	$-\frac{d^2\Phi^-}{dz^2} + \Phi^- = 0$

μ	z	$\Omega \cdot \mathbf{n}$	Boundary Conditions	
+1	0	-1	$-\Phi^+ + \frac{d\Phi^+}{dz} = -1$	$-\Phi^- + \frac{d\Phi^-}{dz} = -1$
+1	1	+1	$+\Phi^+ + \frac{d\Phi^+}{dz} = 0$	$+\Phi^- + \frac{d\Phi^-}{dz} = 0$
-1	0	+1	$+\Phi^+ - \frac{d\Phi^+}{dz} = 1$	$+\Phi^- - \frac{d\Phi^-}{dz} = -1$
-1	1	-1	$-\Phi^+ - \frac{d\Phi^+}{dz} = 0$	$-\Phi^- - \frac{d\Phi^-}{dz} = 0$

μ	Solutions	
+1	$\Phi^+(z) = \frac{e^{-z}}{2}$	$\Phi^-(z) = \frac{e^{-z}}{2}$
-1	$\Phi^+(z) = \frac{e^{-z}}{2}$	$\Phi^-(z) = -\frac{e^{-z}}{2}$

The computational convergence rate is determined by performing a linear fit to a log-log plot of the L^2 norm of the error vs. the number of elements in the mesh.

Figure 3: L^2 norm of the error vs. the number of elements for test problem 1.

With linear interpolation functions, the L^2 norm shows quadratic convergence, based on the data in the following table:

number of elements	L^2 norm of error: linear interpolation functions	
	even-parity fluence	odd-parity fluence
5	8.737×10^{-4}	8.737×10^{-4}
10	2.188×10^{-4}	2.188×10^{-4}
20	5.471×10^{-5}	5.471×10^{-5}
40	1.368×10^{-5}	1.368×10^{-5}
80	3.420×10^{-6}	3.420×10^{-6}
160	8.550×10^{-7}	8.550×10^{-7}
convergence rate	2.000	2.000

With quadratic interpolation functions, the L^2 norm shows cubic convergence, which is verified with the data in the following table:

number of elements	L^2 norm of error: quadratic interpolation functions	
	even-parity fluence	odd-parity fluence
5	1.506×10^{-5}	1.506×10^{-5}
10	1.889×10^{-6}	1.889×10^{-6}
20	2.363×10^{-7}	2.363×10^{-7}
40	2.954×10^{-8}	2.954×10^{-8}
80	3.693×10^{-9}	3.693×10^{-9}
convergence rate	2.999	2.999

10.1.2 No Scattering, Unit Distributed Source, No Boundary Source

With a unit isotropic distributed source,

$$Q^+ = 1,$$

the even- and odd-parity equations, boundary conditions, and solutions are listed in the following tables,

μ	Equations	
+1	$-\frac{d^2\Phi^+}{dz^2} + \Phi^+ = 1$	$-\frac{d^2\Phi^-}{dz^2} + \Phi^- = 0$
-1	$-\frac{d^2\Phi^+}{dz^2} + \Phi^+ = 1$	$-\frac{d^2\Phi^-}{dz^2} + \Phi^- = 0$

μ	z	$\Omega \cdot \mathbf{n}$	Boundary Conditions	
+1	0	-1	$-\Phi^+ + \frac{d\Phi^+}{dz} = 0$	$-\Phi^- + \frac{d\Phi^-}{dz} = 1$
+1	1	+1	$+\Phi^+ + \frac{d\Phi^+}{dz} = 0$	$+\Phi^- + \frac{d\Phi^-}{dz} = 1$
-1	0	+1	$+\Phi^+ - \frac{d\Phi^+}{dz} = 0$	$+\Phi^- - \frac{d\Phi^-}{dz} = 1$
-1	1	-1	$-\Phi^+ - \frac{d\Phi^+}{dz} = 0$	$-\Phi^- - \frac{d\Phi^-}{dz} = 1$

μ	Solutions	
1	$\Phi^+(z) = 1 - \frac{e^{-z} + e^{-(1-z)}}{2}$	$\Phi^-(z) = -\frac{e^{-z} - e^{-(1-z)}}{2}$
-1	$\Phi^+(z) = 1 - \frac{e^{-z} + e^{-(1-z)}}{2}$	$\Phi^-(z) = +\frac{e^{-z} - e^{-(1-z)}}{2}$

Figure 4: L^2 norm of the error vs. the number of elements for test problem 2.

