SAND REPORT

SAND2002-1880
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Printed June 2002

Discrete Ordinates Approximations to the First- and Second-Order Radiation Transport Equations

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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Abstract

The conventional discrete ordinates approximation to the Boltzmann transport equation can be described in a matrix form. Specifically, the within-group scattering integral can be represented by three components: a moment-to-discrete matrix, a scattering cross-section matrix and a discrete-to-moment matrix. Using and extending these entities, we derive and summarize the matrix representations of the second-order transport equations.

Acknowledgements

We would like to express our sincere gratitude to Len Lorence and Gary Scrivner for their continuing support of this work. We also thank Tom Laub for reviewing this manuscript and making valuable suggestions.

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1. Introduction

The CEPTRE code, which stands for **C**oupled **E**lectron-**P**hoton **T**ransport for **R**adiation **E**ffects, is under development under the ASCI program at Sandia. It is designed to provide radiation transport capabilities for the subsequent mechanical and electrical analysis. The major features of the code include:

- multigroup energy discretization,[1]
- angular discretization with discrete ordinates approximation and with arbitrary order of anisotropic scattering,[1]
- continuous linear or quadratic finite-element approximations on unstructured mesh,[2]
- parallel options with message passing interface,
- object-oriented program architecture to allow ease of maintenance and extension.

Moreover, the CEPTRE code is based on a novel approach in which the space-angle dependence is solved simultaneously by using the conjugate gradient method.[3] This solution technique offers two advantages over the conventional source iteration. First, it eliminates the need for the inner iterations which is notoriously slow for electron transport. Second, the global system is built and processed in a distributed fashion which is well suited for massively parallel computers.

The objective of this report is to document the mathematical basis of the CEPTRE code including both the first- and second-order formulation of the radiation transport equation. We emphasize the energy and angular discretizations while the finite element analyses are presented in a follow-up report. We begin by discussing the first-order Boltzmann transport equation in a general context. The multigroup Legendre expansion to treat the scattering cross section and the discrete ordinants approximation to treat the angular dependence are introduced to reduce the transport equation to a system of energy-independent, discrete equations. We then outline a procedure to cast the discrete equations into a matrix form by expressing the within-group scattering integral with three components: a moment-to-discrete matrix, a scattering cross-section matrix and a discrete-to-moment matrix. This matrix representation involves combining the discrete angular flux into a vector which constitutes the fundamental unknown of the simultaneous space-angle solution.

The discrete ordinates approximation can also be applied to the second-order forms of the transport equation which are recognized as the self-adjoint angular flux (SAAF)[4] and the even-odd parity (EOP)[2] equations. The fundamental unknowns of the SAAF equation are the full-range angular flux while that of the EOP equations are the even- and odd-components of the angular flux. Nevertheless, we demonstrate that these discrete, second-order transport equations can be structured into a unified form with properly defined matrix components. This unified formulation not only allows us to derive the corresponding finite-element equations in a generalized fashion, but also mitigate the complexity in program structure to accommodate both the SAAF and EOP equations.

2. Boltzmann Transport Equation

The vast majority of numerical transport calculations are carried out by solving the linear Boltzmann equation in which the radiation field of the problem space is characterized by the angular flux distribution over the phase space of time, position, direction, and energy. For a time-independent problem with an external source, this equation has the form of[1]

$$\begin{aligned}&\Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega, E) + \sigma(\boldsymbol{r}, E)\psi(\boldsymbol{r}, \Omega, E) \\ &= \int_0^{\infty}\int_{4\pi}\sigma_s(\boldsymbol{r}, \Omega' \to \Omega, E' \to E)\psi(\boldsymbol{r}, \Omega', E')d\Omega' dE' + S(\boldsymbol{r}, \Omega, E)\end{aligned} \tag{1}$$

where ∇ is the gradient operator in the cartesian geometry, and

$\psi(\boldsymbol{r}, \Omega, E)$ = the angular flux of energy E at position $\boldsymbol{r}$ in the direction Ω,

$\sigma(\boldsymbol{r}, E)$ = the macroscopic cross section which gives the probability of collision per unit path length,

$\sigma_s(\boldsymbol{r}, \Omega' \to \Omega, E' \to E)$ = the differential scattering cross section where $\sigma_s(\boldsymbol{r}, \Omega' \to \Omega, E' \to E)d\Omega dE$ gives the probability per unit path length that particles at position $\boldsymbol{r}$ with energy E' in the direction Ω' scatter into dE about E and into a cone of direction $d\Omega$ about Ω,

$S(\boldsymbol{r}, \Omega, E)$ = the external particle source distribution.

In this manuscript, we will use the symbol V to denote the spatial domain which is bounded by an external boundary A. The particle direction spans the entire solid angle of 4π. The particle energy is defined within a range, $E \in [E_{\min}, E_{\max}]$.

The appropriate boundary conditions to Eq. (1) are usually given by specifying in that the incoming flux at an external boundary:

$$\psi(\boldsymbol{r}_b, \Omega, E) = \psi_b(\Omega, E) \qquad \text{for } \Omega \cdot \boldsymbol{n}_b < 0 \tag{2}$$

where $\boldsymbol{r}_b$ and $\boldsymbol{n}_b$ are the position vector and outward normal on the external boundary, respectively.

Equation (1) is often referred to as the first-order form of the Boltzmann transport equation. Physically, it is a mathematical statement of particle balance over a differential volume in the phase space of $(\boldsymbol{r}, \Omega, E)$. The first term on the left of Eq. (1) represents change in particle angular density due to the motion of the particles in a straight line without any collisions while the second term represents the rate of removal due to collisions with matter. The two terms on the right of Eq. (1) represent the particle contribution from collision and external source.

Two physical quantities of interest can be computed directly from the angular flux. The scalar flux is defined as the angular integral of the angular flux:

$$\phi(r, E) = \int_{4\pi} \psi(\boldsymbol{r}, \Omega, E) d\Omega \tag{3}$$

The current is defined as the angular integral of the angular current:

$$\mathbf{J}(r, E) = \int_{4\pi} \Omega \psi(\boldsymbol{r}, \Omega, E) d\Omega \tag{4}$$

Integrating Eq. (1) over the entire angular, energy and spatial domain, we obtain the global balance equation:

$$\int_V \nabla \cdot \mathbf{J}(r) dV + \int_V \sigma_a(r)\phi(r) dV = \int_A n \cdot \mathbf{J}(r) dA + \int_V \sigma_a(r)\phi(r) dV = \int_V S(r) dV \tag{5}$$

where $\phi(r)$, $\mathbf{J}(r)$ and $S(r)$ are the integrals of the scalar flux, current and external source over the energy range, $\sigma_a(r) = \sigma_t(r) - \sigma_s(r)$ is the particle absorption cross section.

2.1 Multigroup Legendre Approximation

The total and scattering cross sections are strongly dependent on material composition. Furthermore, they are complicated functions in terms of particle energy and scattering angle. For computational purposes it is customary to reduce the Boltzmann transport equation to a more manageable form before applying any numerical methods. Traditionally, the differential scattering cross section in Eq. (1) is expanded in terms of orthogonal functions, typically, the Legendre polynomials,[1] $P_l(\mu_0)$, where $\mu_0 = \Omega' \cdot \Omega$ is the cosine of the scattering angle in the laboratory system.

$$\begin{aligned}\sigma_s(\boldsymbol{r}, \Omega' \to \Omega, E' \to E) &= \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega, E' \to E) \\ &= \sigma_s(\boldsymbol{r}, \mu_0, E' \to E) \\ &= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sigma_l(\boldsymbol{r}, E' \to E) P_l(\mu_0)\end{aligned} \tag{6}$$

The scattering moments are determined from the orthogonal property of the Legendre polynomials,

$$\sigma_l(\boldsymbol{r}, E' \to E) = 2\pi \int_{-1}^{1} \sigma_s(\boldsymbol{r}, \mu_0, E' \to E) P_l(\mu_0) d\mu_0 . \tag{7}$$

The expansion in Eq. (6) is usually truncated, retaining only as many terms as is consistent with the level of approximation being applied to the angular flux and with the severity of anisotropy presented in the differential cross sections. This is known as the P_L approximation. For neutron and photon transport, only the first few terms in the series are required to accurately model the scattering process. For electron transport, higher order of expansions are required to adequately model the forward-peak scattering.