For linear interpolation functions, the L^2 norm shows quadratic convergence:

number of elements	L^2 norm of error: linear interpolation functions	
	even-parity fluence	odd-parity fluence
5	1.638×10^{-3}	6.083×10^{-4}
10	4.095×10^{-4}	1.541×10^{-4}
20	1.024×10^{-4}	3.865×10^{-5}
40	2.559×10^{-5}	9.671×10^{-6}
80	6.398×10^{-6}	2.418×10^{-6}
160	1.600×10^{-6}	6.046×10^{-7}
convergence rate	2.000	1.996

For quadratic interpolation functions, the L^2 norm shows cubic convergence:

number of elements	L^2 norm of error: quadratic interpolation functions	
	even-parity fluence	odd-parity fluence
5	8.068×10^{-6}	2.902×10^{-5}
10	1.026×10^{-6}	3.635×10^{-6}
20	1.289×10^{-7}	4.546×10^{-7}
40	1.612×10^{-8}	5.683×10^{-8}
80	2.016×10^{-9}	7.105×10^{-9}
convergence rate	2.993	2.999

10.1.3 Unit Isotropic Scattering, Unit Distributed Source, and Unit Boundary Source

For unit isotropic scattering and unit total cross section,

$$\sigma_s = \sigma_t = 1,$$

the equations, boundary conditions, and solutions are listed in the following tables. For this example, the odd-parity equation is undefined, since the inverse of the even-parity scattering operator is undefined. The odd-parity fluence can be computed from the derivative of the even-parity fluence, with a loss of accuracy:

μ	Equations	
+1	$-\frac{d^2\Phi^+}{dz^2} + \Phi^+ - \frac{\Phi^+ + \Phi^-}{2} = 1$	$\Phi^- = -\frac{d\Phi^+}{dz}$
-1	$-\frac{d^2\Phi^+}{dz^2} + \Phi^+ - \frac{\Phi^+ + \Phi^-}{2} = 1$	$\Phi^- = \frac{d\Phi^+}{dz}$

μ	z	$\Omega \cdot \mathbf{n}$	Boundary Conditions
+1	0	-1	$-\Phi^+ + \frac{d\Phi^+}{dz} = -1$
+1	1	+1	$+\Phi^+ + \frac{d\Phi^+}{dz} = 0$
-1	0	+1	$+\Phi^+ - \frac{d\Phi^+}{dz} = 1$
-1	1	-1	$-\Phi^+ - \frac{d\Phi^+}{dz} = 0$

μ	Solutions	
1	$\Phi^+(z) = \frac{7}{6} + \frac{z}{6} - \frac{z^2}{2}$	$\Phi^-(z) = z - \frac{1}{6}$
-1	$\Phi^+(z) = \frac{7}{6} + \frac{z}{6} - \frac{z^2}{2}$	$\Phi^-(z) = -(z - \frac{1}{6})$

Figure 5: L^2 norm of the error vs. the number of elements for test problem 3.

For linear interpolation functions, the L^2 norm of the error in the even-parity fluence shows quadratic convergence. Computing the odd-parity fluence from the derivative of the even-parity fluence shows linear convergence in the L^2 norm of the error.

number of elements	L^2 norm of error: linear interpolation functions	
	even-parity fluence	odd-parity fluence
5	3.651×10^{-3}	5.773×10^{-2}
10	9.129×10^{-4}	2.887×10^{-2}
20	2.282×10^{-4}	1.443×10^{-2}
40	5.705×10^{-5}	7.217×10^{-3}
80	1.426×10^{-5}	3.608×10^{-3}
160	3.566×10^{-6}	1.084×10^{-3}
convergence rate	2.000	1.000

Because the analytic solution of the even-parity fluence is quadratic, using quadratic interpolation functions results in essentially perfect computation of the quadratic even-parity fluence, for any number of elements.

10.2 Two-Dimensional Spatial Domain

For a uniform square region,

$$0 < x < 1, 0 < y < 1,$$

with unit total cross section,

$$\sigma_t = 1,$$

and no scattering,

$$\sigma_s = 0,$$

consider four directions,

$$\mu_x = \pm \frac{1}{\sqrt{3}}, \mu_y = \pm \frac{1}{\sqrt{3}}.$$

10.2.1 No Distributed Source, Unit Planar Source

Consider a unit planar source incident from the lower right with direction cosines

$$\mu_x = -\frac{1}{\sqrt{3}}, \mu_y = +\frac{1}{\sqrt{3}}.$$

For a source uniform across bottom, $y = 0$, and right side, $x = 1$, the equations, boundary conditions, and analytic solutions are given in the following tables. Because there is no scattering, the only direction that needs to be considered is the source direction. In the opposite direction, the even-parity fluence is the same as that in the source direction, and the odd-parity fluence is the same in magnitude with the opposite sign as that in the source direction. The gradient term in the boundary condition is

$$\Omega \cdot \nabla \Phi^\pm = -\frac{1}{\sqrt{3}} \frac{\partial \Phi^\pm}{\partial x} + \frac{1}{\sqrt{3}} \frac{\partial \Phi^\pm}{\partial y}$$

μ_x	μ_y	Equations	
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	$-\frac{1}{3} \frac{\partial^2 \Phi^+}{\partial x^2} + \frac{2}{3} \frac{\partial^2 \Phi^+}{\partial x \partial y} - \frac{1}{3} \frac{\partial^2 \Phi^+}{\partial y^2} + \Phi^+ = 0$	$-\frac{1}{3} \frac{\partial^2 \Phi^-}{\partial x^2} + \frac{2}{3} \frac{\partial^2 \Phi^-}{\partial x \partial y} - \frac{1}{3} \frac{\partial^2 \Phi^-}{\partial y^2} + \Phi^- = 0$

μ_x	μ_y	x	y	$\Omega \cdot \mathbf{n}$	Boundary Conditions	
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	0 : 1	0	< 0	$-\Phi^+ + \Omega \cdot \nabla \Phi^+ = -1$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = -1$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	1	0 : 1	< 0	$-\Phi^+ + \Omega \cdot \nabla \Phi^+ = -1$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = -1$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	0 : 1	1	> 0	$+\Phi^+ + \Omega \cdot \nabla \Phi^+ = 0$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = 0$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	0	0 : 1	> 0	$+\Phi^+ + \Omega \cdot \nabla \Phi^+ = 0$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = 0$

μ_x	μ_y	spatial domain	Solutions	
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	$x + y \leq 1$	$\Phi^+(z) = \frac{e^{-\sqrt{3}y}}{2}$	$\Phi^-(z) = \frac{e^{-\sqrt{3}y}}{2}$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	$x + y \geq 1$	$\Phi^+(z) = \frac{e^{-\sqrt{3}(1-x)}}{2}$	$\Phi^-(z) = \frac{e^{-\sqrt{3}(1-x)}}{2}$

Although the analytic solution is continuous, there is a discontinuity in the derivative for $x + y = 1$, so quadratic convergence is not obtained for this problem. The L^2 norm showed sub-linear convergence.

With a slight change in the boundary conditions, however, a solution with continuous derivatives is obtained, which exhibits the expected convergence rate. The modified boundary conditions and analytic solutions are shown in the following tables.

μ_x	μ_y	x	y	$\Omega \cdot \mathbf{n}$	Boundary Conditions	
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	0 : 1	0	< 0	$-\Phi^+ + \Omega \cdot \nabla \Phi^+ = -\frac{e^{\sqrt{3}x/2}}{2}$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = -\frac{e^{\sqrt{3}x/2}}{2}$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	1	0 : 1	< 0	$-\Phi^+ + \Omega \cdot \nabla \Phi^+ = -\frac{e^{\sqrt{3}(1-y)/2}}{2}$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = -\frac{e^{\sqrt{3}(1-y)/2}}{2}$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	0 : 1	1	> 0	$+\Phi^+ + \Omega \cdot \nabla \Phi^+ = 0$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = 0$
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	0	0 : 1	> 0	$+\Phi^+ + \Omega \cdot \nabla \Phi^+ = 0$	$-\Phi^- + \Omega \cdot \nabla \Phi^- = 0$