Substituting Eq. (6) into Eq. (1), the scattering source term becomes

$$
\begin{aligned}
Q_s(\boldsymbol{r}, \Omega, E) &= \int_0^{\infty}\int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \rightarrow \Omega, E' \rightarrow E)\psi(\boldsymbol{r}, \Omega', E')d\Omega' dE' \\
&= \sum_{l=0}^{L} \frac{2l+1}{4\pi}\int_0^{\infty}\int_{4\pi} \sigma_l(r, E' \rightarrow E)P_l(\mu_0)\psi(\boldsymbol{r}, \Omega', E')d\Omega' dE' \\
&= \sum_{l=0}^{L}\sum_{m=-l}^{l} Y_{lm}(\Omega)\int_0^{\infty}\int_{4\pi} \sigma_l(r, E' \rightarrow E)Y^*_{lm}(\Omega')\psi(\boldsymbol{r}, \Omega', E')d\Omega' dE'
\end{aligned}
\tag{8}
$$

where we have applied the addition theorem of spherical harmonics, and $Y_{lm}(\Omega)$ is the spherical harmonics and $Y^*_{lm}(\Omega')$ is its complex conjugate, as described in Appendix A.

The next step is to divide the energy range of interest, that is, $E_{min} \le E \le E_{max}$, into a finite number, G, of intervals. Each energy interval is called a group which is bounded by the energy values E_{g+1} and E_g. The particles in group g are taken to be those with energies between E_{g+1} and E_g. The group angular flux is defined by

$$
\psi_g(\boldsymbol{r}, \Omega) = \int_{E_{g+1}}^{E_g} \psi(\boldsymbol{r}, \Omega, E)dE. \tag{9}
$$

Furthermore, the integral over the entire energy range is represented by

$$
\int_0^{\infty} dE \approx \int_{E_{min}}^{E_{max}} dE = \sum_{g=1}^{G}\int_{E_{g+1}}^{E_g} dE. \tag{10}
$$

With these definitions, the continuous-energy form of Eq. (1) can be approximated by the multigroup transport equations:

$$
\begin{aligned}
&\Omega \cdot \nabla\psi_g(\boldsymbol{r}, \Omega) + \sigma_g(\boldsymbol{r})\psi_g(\boldsymbol{r}, \Omega) \\
&= \sum_{g'=1}^{G}\sum_{l=0}^{L}\sum_{m=-l}^{l} \sigma_{lg'g}(\boldsymbol{r})Y_{lm}(\Omega)\int_{4\pi} Y^*_{lm}(\Omega')\psi_g(\boldsymbol{r}, \Omega')d\Omega' + Q_g(\boldsymbol{r}, \Omega)
\end{aligned}
\tag{11}
$$

for $g = 1, G$, where $\sigma_g(\boldsymbol{r})$ is the group-averaged total cross section and $\sigma_{lg'g}(\boldsymbol{r})$ is the group-to-group scattering moment. These multigroup parameters have to be evaluated with the detailed energy dependence of the cross section data and the spectral weighting functions to accurately characterize the system under consideration.

The multigroup approximation effectively converts the continuous-energy transport equation to a set of simultaneous equations for the discrete energy groups. In practice one will solve these equations successively as a sequence of one-group problems in which the contributions from other groups are combined with the external source $S_g(\boldsymbol{r}, \Omega)$ to be treated as an inhomogeneous source term:

$$Q_g(\boldsymbol{r}, \Omega) = \sum_{g' \neq g} \sum_{l=0}^{L} \sigma_{lg'g}(\boldsymbol{r}) \sum_{m=-l}^{l} Y_{lm}(\Omega) \int_{4\pi} Y^*_{lm}(\Omega') \psi_{g'}(\boldsymbol{r}, \Omega') d\Omega' + S_g(\boldsymbol{r}, \Omega). \quad (12)$$

Thus, the multigroup transport equation becomes

$$\begin{aligned} &\Omega \cdot \nabla \psi_g(\boldsymbol{r}, \Omega) + \sigma_g(\boldsymbol{r}) \psi_g(\boldsymbol{r}, \Omega) \\ &= \sum_{l=0}^{L} \sigma_{lg}(\boldsymbol{r}) \sum_{m=-l}^{l} Y_{lm}(\Omega) \int_{4\pi} Y^*_{lm}(\Omega') \psi_g(\boldsymbol{r}, \Omega') d\Omega' + Q_g(\boldsymbol{r}, \Omega) \end{aligned} \quad (13)$$

It is noted the second term on the left accounts for removal of particles from collisions while the first term on the right represents contribution from scattering in which particles change their directions of motion but remain in the same energy group. The difference of these two terms is the net removal of particles from an energy group. For this reason, we can define a removal operator

$$\begin{aligned} &R_g \psi_g(\boldsymbol{r}, \Omega) \\ &= \sigma_g(\boldsymbol{r}) \psi_g(\boldsymbol{r}, \Omega) - \sum_{l=0}^{L} \sigma_{lg}(\boldsymbol{r}) \sum_{m=-l}^{l} Y_{lm}(\Omega) \int_{4\pi} Y^*_{lm}(\Omega') \psi_g(\boldsymbol{r}, \Omega') d\Omega' \end{aligned} \quad (14)$$

and express Eq. (13) in a simple form

$$\Omega \cdot \nabla\psi_g(\boldsymbol{r}, \Omega) + R_g\psi_g(\boldsymbol{r}, \Omega) = Q_g(\boldsymbol{r}, \Omega). \tag{15}$$

Conventionally, the scattering terms in Eq. (13) are evaluated in terms of the angular moments. As shown in Appendix A, the spherical harmonics satisfy the following relationship:

$$P_l(\Omega \cdot \Omega') = \frac{4\pi}{2l+1} \sum_{m=0}^{l} \left[Y_{lm}^c(\Omega) Y_{lm}^c(\Omega') + Y_{lm}^s(\Omega) Y_{lm}^s(\Omega') \right], \tag{16}$$

where $Y_{lm}^c(\Omega)$ and $Y_{lm}^s(\Omega)$ are the cosine- and sine-components of the spherical harmonics, respectively. This allows us to rewrite Eq. (13) as

$$\begin{aligned} &\Omega \cdot \nabla\psi_g(\boldsymbol{r}, \Omega) + \sigma_g(\boldsymbol{r})\psi_g(\boldsymbol{r}, \Omega) \\ &= \sum_{l=0}^{L} \sigma_{lg}(\boldsymbol{r}) \sum_{m=0}^{l} \int_{4\pi} \left[Y_{lm}^c(\Omega) Y_{lm}^c(\Omega') + Y_{lm}^s(\Omega) Y_{lm}^s(\Omega') \right] \psi_g(\boldsymbol{r}, \Omega') d\Omega' + Q_g(\boldsymbol{r}, \Omega) \\ &= \sum_{l=0}^{L} \sigma_{lg}(\boldsymbol{r}) \sum_{m=0}^{l} \left[Y_{lm}^c(\Omega) \phi_{glm}^c(r) + Y_{lm}^s(\Omega) \phi_{glm}^s(r) \right] + Q_g(\boldsymbol{r}, \Omega) \end{aligned} \tag{17}$$

where the angular moments are defined by

$$\phi_{glm}^c(r) = \int_{4\pi} Y_{lm}^c(\Omega)\psi_g(\boldsymbol{r}, \Omega)d\Omega \text{ and } \phi_{glm}^s(r) = \int_{4\pi} Y_{lm}^s(\Omega)\psi_g(\boldsymbol{r}, \Omega)d\Omega. \tag{18}$$