μ_x	μ_y	Solutions	
$-\frac{1}{\sqrt{3}}$	$+\frac{1}{\sqrt{3}}$	$\Phi^+(z) = \frac{e^{-\sqrt{3}(y-x)/2}}{2}$	$\Phi^-(z) = \frac{e^{-\sqrt{3}(y-x)/2}}{2}$

The L^2 norm appears to show nearly quadratic convergence, as expected for linear interpolation functions,

maximum element size	L^2 norm of error: linear interpolation functions	
	even-parity fluence	odd-parity fluence
0.5	1.178×10^{-2}	1.178×10^{-2}
0.2	1.812×10^{-3}	1.812×10^{-3}
0.1	4.471×10^{-4}	4.471×10^{-4}
0.05	9.937×10^{-5}	9.937×10^{-5}
0.01	4.983×10^{-6}	4.983×10^{-6}
convergence rate	1.992	1.992

Figure 6: L^2 norm of the error vs. the inverse of the maximum element size for 2D test problem.

10.3 Convergence of Angular Quadrature

10.3.1 One-Dimensional Spatial Domain

For a function, $f(\mathbf{r}, \Omega)$, in space and angle, the L^2 norm of the error is

$$\epsilon = \sqrt{\iint |f(\mathbf{r}, \Omega) - \tilde{f}(\mathbf{r}, \Omega)|^2 d\mathbf{r} d\Omega},$$

where $\tilde{f}(\mathbf{r}, \Omega)$ is an approximate solution. However, for a discrete ordinates treatment in angle, the approximate solution is known only at the quadrature points, so this expression cannot be calculated. The following three error norms can be calculated and will be compared,

$$\epsilon_1 = \sqrt{\sum_m w_m \int |f(\mathbf{r}, \Omega_m) - \tilde{f}(\mathbf{r}, \Omega_m)|^2 d\mathbf{r}},$$

$$\epsilon_2 = \max_m \sqrt{\int |f(\mathbf{r}, \Omega_m) - \tilde{f}(\mathbf{r}, \Omega_m)|^2 d\mathbf{r}},$$

and

$$\epsilon_3 = \max_{m,i} |f(\mathbf{r}_i, \Omega_m) - \tilde{f}(\mathbf{r}_i, \Omega_m)|,$$

where $\tilde{f}(\mathbf{r}, \Omega_m)$ is the approximate solution at the m -th quadrature point.

For isotropic scattering, the scattering cross section, σ_s , is proportional to the total cross section,

$$\sigma_s = c\sigma_t,$$

where c is the scattering ratio, which is in the range, $0 \leq c < 1$. For isotropic scattering and unit total cross section, the even-parity transport equation is

$$-\mu^2 \frac{d^2 \Phi^+(z, \mu)}{dz^2} + \Phi^+(z, \mu) = \frac{c}{2} \int_{-1}^1 \Phi^+(z, \mu') d\mu' + Q^+(z, \mu),$$

with boundary conditions,

$$\pm \Phi^+(z, \mu) + \mu \frac{d\Phi^+(z, \mu)}{dz} = \pm \Phi_b(z, \pm \mu) + Q^-(z, \mu), \text{ for } \Omega \cdot \mathbf{n} \gtrless 0, z = 0, 1. \quad (147)$$

In order to investigate the convergence of the error norms as a function of the angular approximation, specify a simple analytic solution,

$$\begin{aligned} \Phi^+(z, \mu) &= \mu^2, \\ \Phi^-(z, \mu) &= 0, \end{aligned}$$

which is the solution resulting from source terms,

$$Q^+(z, \mu) = \mu^2 - \frac{c}{3},$$

and

$$Q^-(z, \mu) = 0.$$

For this problem, the three error norms are listed in the following table, showing nearly quadratic convergence in the error norm. In order to investigate the error in the angular approximation, the angular mesh is divided uniformly into a number of angle meshes, and the integral over each angle mesh is approximated by a low-order Gauss quadrature over the mesh. Using a single Gauss quadrature point per angle mesh, which is located at the midpoint of the mesh, the three error norms are as follows.

number of angle meshes	1 Gauss Point per Angle Mesh		
	ϵ_1	ϵ_2	ϵ_3
2	9.38×10^{-3}	1.14×10^{-2}	1.32×10^{-2}
4	2.40×10^{-3}	3.34×10^{-3}	3.79×10^{-3}
8	6.03×10^{-4}	8.89×10^{-4}	9.69×10^{-4}
16	1.51×10^{-4}	2.28×10^{-4}	2.43×10^{-4}
convergence rate	1.99	1.88	1.93

Figure 7: L^2 of the error vs. number of angle meshes for test problem 5.

Using higher-order Gauss quadrature results in essentially perfect modeling of this test problem, since the analytic solution is quadratic, which is integrated exactly by Gauss quadrature of orders 2 or greater.

Another test problem is as follows,

$$\begin{aligned}\Phi^+(z, \mu) &= \cos(\mu), \\ \Phi^-(z, \mu) &= 0,\end{aligned}$$

which is the analytic solution for distributed source terms of,

$$Q^+(z, \mu) = \cos(\mu) - c \sin(1),$$

and

$$Q^-(z, \mu) = 0.$$

Using 2 Gauss points per angle mesh reduced the error to such an extent that the Aztec tolerance had to be reduced to 10^{-12} ,

$$\frac{\|\mathbf{r}^{(k)}\|_2}{\|\mathbf{r}^{(0)}\|_2} < 10^{-12},$$

where $\mathbf{r}^{(k)}$ is the residual at the k^{th} conjugate gradient iteration.

The three error norms are for one and two Gauss points per angle mesh are as follows. Using one Gauss point per angle mesh results in quadratic convergence, and using two Gauss points per angle mesh results in fourth-order convergence, since one-point Gauss quadrature integrates linear terms exactly, and two-point Gauss quadrature integrates up to cubic terms exactly.

number of angle meshes	1 Gauss Point per Angle Mesh			2 Gauss Points per Angle Mesh		
	ϵ_1	ϵ_2	ϵ_3	ϵ_1	ϵ_2	ϵ_3
2	3.98×10^{-3}	4.85×10^{-3}	5.57×10^{-3}	5.71×10^{-6}	8.05×10^{-6}	9.02×10^{-6}
4	1.01×10^{-3}	1.41×10^{-3}	1.59×10^{-3}	3.54×10^{-7}	5.26×10^{-7}	5.67×10^{-7}
8	2.54×10^{-4}	3.75×10^{-4}	4.08×10^{-4}	2.21×10^{-8}	3.36×10^{-8}	3.55×10^{-8}
16	6.36×10^{-5}	9.64×10^{-5}	1.02×10^{-4}	1.38×10^{-9}	2.12×10^{-9}	2.22×10^{-9}
convergence rate	1.99	1.89	1.95	4.00	3.96	4.00

Figure 8: L^2 of the error vs. number of angle meshes for test problem 6.

10.4 Lockwood Data

Lockwood et al.[8] used a calorimetric technique to measure energy-deposition profiles in one-dimensional geometries for electron sources. In this section we compare the results of one of their sets of measurements with FEM modeling. The reported experimental uncertainties are less than a few percent. The problem considered here is that of 1-MeV normally incident on aluminum. The parameters for the FEM modeling are: 40 electron energy groups, no coupling with photons, P-15 Legendre expansion of the scattering cross section angular dependence, S-16 angular quadrature, 50 uniform spatial elements, with quadratic interpolation functions. The comparison between calculation and experiment is shown in Fig. 9, with excellent agreement.

Figure 9: Energy deposition profiles for 1-MeV electrons normally incident on aluminum.

11 Discussion

The solver is currently based on a Pro/E triangular mesh of a two-dimensional region. Extension to three-dimensional, unstructured tetrahedrons would be straightforward, resulting in double the number of discrete directions and increasing the number of FEM nodes. The structure of the code would not need to be changed a great deal, although the size of the problem will increase greatly. Compatibility with other mesh generation software (IDEAS) is currently under way.

Modeling photon transport with Eq. (1) is straightforward. However, modeling electron transport with Eq. (1) requires specially modified electron cross sections[3]. The reference describes a Goudsmit-Saunders modification to CEPXS electron cross sections[9], resulting in electron cross sections that are compatible with neutral-particle transport codes. For some applications, this method requires a very high order Legendre expansion of the electron cross sections, which is inefficient. A better approach would be to include a CSD term directly in the transport equation, and this modification is currently under way.