The group-to-group scattering source can be evaluated accordingly as

$$\begin{aligned} &Q_g(\boldsymbol{r}, \Omega) \\ &= \sum_{g' \neq g} \sum_{l=0}^{L} \sigma_{lg'g}(\boldsymbol{r}) \sum_{m=0}^{l} \left[Y_{lm}^c(\Omega) \phi_{g'lm}^c(r) + Y_{lm}^s(\Omega) \phi_{g'lm}^s(r) \right] + S_g(\boldsymbol{r}, \Omega) \end{aligned} \tag{19}$$

From this point forward, we will omit the subscript g in the multigroup transport equation (17) with the notion that this equation will be solved group by group. Hence, we will concentrate on the one-group transport equation in the form of

$$T\psi(\boldsymbol{r}, \Omega) = Q(\boldsymbol{r}, \Omega) \tag{20}$$

with

$$T\psi(\boldsymbol{r}, \Omega) = \Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega) + R\psi(\boldsymbol{r}, \Omega) \tag{21}$$

$$\begin{aligned} & R\psi(\boldsymbol{r}, \Omega) \\ & = \sigma(\boldsymbol{r})\psi(\boldsymbol{r}, \Omega) - \sum_{l=0}^{L} \sigma_l(\boldsymbol{r}) \sum_{m=-l}^{l} Y_{lm}(\Omega)\int_{4\pi} Y^*_{lm}(\Omega')\psi(\boldsymbol{r}, \Omega')d\Omega' \\ & = \sigma(\boldsymbol{r})\psi(\boldsymbol{r}, \Omega) - \sum_{l=0}^{L} \sigma_l(\boldsymbol{r}) \sum_{m=0}^{l} \left[Y^c_{lm}(\Omega)\phi^c_{lm}(r) + Y^s_{lm}(\Omega)\phi^s_{lm}(r)\right] \end{aligned} \tag{22}$$

In two-dimensional cartesian geometry, the angular flux is independent of the z-coordinate and has mirror symmetry about the x-y plane. If a direction Ω is represented by a polar angle $\theta(= \cos^{-1}\mu)$ measured from the positive z-axis and an azimuthal angle φ measured from the positive x-axis (see Figure A-1), we can express this symmetry condition as

$$\psi(\boldsymbol{r}, -\mu, \varphi) = \psi(\boldsymbol{r}, \mu, \varphi). \tag{23}$$

Hence, we only need to consider the angular flux over half of the directions, $0 \le \mu \le 1$ and $0 \le \varphi \le 2\pi$. Using the following property of the associated Legendre polynomial

$$P^m_l(-\mu) = (-1)^{l+m}P^m_l(\mu) , \tag{24}$$

it can be shown that those terms with odd $l + m$ vanish from the within-group scattering integral. The values of m in the summation are restricted to even $l + m$:

$$R\psi(\boldsymbol{r},\Omega)$$
$$= \sigma(\boldsymbol{r})\psi(\boldsymbol{r},\Omega) - \sum_{l=0}^{L}\sigma_l(\boldsymbol{r})\sum_{\substack{m=0 \\ \text{even } l+m}}^{l}\left[Y^c_{lm}(\Omega)\phi^c_{lm}(r) + Y^s_{lm}(\Omega)\phi^s_{lm}(r)\right] \tag{25}$$

and the angular moments are evaluated over half of the angular domain

$$\phi^c_{lm}(r) = \int_{2\pi} Y^c_{lm}(\Omega)\psi(\boldsymbol{r},\Omega)d\Omega \text{ and } \phi^s_{lm}(r) = \int_{2\pi} Y^s_{lm}(\Omega)\psi(\boldsymbol{r},\Omega)d\Omega. \tag{26}$$

2.2 Discrete Ordinates Approximation

In this section, we will briefly discuss the classical Discrete Ordinates (S_N) method commonly used to approximate the angular dependence in the multigroup transport equation. In this approach, the angular variable Ω is discretized into a number of directions (angles) and the transport equation is then derived for each direction. The integral over direction, which describes the direction-to-direction transfer, is replaced by a corresponding quadrature integration:

$$\int_{4\pi} f(\Omega)d\Omega = \sum_{n=1}^{N_d} w_n f(\Omega_n) \tag{27}$$

where Ω_n and w_n is the nth pair of direction and weight, respectively. Furthermore, it is assumed that $f(\Omega)$ is constant within an angular bin $\Delta\Omega_n$ about Ω_n. Selection of the value of N, hence the number of directions, depends on the required degree of accuracy. For a truncated cross-section expansion, the number of directions is often chosen so that the angular moments and the scattering source can be evaluated as accurately as possible. In the case of a $S_N P_L$ approximation, the corresponding number of directions (N_d) and angular moments (N_m) are given in Table 1 with conventional choice of even value of N and odd value of L.

Table 1. Number of Discrete Directions (N_d) and Angular Moments (N_m) for the Angular Flux with a Standard S_NP_L Approximation.

Dimensionality	N_d	N_m
1	N	L
2	$\frac{N}{2}(N+2)$	$\frac{1}{2}(L+1)(L+2)$
3	$N(N+2)$	$(L+1)^2$

Using the quadrature formula, the angular moments given in Eq. (18) can be evaluated by

$$\phi^C_{lm}(\boldsymbol{r}) = \sum_{n=1}^{N_d} w_n Y^C_{lm}(\Omega_n)\psi_n(\boldsymbol{r}) \text{ and } \phi^S_{lm}(\boldsymbol{r}) = \sum_{n=1}^{N_d} w_n Y^S_{lm}(\Omega_n)\psi_n(\boldsymbol{r}), \tag{28}$$

where $\psi_n(\boldsymbol{r}) = \psi(\boldsymbol{r}, \Omega_n)$ and is assumed to be constant within an incremental angular range about Ω_n. We can then define a discrete-to-moment matrix which maps the discrete angular flux to the angular moments:

$$\vec{\phi} = [D]\vec{\psi} \tag{29}$$

where

$\vec{\phi}$ = a column vector of size N_m containing the angular moments,

$\vec{\psi}$ = a column vector of size N_d containing the discrete angular flux

$= \left[\psi_1(\boldsymbol{r})\ \psi_2(\boldsymbol{r})\ \ldots\ \psi_{N_d}(\boldsymbol{r})\right]^T$

and

$[D]$ = the discrete-to-moment matrix of size $N_m \times N_d$.

As shown in Appendix B, it is possible to arrange the angular moments in an orderly vector and assign a unique index k to a specified moment. This allows us to define the components in the discrete-to-moment matrix by

$$D_{kn} = w_n Y^c_{lm}(\Omega_n) \text{ or } w_n Y^s_{lm}(\Omega_n) \qquad \text{for } 1 \le k \le N_m \text{ and } 1 \le n \le N_d, \tag{30}$$

where k is determined by a pair of l and m.

The discrete form of the multigroup transport equation can be obtained by integrating Eq. (17) over an incremental range about the direction Ω_n:

$$\begin{aligned} & w_n \Omega_n \cdot \nabla \psi_n(\boldsymbol{r}) + w_n \sigma(\boldsymbol{r}) \psi_n(\boldsymbol{r}) \\ &= w_n \sum_{l=0}^{L} \sigma_l(\boldsymbol{r}) \sum_{m=0}^{l} \left[Y^c_{lm}(\Omega_n) \phi^c_{lm}(r) + Y^s_{lm}(\Omega_n) \phi^s_{lm}(r) \right] + w_n Q_n(\boldsymbol{r}) \\ &= w_n \sum_{l=0}^{L} \sigma_l(\boldsymbol{r}) \sum_{m=0}^{l} \sum_{n'=1}^{N_d} w_{n'} \left[Y^c_{lm}(\Omega_n) Y^c_{lm}(\Omega_{n'}) + Y^s_{lm}(\Omega_n) Y^s_{lm}(\Omega_{n'}) \right] \psi_{n'}(\boldsymbol{r}) + w_n Q_n(\boldsymbol{r}) \end{aligned} \tag{31}$$

for $1 \le n \le N_d$. Combining the last equations for all directions and arranging these results in a matrix form lead to a compact expression for the discrete-ordinates approximation:

$$[\Lambda]\vec{\psi} + [R]\vec{\psi} = [W]\vec{Q}, \tag{32}$$

where $\vec{\psi}$ and $\vec{Q}$ are vectors containing the angular flux and the external source, respectively. The matrix $[\Lambda]$ is a diagonal matrix consisting of the streaming operator along the discrete directions

$$[\Lambda] = diag\left[\Lambda_1 \Lambda_2 \ldots \Lambda_{N_d}\right], \tag{33}$$

where $\Lambda_n f = w_n \Omega_n \cdot \nabla f$. The removal matrix $[R]$ is a square matrix and has the form of:

$$[R] = \sigma[W] - [W][M][\Sigma][D] \tag{34}$$

where $\sigma = \sigma(r)$,

$[W]$ = a $N_d \times N_d$ diagonal matrix = $diag\left[w_1\ w_2\ \ldots\ w_{N_d}\right]$,

$[\Sigma]$ = a $N_m \times N_m$ diagonal matrix = $diag\left[\sigma_0(\boldsymbol{r})\ \sigma_1(\boldsymbol{r})\ \ldots\ \sigma_L(\boldsymbol{r})\right]$,

$[M]$ = the moment-to-discrete matrix of size $N_d \times N_m$,

with $M_{nk} = Y^c_{lm}(\Omega_n)$ or $Y^s_{lm}(\Omega_n)$ for $1 \le k \le N_m$ and $1 \le n \le N_d$, and $[D]$ is the discrete-to-moment matrix as defined in Eq. (30).

The matrix $[R]$ is simply a discrete representation of the operator $\boldsymbol{R}$ given in Eq. (22). The scattering matrix $[S] = [M][\Sigma][D]$ comprises of three components and represents the discrete form of the within-group scattering integral in Eq. (17). In other words, it defines a mapping between the discrete angular flux and the discrete scattering source. It is interesting to note that the matrices $[W][S]$ and $[R]$ are *symmetric* for any standard quadrature sets. These result directly from the assumption that the scattering kernel depends only on the direction cosine between two scattering angles. In addition, the discrete-to-moment and moment-to-discrete matrices satisfy the relationship

$$[D]^T = [W][M]. \tag{35}$$

Furthermore, the matrix $[\Sigma]$ depends on the indexing scheme in which the angular moments are ordered. For example, for a three-dimensional P_3 approximation, the moment vector is arranged as

$$\left[\phi^c_{00}\phi^c_{10}\phi^c_{11}\phi^s_{11}\phi^c_{20}\phi^c_{21}\phi^c_{22}\phi^s_{21}\phi^s_{22}\phi^c_{30}\phi^c_{31}\phi^c_{32}\phi^c_{33}\phi^s_{31}\phi^s_{32}\phi^s_{33}\right]$$

and the corresponding scattering cross-section matrix is given by

$$[\Sigma] = diag\left[\sigma_0\sigma_1\sigma_1\sigma_1\sigma_2\sigma_2\sigma_2\sigma_2\sigma_2\sigma_3\sigma_3\sigma_3\sigma_3\sigma_3\sigma_3\sigma_3\right].$$

2.3 Galerkin Quadrature Method

In the last section, we outlined the procedure to construct the scattering matrix in terms of the moment-to-discrete and discrete-to-moment matrices with the standard S_N method in which a set of directions and weights is specified. An alternative approach was proposed by Morel[5] to compose the scattering matrix based the Galerkin finite-element method, while the rest of transport equation is treated by the standard S_N method. In this approach, the angular flux is first represented by a set of interpolation functions (spherical harmonics). The matrices $[M]$ and $[D]$ are then obtained by requiring that the discrete scattering source from the interpolatory representation provides the same angular moments as the scattering source calculated with the interpolatory representation of the angular flux. This requirement translates into the relationship:

$$[D] = [M]^{-1}. \tag{36}$$

and implies that one need only to invert the moment-to-discrete matrix to obtain the discrete-to-moment matrix.

For multi-dimensional geometries, the number of directions in the standard S_N quadrature set is greater than the number of moments to expand the P_{N-1} scattering source. Thus, it is necessary to incorporate higher-order angular moments (with $L < l$) to make $[M]$ square and invertible. A suitable recipe suggested by Morel is summarized in Table 2 where the components of the matrix $[M]$ and the ranges of l and m are given for two- and three-dimensional geometries.

The scattering matrix produced by the Galerkin quadrature method may not be symmetric but this method offers two distinctive advantages over the standard S_N quadrature. First, a delta-function scattering is treated exactly with the Galerkin scattering matrix due to the requirement of Eq. (36). Conversely, the standard quadrature set often produces an unstable scattering matrix. Second, the extra angular moments needed to make $[M]$ a square matrix also make it possible to use the higher-order cross-section moments (see Table 2) moments in computing the scattering source. This may lead to a more accurate solution if the angular flux and cross section are highly anisotropic.

Table 2. Subsets of Spherical Harmonics Used to Construct the Moment-to-Discrete Matrix for the Angular Flux.

Two-Dimensional Geometry			
$Y^c_{lm}(\Omega)$		$Y^s_{lm}(\Omega)$	
l	m	l	m
$[0, N-1]$	$[0, l]$ even $l+m$	$[1, N-1]$	$[1, l]$ even $l+m$
----	----	N	$[1, l]$ even $l+m$
Three-Dimensional Geometry			
$Y^c_{lm}(\Omega)$		$Y^s_{lm}(\Omega)$	
l	m	l	m
$[0, N-1]$	$[0, l]$	$[1, N-1]$	$[1, l]$
N	$[1, N-1]$ odd m	N	$[1, N]$
----	----	$N+1$	$[2, N]$ even m

1. The symbol [a, b] indicates the index ranges from a to b with the footnote indicating the restricted values.
2. The shaded entries are the additional spherical harmonics to make the moment-to-discrete matrix invertible.

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3. Self-Adjoint Angular Flux Equation

The self-adjoint angular flux (SAAF) equation has recently been brought into attention as a basis for numerical transport methods.[4] In this section, we will first derive the SAAF equation by manipulating the Boltzmann transport equation and formally inverting the removal operator. The result is a differential-integral equation for the angular flux but containing a second-order differential operator in space. We then apply the discrete ordinates approximation and structure the discrete equations into a matrix form.

3.1 Derivation

The SAAF equation can be derived symbolically in two steps. First, we solve $\psi(\boldsymbol{r}, \Omega)$ from Eq. (20)

$$\psi(\boldsymbol{r}, \Omega) = R^{-1}\Big[Q(\boldsymbol{r}, \Omega) - \Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega)\Big] \tag{37}$$

and then substitute the result into the streaming operator in Eq. (20):

$$-\Omega \cdot \nabla\Big[R^{-1}\Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega)\Big] + R\psi(\boldsymbol{r}, \Omega) = Q(\boldsymbol{r}, \Omega) - \Omega \cdot \nabla\Big[R^{-1}Q(\boldsymbol{r}, \Omega)\Big]. \tag{38}$$

As shown in Appendix C, the second-order transport operator as defined by

$$T_S\,\psi(\boldsymbol{r}, \Omega) = -\Omega \cdot \nabla\Big[R^{-1}\Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega)\Big] + R\psi(\boldsymbol{r}, \Omega), \tag{39}$$

along with the operators R and R^{-1} are symmetric (self-adjoint) and positive definite (SPD). This allows us to apply the Galerkin finite element method to treat the spatial dependence and obtain the same system of equations as in the Rayleigh-Ritz method which exhibits the SPD properties.