The two-dimensional FEM analysis is currently based on linear-continuous interpolation functions, which are fairly inaccurate in regions with steep gradients in the solution, which are common in radiation transport problems. Inclusion of either quadratic or linear-discontinuous interpolation functions is needed. Quadratic interpolation functions have already been included in a 1-D version of the code, and inclusion in the two-dimensional code would be straightforward. Linear-discontinuous interpolation functions would require a more significant modification to the code, and 1-D analyses are currently under way to evaluate the effectiveness of using linear-discontinuous interpolation functions.

The conjugate-gradients iterations in the current version of the code converge fairly slowly, since the only preconditioning included so far is point Jacobi. More effective preconditioning and acceleration techniques are currently being investigated.

12 References

- [1] J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, and G. D. Valdez, "TTS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," SAND91-1634, Sandia National Laboratories Report, 1992.
- [2] G. Bell and S. Glasstone, *Nuclear Reactor Theory* (Van Nostrand Reinhold, New York, 1970).
- [3] C. R. Drumm, "Multidimensional Electron-Photon Transport with Standard Discrete Ordinates Codes," *Nuclear Science and Engineering*, **127**, 1-21, (September, 1997).
- [4] R. T. Ackroyd, *Finite Element Methods for Particle Transport* (Wiley, New York, 1997).
- [5] S. Hutchinson, J. Shadid, and R. Tuminaro, *Aztec User's Guide Version 1.1*, SAND95-1559, Sandia National Laboratories Report, 1995.
- [6] J. Duderstadt and W. Martin, *Transport Theory* (Wiley, New York, 1979).
- [7] J. Reddy, *An Introduction to the Finite Element Method* (McGraw-Hill, New York, 1993).
- [8] G. J. Lockwood, L. E. Ruggles, G. H. Miller, and J. A. Halbleib, "Calorimetric Measurement of Electron energy Deposition in Extended Media-Theory vs. Experiment," SAND79-0414, Sandia National Laboratories Report, 1979.
- [9] L. J. Lorence, Jr., J. E. Morel, and G. D. Valdez, "Physics Guide to CEPXS: A Multigroup Coupled Electron Photon Cross-Section Generating Code, Version 1.0," SAND89-1685, Sandia National Laboratories Report, 1989.

Appendix A. Code Description

A.1 Structs and Prototypes

```
#include "az_aztec.h"
typedef struct
{
    int quad_order ;
    int n_directions ;
    double *quad_weight ;
    double *dir_cos_x ;
    double *dir_cos_y ;
    double *dir_cos_z ;
    double mux_source ; /* source x-direction cosine */
    double muy_source ; /* source y-direction cosine */
} Quad_data ;
void lobatto(Quad_data q) ;
void gauss_quadrature(Quad_data q) ;
void quadrature2d(Quad_data q) ;
void quadrature3d(Quad_data q) ;
double associated_legendre_polynomial(int l,int m,double x) ;
typedef struct
{
    int n_dimensions ;          /* 1: 1-D slab
                                2: two-dimensional x-y
                                3: three-dimensional x-y-z */
    int element_type ;          /* 1: linear continuous
                                2: quadratic continuous */
    int n_nodes_per_element ;
    int n_nodes ;
    int n_elements ;
    int n_zones ;               /* number of material zones */
    double *x, *y, *z ;         /* x, y, z coordinates of nodes */
    int *node_number ;           /* global node number of storage location */
    int *element_material_number ; /* material number by element */
    int **global_node ;          /* mapping from local to global node numbers
                                by element and local node number */
    double *delx ;               /* mesh widths for 1D geometry */
    double *element_area ;       /* element areas for 2D geometry */
    char **surface_flag ;        /* 0 for non-boundary surfaces
                                1 for boundary surfaces */
    char **connectivity_flag ;   /* 0 for non-adjacent nodes
                                1 for adjacent nodes */
} FEM_data ;
void setup_fem(FEM_data *fem, Quad_data quad) ;
void form_global_node_1d(FEM_data fem) ; /* compute mapping from local
to global node numbering
for 1-D geometry */
```

```

void readfnf(char *fnf_file, FEM_data *fem) ; /* read Pro/E fnf file */
void compute_element_areas(int n_elements, double *element_area,
    int **global_node, double *x, double *y) ;
void find_boundary_surfaces(int n_elements, int n_nodes_per_element,
    char **surface_flag, int **global_node) ;
typedef struct
{
    int n_particles ;    /* number of particle types */
    int icoup ;          /* cepxs coupling parameter:
                        0: no coupling
                        1: electron to photon (partial)
                        2: photon to electron (partial)
                        3: electron to photon (full)
                        4: photon to electron (full) */
    int neg ;            /* number of electron groups */
    int npg ;            /* number of photon groups */
    int n_groups ;       /* total number of energy groups */
    int ihm ;            /* cross section table length */
    int iht ;            /* position of total cross section */
    int ihs ;            /* position of scattering cross sections */
    int n_moments ;      /* number of legendre moments in cross sections */
    int n_materials ;    /* number of materials in cross section set */
    double *eeg ;         /* electron energy group boundaries */
    double *peg ;         /* photon energy group boundaries */
    double *eavg ;        /* energy group midpoints */
    double *dele ;        /* energy group widths */
    double *material_density ; /* material densities */
    double *range ;       /* electron range at upper energy by material */
    double **bound_restr_spower ; /* restricted stopping powers
                                at electron group boundaries
                                by material */
    double ****xsec ;      /* xslib cross sections by
                                material
                                legendre moment
                                energy group
                                position

                                position      cross section
                                -----
                                0      equilibrium energy deposition
                                1      charge deposition
                                2      secondary produciton
                                3      energy deposition
                                4      absorption
                                5
                                6      total
                                7      self scatter
*/
} Xsec_data ;