We still need to derive a formal expression of R^{-1}. From Eqs. (20-22), we have

$$
\begin{aligned}
&\sigma(\boldsymbol{r})\psi(\boldsymbol{r},\Omega) - \sum_{l=0}^{L}\sigma_l(\boldsymbol{r})\sum_{m=-l}^{l}Y_{lm}(\Omega)\int_{4\pi}Y_{lm}^*(\Omega')\psi(\boldsymbol{r},\Omega')d\Omega' \\
&= Q(\boldsymbol{r},\Omega) - \Omega\cdot\nabla\psi(\boldsymbol{r},\Omega)
\end{aligned}
\tag{40}
$$

Multiplying the last equation by $Y_{lm}^*(\Omega)$ and integrating the result over 4π leads to

$$
\begin{aligned}
&\sigma(\boldsymbol{r})\int_{4\pi}Y_{lm}^*(\Omega)\psi(\boldsymbol{r},\Omega)d\Omega - \sigma_l(\boldsymbol{r})\int_{4\pi}Y_{lm}^*(\Omega)\psi(\boldsymbol{r},\Omega)d\Omega \\
&= \int_{4\pi}Y_{lm}^*(\Omega)\Big[Q(\boldsymbol{r},\Omega) - \Omega\cdot\nabla\psi(\boldsymbol{r},\Omega)\Big]d\Omega
\end{aligned}
$$

and

$$
\int_{4\pi}Y_{lm}^*(\Omega)\psi(\boldsymbol{r},\Omega)d\Omega = \Big[\sigma(\boldsymbol{r}) - \sigma_l(\boldsymbol{r})\Big]^{-1}\int_{4\pi}Y_{lm}^*(\Omega)\Big[Q(\boldsymbol{r},\Omega) - \Omega\cdot\nabla\psi(\boldsymbol{r},\Omega)\Big]d\Omega .
$$

Replacing the integral term in Eq. (40) by the last expression and solving for $\psi(\boldsymbol{r},\Omega)$ yield

$$
\begin{aligned}
\psi(\boldsymbol{r},\Omega) &= \frac{1}{\sigma(\boldsymbol{r})}\Big[Q(\boldsymbol{r},\Omega) - \Omega\cdot\nabla\psi(\boldsymbol{r},\Omega)\Big] \\
&+ \frac{1}{\sigma(\boldsymbol{r})}\sum_{l=0}^{L}\frac{\sigma_l(\boldsymbol{r})}{\sigma(\boldsymbol{r})-\sigma_l(\boldsymbol{r})}\sum_{m=-l}^{l}Y_{lm}(\Omega)\int_{4\pi}Y_{lm}^*(\Omega')\Big[Q(\boldsymbol{r},\Omega') - \Omega'\cdot\nabla\psi(\boldsymbol{r},\Omega')\Big]d\Omega'
\end{aligned}
\tag{41}
$$

Comparing Eqs. (37) and (41), we can identify the functional form of the inverse removal operator:

$$
\begin{aligned}
&R^{-1}f(\boldsymbol{r},\Omega) \\
&= \frac{1}{\sigma(\boldsymbol{r})}\left[f(\boldsymbol{r},\Omega) + \sum_{l=0}^{L}\frac{\sigma_l(\boldsymbol{r})}{\sigma(\boldsymbol{r})-\sigma_l(\boldsymbol{r})}\sum_{m=-l}^{l}Y_{lm}(\Omega)\int_{4\pi}Y_{lm}^*(\Omega')f(\boldsymbol{r},\Omega')d\Omega'\right]
\end{aligned}
\tag{42}
$$

There are several characteristics of the SAAF equation worth noting. First, the unknown in the SAAF equation is still the angular flux over the entire angular domain. The vacuum and reflective boundary conditions for the incoming directions of the first-order transport equation can be applied with no alteration. However, as shown in Eq. (38), the SAAF equation contains second-order spatial derivatives and thus requires additional boundary conditions to properly formulate the problem. One stipulation is to require the angular flux in the outgoing directions to satisfy the first-order transport equation at the boundary:

$$\Omega \cdot \nabla\psi(\boldsymbol{r}_b, \Omega) + R\psi(\boldsymbol{r}_b, \Omega) = Q(\boldsymbol{r}_b, \Omega) \qquad \text{for } \Omega \cdot \boldsymbol{n}_b > 0 \tag{43}$$

Second, the previous derivation of the SAAF equation breaks down when applying it to a void region due to the presence of the total cross section in the denominator of the inverse removal operator. One possible remedy[4] is to start with the SAAF equation for a purely absorbing medium with uniform cross section:

$$-\Omega \cdot \nabla\left[\frac{1}{\sigma_a}\Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega)\right] + \sigma_a\psi(\boldsymbol{r}, \Omega) = 0 .$$

Multiplying the last expression by σ_a and taking the limit as $\sigma_a \to 0$, we obtain the SAAF equation for a void region:

$$-\Omega \cdot \nabla\left[\Omega \cdot \nabla\psi(\boldsymbol{r}, \Omega)\right] = 0 .$$

3.2 Discrete Ordinates Approximation

The discrete SAAF equation can be obtained by integrating Eq. (38) over an incremental range in the directional space and collecting terms:

$$-[\Lambda][\tilde{R}][\Lambda]\vec{\psi} + [R]\vec{\psi} = [W]\vec{Q} - [\Lambda][\tilde{R}][W]\vec{Q} \tag{44}$$

where $\vec{\psi}$ and $\vec{Q}$ are vectors containing the discrete angular flux and the extraneous source, respectively. The streaming matrix $[\Lambda]$, the removal matrix $[R]$ and the diagonal matrix $[W]$ are previously defined in Section 2.2. The matrix $[\tilde{R}]$ has the same form as the removal matrix and is defined as

$$[\tilde{R}] = \frac{1}{\sigma}\left[[W]^{-1} + [M][\tilde{\Sigma}][D][W]^{-1}\right] \tag{45}$$

where $[M]$ and $[D]$ are the moment-to-discrete and discrete-to-moment matrices. and

$$\begin{aligned}[\tilde{\Sigma}] &= \text{a } N_m \times N_m \text{ diagonal matrix} \\ &= diag\left[\frac{\sigma_0(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_0(\boldsymbol{r})}\ \frac{\sigma_1(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_1(\boldsymbol{r})}\ \cdots\ \frac{\sigma_L(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_L(\boldsymbol{r})}\right]\end{aligned}$$

We can make two observations about the matrix $[\tilde{R}]$. First, like $[R]$, the matrix $[\tilde{R}]$ is symmetric for any standard quadrature sets but asymmetric for the Galerkin quadrature method. It is not obvious that there is an effortless way to symmetrize these matrices $[R]$ and $[\tilde{R}]$ for the latter case.

Second, it is noted that the operators $\boldsymbol{R}$ and $\boldsymbol{R}^{-1}$ given in Eqs. (22) and (42) satisfy the following condition

$$\psi(\boldsymbol{r}, \Omega) = \boldsymbol{R}^{-1}\boldsymbol{R}\psi(\boldsymbol{r}, \Omega), \tag{46}$$

which can be easily verified by applying the following orthonormal properties of the spherical harmonics:

$$\int_{4\pi} Y^c_{lm}(\Omega) Y^c_{l'm'}(\Omega) d\Omega = \delta_{ll'}\delta_{mm'}, \tag{47}$$

$$\int_{4\pi} Y^s_{lm}(\Omega) Y^s_{l'm'}(\Omega) d\Omega = (1 - \delta_{m0})\delta_{ll'}\delta_{mm'}. \tag{48}$$

On the contrary, the matrix $[\tilde{R}]$ is the exact inverse of $[R]$ *if and only if* the product of $[M]$ and $[D]$ is an identity matrix. This condition may not be satisfied by the matrices $[M]$ and $[D]$ generated from a standard quadrature set since the standard quadrature set does not guarantee to integrate Eqs. (47-48) exactly for any given orders of l and m. However, this condition is guaranteed by the Galerkin scattering matrices as stated in Section 2.3.

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4. Even-Odd Parity Equations

The even- and odd-parity (EOP) equations have been employed for a wide variety of numerical transport codes,[2] especially in the applications of the continuous finite element methods in nuclear reactor analysis. In the following sections, we will present the derivation of the EOP equations by following a standard procedure. The results are two differential-integral equations similar to the SAAF equation, but are for the even- and odd-components of the angular flux. We then apply the discrete ordinates approximation and package the discrete equations into a matrix form.

4.1 Derivation

We start with the one-group transport equation expressed in the form of

$$\begin{aligned}&\Omega\cdot\nabla\psi(\boldsymbol{r},\Omega)+\sigma(\boldsymbol{r})\psi(\boldsymbol{r},\Omega)\\&=\sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}P_l(\Omega\cdot\Omega')\psi(\boldsymbol{r},\Omega')d\Omega'+Q(\boldsymbol{r},\Omega)\end{aligned} \tag{49}$$

and decompose the angular flux into the even-(symmetric) and odd-parity (asymmetric) components as

$$\psi(\boldsymbol{r},\Omega)=\psi^e(\boldsymbol{r},\Omega)+\psi^o(\boldsymbol{r},\Omega), \tag{50}$$

where the even-parity angular flux is defined by

$$\psi^e(\boldsymbol{r},\Omega)=\frac{1}{2}\left[\psi(\boldsymbol{r},\Omega)+\psi(\boldsymbol{r},-\Omega)\right], \tag{51}$$

and the odd-parity angular flux is defined by

$$\psi^o(\boldsymbol{r},\Omega) = \frac{1}{2}\Big[\psi(\boldsymbol{r},\Omega) - \psi(\boldsymbol{r},-\Omega)\Big]. \tag{52}$$

Since Eq. (49) holds for $-\Omega$, we have

$$\begin{aligned} &-\Omega\cdot\nabla\psi(\boldsymbol{r},-\Omega) + \sigma(\boldsymbol{r})\psi(\boldsymbol{r},-\Omega) \\ &= \sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}P_l(-\Omega\cdot\Omega')\psi(\boldsymbol{r},\Omega')d\Omega' + Q(\boldsymbol{r},-\Omega) \end{aligned} \tag{53}$$

Adding Eqs. (49) and (53) and utilizing Eqs. (51) and (52) lead to

$$\begin{aligned} &\Omega\cdot\nabla\psi^o(\boldsymbol{r},\Omega) + \sigma(\boldsymbol{r})\psi^e(\boldsymbol{r},\Omega) \\ &= \frac{1}{2}\sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}\Big[P_l(\Omega\cdot\Omega') + P_l(-\Omega\cdot\Omega')\Big]\psi(\boldsymbol{r},\Omega')d\Omega' + Q^e(\boldsymbol{r},\Omega) \\ &= \sum_{\text{even } l}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}P_l(\Omega\cdot\Omega')\psi^e(\boldsymbol{r},\Omega')d\Omega' + Q^e(\boldsymbol{r},\Omega) \end{aligned} \tag{54}$$

where

$$Q^e(\boldsymbol{r},\Omega) = \frac{1}{2}\Big[Q(\boldsymbol{r},\Omega) + Q(\boldsymbol{r},-\Omega)\Big]$$

It is noted that the terms with odd values of l in the summation vanish as results of $P_l(-\Omega\cdot\Omega') = (-1)^l P_l(\Omega\cdot\Omega')$.

Subtracting Eq. (53) from (49) yields

$$\begin{aligned} &\Omega\cdot\nabla\psi^e(\boldsymbol{r},\Omega) + \sigma(\boldsymbol{r})\psi^o(\boldsymbol{r},\Omega) \\ &= \frac{1}{2}\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}\Big[P_l(\Omega\cdot\Omega') - P_l(-\Omega\cdot\Omega')\Big]\psi(\boldsymbol{r},\Omega')d\Omega' + Q^o(\boldsymbol{r},\Omega) \\ &= \sum_{\text{odd } l}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}P_l(\Omega\cdot\Omega')\psi^o(\boldsymbol{r},\Omega')d\Omega' + Q^o(\boldsymbol{r},\Omega) \end{aligned} \tag{55}$$

where

$$Q^o(\boldsymbol{r},\Omega) = \frac{1}{2}\Big[Q(\boldsymbol{r},\Omega) - Q(\boldsymbol{r},-\Omega)\Big].$$

Analogous to the Boltzmann transport equation, we can define the removal operators for the even- and odd-parity angular flux:

$$\begin{aligned}
&R_e\psi^e(\boldsymbol{r},\Omega)\\
&= \sigma(\boldsymbol{r})\psi^e(\boldsymbol{r},\Omega) - \sum_{\text{even } l}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}P_l(\Omega\cdot\Omega')\psi^e(\boldsymbol{r},\Omega')d\Omega'\\
&= \sigma(\boldsymbol{r})\psi^e(\boldsymbol{r},\Omega) - \sum_{\text{even } l}\sigma_l(\boldsymbol{r})\sum_{m=-l}^{l}Y_{lm}(\Omega)\int_{4\pi}Y^*_{lm}(\Omega')\psi^e(\boldsymbol{r},\Omega')d\Omega'\\
&= \sigma(\boldsymbol{r})\psi^e(\boldsymbol{r},\Omega) - \sum_{\text{even } l}\sigma_l(\boldsymbol{r})\sum_{m=0}^{l}\left[Y^c_{lm}(\Omega)\phi^{ec}_{lm}(r) + Y^s_{lm}(\Omega)\phi^{es}_{lm}(r)\right]
\end{aligned} \tag{56}$$

$$\begin{aligned}
&R_o\psi^o(\boldsymbol{r},\Omega)\\
&= \sigma(\boldsymbol{r})\psi^o(\boldsymbol{r},\Omega) - \sum_{\text{odd } l}\frac{2l+1}{4\pi}\sigma_l(\boldsymbol{r})\int_{4\pi}P_l(\Omega\cdot\Omega')\psi^o(\boldsymbol{r},\Omega')d\Omega'\\
&= \sigma(\boldsymbol{r})\psi^o(\boldsymbol{r},\Omega) - \sum_{\text{odd } l}\sigma_l(\boldsymbol{r})\sum_{m=-l}^{l}Y_{lm}(\Omega)\int_{4\pi}Y^*_{lm}(\Omega')\psi^o(\boldsymbol{r},\Omega')d\Omega'\\
&= \sigma(\boldsymbol{r})\psi^o(\boldsymbol{r},\Omega) - \sum_{\text{odd } l}\sigma_l(\boldsymbol{r})\sum_{m=1}^{l}\left[Y^c_{lm}(\Omega)\phi^{oc}_{lm}(r) + Y^s_{lm}(\Omega)\phi^{os}_{lm}(r)\right]
\end{aligned} \tag{57}$$