```

```

void read_cepdat(Xsec_data *xs) ;
void read_xslib(Xsec_data *xs) ;
void broadcast_xs(int proc_config[AZ_PROC_SIZE], Xsec_data *xs) ;
void broadcast_fem(int proc_config[AZ_PROC_SIZE], FEM_data *fem) ;
void assemble_lhs(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ig, int N_update, int *update,
    int **bindx, double **val) ;

void form_connectivity_flag(int n_elements, int n_nodes,
    int n_nodes_per_element, int n_directions,
    int **global_node, int N_update, int *update,
    char **connectivity_flag) ;
void setup_msr(int N_update, int *update, int n_nodes,
    int n_directions,
    char **connectivity_flag, int **bindx, double **val) ;

void form_element_A_1d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ele, int ig, double ***element_A) ;
void form_element_A_2d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ele, int ig, double ***element_A) ;
void assemble_rhs(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ig, int source_direction_index,
    double ***even_parity_fluence,
    double ***odd_parity_fluence, double *F) ;
void boundary_source_2d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ele, int source_direction_index,
    double **element_F) ;
void form_element_F_1d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ele, int ig, double ***even_parity_fluence,
    double ***odd_parity_fluence, double **element_F) ;
void form_element_F_2d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int parity, int ele, int ig, double ***even_parity_fluence,
    double ***odd_parity_fluence, int source_direction_index,
    double **element_F) ;

void partition_rhs(int N_update, int *update, int n_nodes,
    int n_directions,
    double *F, double *b) ;

void ludecomp(int n, double **A) ;
void lubacksub(int n, double **A, double *X) ;
void write_tecplot1d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int source_direction_index,
    double ***even_parity_fluence, double ***odd_parity_fluence,
    double **fluence, double *total_fluence, double *energy_deposition,
    double *charge_deposition, double **dose) ;
void write_tecplot2d(Quad_data quad, FEM_data fem, Xsec_data xs,
    int source_direction_index,

```



```
double ***even_parity_fluence, double ***odd_parity_fluence,  
double **fluence, double *total_fluence, double *energy_deposition,  
double *charge_deposition, double **dose, double **cdep) ;
```

A.2 High-Level Description

1. Initialize MPI and Aztec options.
2. Read and broadcast input data.
3. Read and broadcast cross section data.
4. Compute quadrature data.
5. Read and process finite-element data.
 - a. compute element areas.
 - b. find external boundary surfaces.
6. Define Aztec partitioning of matrix.
7. Begin loop over energy groups.
 - a. Begin even-odd parity loop.
 - i. assemble bindx and val arrays in MSR format.
 - ii. assemble forcing vector.
 - iii. Aztec conjugate-gradients solve.
 - iv. gather solution.
 - b. End of even-odd parity loop.
8. End of energy loop.
9. Postprocess solution.

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