The angular moments for the parity flux are

$$\phi^{\alpha\beta}_{lm}(r) = \int_{4\pi}Y^{\beta}_{lm}(\Omega)\psi^{\alpha}(\boldsymbol{r},\Omega)d\Omega, \tag{58}$$

where the symbol $\alpha \in \{e, o\}$ is used to distinguish the even- or odd-parity angular flux and the symbol $\beta \in \{c, s\}$ is used to denote the cosine- or sine-moment. With the removal operators defined, we can rewrite Eqs. (54) and (55) as

$$\Omega\cdot\nabla\psi^o(\boldsymbol{r},\Omega) + R_e\psi^e(\boldsymbol{r},\Omega) = Q^e(\boldsymbol{r},\Omega), \tag{59}$$

$$\Omega\cdot\nabla\psi^e(\boldsymbol{r},\Omega) + R_o\psi^o(\boldsymbol{r},\Omega) = Q^o(\boldsymbol{r},\Omega). \tag{60}$$

Solving $\psi^o(\boldsymbol{r}, \Omega)$ from Eq. (60)

$$\psi^o(\boldsymbol{r}, \Omega) = R_o^{-1}\left[Q^o(\boldsymbol{r}, \Omega) - \Omega \cdot \nabla\psi^e(\boldsymbol{r}, \Omega)\right] \tag{61}$$

and substituting the result into the streaming operator in Eq. (59), we obtain the even-parity equation:

$$-\Omega \cdot \nabla\left[R_o^{-1}\Omega \cdot \nabla\psi^e(\boldsymbol{r}, \Omega)\right] + R_e\psi^e(\boldsymbol{r}, \Omega) = Q^e(\boldsymbol{r}, \Omega) - \Omega \cdot \nabla\left[R_o^{-1}Q^o(\boldsymbol{r}, \Omega)\right]. \tag{62}$$

One can repeat this process and obtain the odd-parity equation

$$-\Omega \cdot \nabla\left[R_e^{-1}\Omega \cdot \nabla\psi^e(\boldsymbol{r}, \Omega)\right] + R_o\psi^o(\boldsymbol{r}, \Omega) = Q^o(\boldsymbol{r}, \Omega) - \Omega \cdot \nabla\left[R_e^{-1}Q^e(\boldsymbol{r}, \Omega)\right]. \tag{63}$$

The EOP equations, Eqs. (62-63), have the same basic form as the SAAF equation. Consequently, we can derive the functional form of the inverse operators by following the same procedure used in deriving the SAAF equation.

$$\begin{aligned} &R_e^{-1}f(\boldsymbol{r}, \Omega) \\ &= \frac{1}{\sigma(\boldsymbol{r})}\left[f(\boldsymbol{r}, \Omega) + \sum_{\text{even } l}\frac{\sigma_l(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_l(\boldsymbol{r})}\sum_{m=-l}^{l} Y_{lm}(\Omega)\int_{4\pi} Y_{lm}^*(\Omega')f(\boldsymbol{r}, \Omega')d\Omega'\right] \end{aligned} \tag{64}$$

$$\begin{aligned} &R_o^{-1}f(\boldsymbol{r}, \Omega) \\ &= \frac{1}{\sigma(\boldsymbol{r})}\left[f(\boldsymbol{r}, \Omega) + \sum_{\text{odd } l}\frac{\sigma_l(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_l(\boldsymbol{r})}\sum_{m=-l}^{l} Y_{lm}(\Omega)\int_{4\pi} Y_{lm}^*(\Omega')f(\boldsymbol{r}, \Omega')d\Omega'\right] \end{aligned} \tag{65}$$

Finally, the transport operators for the even- and odd-parity angular flux are defined as:

$$T_e \psi^e(\boldsymbol{r}, \Omega) = -\Omega \cdot \nabla\left[R_o^{-1}\Omega \cdot \nabla\psi^e(\boldsymbol{r}, \Omega)\right] + R_e\psi^e(\boldsymbol{r}, \Omega), \tag{66}$$

$$T_o \psi^o(\boldsymbol{r}, \Omega) = -\Omega \cdot \nabla\left[R_e^{-1}\Omega \cdot \nabla\psi^o(\boldsymbol{r}, \Omega)\right] + R_o\psi^o(\boldsymbol{r}, \Omega). \tag{67}$$

As shown in Reference 3, these operators are symmetric and positive definite. Proofs of these properties are similar to those for the SAAF equation and will not be duplicated here. We also stress the similarity between the EOP equations: they have the same structure except that the limits on summation are different. For this reason, we will express the EOP equations in a common form in the following sections except for the instance where we have to distinguish the even- or odd-parity angular flux.

The corresponding vacuum boundary conditions for the even- and odd-parity flux can be deduced from that for the Boltzmann transport equation. Since the EOP equations are second-order in space, both the incoming and outgoing parity flux are specified to provide proper number of conditions. Consider the boundary conditions where the incoming angular flux are specified:

$$\psi(\boldsymbol{r}_b, \Omega) = \psi_b(\Omega) \qquad \text{for } \Omega \cdot \boldsymbol{n}_b < 0$$

where $\boldsymbol{r}_b$ and $\boldsymbol{n}_b$ are the position vector and outward normal on the external boundary, respectively. Following the decomposition given in Eq. (50), the condition on the incoming flux can be expressed as

$$\psi(\boldsymbol{r}_b, \Omega) = \psi^e(\boldsymbol{r}_b, \Omega) + \psi^o(\boldsymbol{r}_b, \Omega) = \psi_b(\Omega) \qquad \text{for } \Omega \cdot \boldsymbol{n}_b < 0, \tag{68}$$

and it also holds for $-\Omega$

$$\psi(\boldsymbol{r}_b, -\Omega) = \psi^e(\boldsymbol{r}_b, \Omega) - \psi^o(\boldsymbol{r}_b, \Omega) = \psi_b(-\Omega) \qquad \text{for } \Omega \cdot \boldsymbol{n}_b > 0. \tag{69}$$

Utilizing the result in Eq. (61) to eliminate the odd-parity flux from the last two equations, we have the boundary conditions for the even-parity flux

$$-R_o^{-1}\Omega\cdot\nabla\psi^e(\boldsymbol{r}_b,\Omega)+\psi^e(\boldsymbol{r}_b,\Omega) = \psi_b(\Omega)-R_o^{-1}Q^o(\boldsymbol{r}_b,\Omega) \qquad \text{for } \Omega\cdot\boldsymbol{n}_b<0, \quad (70)$$

$$R_o^{-1}\Omega\cdot\nabla\psi^+(\boldsymbol{r}_b,\Omega)+\psi^e(\boldsymbol{r}_b,\Omega) = \psi_b(-\Omega)+R_o^{-1}Q^o(\boldsymbol{r}_b,\Omega) \qquad \text{for } \Omega\cdot\boldsymbol{n}_b>0. \quad (71)$$

Similarly, the boundary conditions for the odd-parity flux are

$$-R_e^{-1}\Omega\cdot\nabla\psi^o(\boldsymbol{r}_b,\Omega)+\psi^o(\boldsymbol{r}_b,\Omega) = \psi_b(\Omega)-R_e^{-1}Q^e(\boldsymbol{r}_b,\Omega) \qquad \text{for } \Omega\cdot\boldsymbol{n}_b<0, \quad (72)$$

$$R_e^{-1}\Omega\cdot\nabla\psi^o(\boldsymbol{r}_b,\Omega)+\psi^o(\boldsymbol{r}_b,\Omega) = -\psi_b(-\Omega)+R_e^{-1}Q^e(\boldsymbol{r}_b,\Omega) \qquad \text{for } \Omega\cdot\boldsymbol{n}_b>0. \quad (73)$$

4.2 Symmetry Conditions

The even- and odd-parity flux defined in Eqs. (51) and (52) are symmetric and asymmetric in Ω, respectively. These conditions allow us to model the angular flux only over half of the angular domain. If a direction Ω is represented by a polar angle $\theta(=\cos^{-1}\mu)$ measured from the positive z-axis and an azimuthal angle φ measured from the positive x-axis, we can express these conditions as

$$\psi^e(\boldsymbol{r},-\Omega) = \psi^e(\boldsymbol{r},\Omega) \Rightarrow \psi^e(\boldsymbol{r},-\mu,\pi+\varphi) = \psi^e(\boldsymbol{r},\mu,\varphi)\ , \quad (74)$$

$$\psi^o(\boldsymbol{r},-\Omega) = -\psi^o(\boldsymbol{r},\Omega) \Rightarrow \psi^o(\boldsymbol{r},-\mu,\pi+\varphi) = -\psi^o(\boldsymbol{r},\mu,\varphi)\ , \quad (75)$$

for $-1\le\mu\le1$ and $0\le\varphi\le\pi$. Furthermore, the spherical harmonics satisfy the following relationships,

$$Y_{lm}^c(\mu,\varphi)+(-1)^l Y_{lm}^c(-\mu,\pi+\varphi) = 2Y_{lm}^c(\mu,\varphi) \quad (76)$$

$$Y^s_{lm}(\mu, \varphi) + (-1)^l Y^s_{lm}(-\mu, \pi + \varphi) = 2Y^s_{lm}(\mu, \varphi) \tag{77}$$

since

$$P^m_l(-\mu) = (-1)^{l+m} P^m_l(\mu)$$

$$\cos m(\pi + \varphi) = (-1)^m \cos m\varphi$$

$$\sin m(\pi + \varphi) = (-1)^m \sin m\varphi$$

Using these identities, we can reduce the range of the integration from 4π to 2π in all the integrals over Ω. Consequently, the angular moments become

$$\phi^{\alpha\beta}_{lm}(r) = \int_{2\pi} Y^{\beta}_{lm}(\Omega)\psi^{\alpha}(r, \Omega)d\Omega, \tag{78}$$

For two-dimensional cartesian geometry, the parity flux have mirror symmetry about the x-y plane. That is, the parity flux are symmetric in μ. We have two additional conditions on the even- and odd-parity flux

$$\psi^e(\boldsymbol{r}, -\mu, \varphi) = \psi^e(\boldsymbol{r}, \mu, \varphi), \tag{79}$$

$$\psi^o(\boldsymbol{r}, -\mu, \varphi) = \psi^o(\boldsymbol{r}, \mu, \varphi), \tag{80}$$

for $0 \le \mu \le 1$. The removal operators defined in Eqs. (56) and (57) become

$$\begin{aligned} &R_e\psi^e(\boldsymbol{r}, \Omega) \\ &= \sigma(\boldsymbol{r})\psi^e(\boldsymbol{r}, \Omega) - \sum_{\text{even } l} \sigma_l(\boldsymbol{r}) \sum_{\substack{m=0 \\ \text{even m}}}^{l} \left[Y^c_{lm}(\Omega)\phi^{ec}_{lm}(r) + Y^s_{lm}(\Omega)\phi^{es}_{lm}(r)\right] \end{aligned} \tag{81}$$

$$\begin{aligned} &R_o\psi^o(\boldsymbol{r}, \Omega) \\ &= \sigma(\boldsymbol{r})\psi^o(\boldsymbol{r}, \Omega) - \sum_{\text{odd } l} \sigma_l(\boldsymbol{r}) \sum_{\substack{m=1 \\ \text{odd m}}}^{l} \left[Y^c_{lm}(\Omega)\phi^{oc}_{lm}(r) + Y^s_{lm}(\Omega)\phi^{os}_{lm}(r)\right] \end{aligned} \tag{82}$$

with

$$\phi_{lm}^{\alpha\beta}(r) = \int_{\pi} Y_{lm}^{\beta}(\Omega)\psi^{\alpha}(r, \Omega)d\Omega, \tag{83}$$

and the limits of the summation are restricted to even $l + m$.

4.3 Discrete Ordinates Approximation

As stated in the last section, we only need to consider the parity flux over half of the angular range due to the symmetry conditions. Hence, when applying the discrete ordinates method, the number of discrete directions employed in the EOP equations is *half* of that for the angular flux. In the case of a standard $S_N P_L$ approximation, the corresponding number of directions (N_d) and angular moments (N_m^e and N_m^o) are given in Table 3 where it is assumed that N is even and L is odd. It is also noted that there are $\frac{1}{2}(L+1)$ less angular moments for the odd-parity flux since all moments with $m = 0$ vanish due to the symmetry conditions.

Table 3. Number of Discrete Directions and Angular Moments for the EOP Equations with a Standard $S_N P_L$ Approximation.

Dimensionality	N_d	N_m^e	N_m^o
1	$\frac{1}{2}N$	L	L
2	$\frac{1}{4}N(N+2)$	$\frac{1}{4}(L+1)(L+3)$	$\frac{1}{4}(L+1)^2$
3	$\frac{1}{2}N(N+2)$	$\frac{1}{2}(L+1)(L+2)$	$\frac{1}{2}L(L+1)$

Using the quadrature formula, the angular moments given in Eq. (83) can be evaluated by

$$\phi_{lm}^{\alpha\beta}(\boldsymbol{r}) = \sum_{n=1}^{N_d} w_n Y_{lm}^{\beta}(\Omega_n)\psi_n^{\alpha}(\boldsymbol{r}) \tag{84}$$

where $\psi_n^{\alpha}(\boldsymbol{r}) = \psi^{\alpha}(\boldsymbol{r}, \Omega_n)$ is assumed to be constant within an incremental range about Ω_n. Again, the letters, $\alpha \in \{e, o\}$ and $\beta \in \{c, s\}$, are used to denote the angular moments of the parity flux. Similar to the angular flux, we can then define two discrete-to-moment matrices which map the discrete parity flux to the angular moments:

$$\vec{\phi}_{\alpha} = [D_{\alpha}]\vec{\psi}_{\alpha} \tag{85}$$

where

$\vec{\phi}_{\alpha}$ = column vectors containing the even- or odd- parity angular moments,

and

$\vec{\psi}_{\alpha}$ = column vectors containing the discrete even- or odd-parity flux.

For a standard quadrature set, the components in the discrete-to-moment matrices have the form of

$$D_{kn}^{\alpha} = w_n Y_{lm}^{c}(\Omega_n) \text{ or } w_n Y_{lm}^{s}(\Omega_n) \qquad \text{for } 1 \le k \le N_m^a \text{ and } 1 \le n \le N_d, \tag{86}$$

where k is a function of l and m, and its value depends on how $\vec{\phi}_a$ is organized. For the Galerkin quadrature method, $[D_{\alpha}]$ is the inverse of the moment-to-discrete matrix $[M_{\alpha}]$, which will be defined next.

The discrete EOP equations can be arranged in the following form:

$$-[\Lambda][\tilde{R}_o][\Lambda]\vec{\psi}_e + [R_e]\vec{\psi}_e = [W]\vec{Q}_e - [\Lambda][\tilde{R}_o][W]\vec{Q}_o, \tag{87}$$

$$-[\Lambda][\tilde{R}_e][\Lambda]\vec{\psi}_o + [R_o]\vec{\psi}_o = [W]\vec{Q}_o - [\Lambda][\tilde{R}_e][W]\vec{Q}_e, \tag{88}$$

where $\vec{Q}_e$ and $\vec{Q}_o$ are vectors containing the discrete extraneous source for the even- and odd-parity flux, respectively. The streaming matrix $[\Lambda]$ is previously defined in Section 2.2. The matrices $[R_\alpha]$ and $[\tilde{R}_\alpha]$ are defined as

$$[R_\alpha] = \sigma[W] - [W][M_\alpha][\Sigma_\alpha][D_\alpha], \tag{89}$$

$$[\tilde{R}_\alpha] = \frac{1}{\sigma}\left[[W]^{-1} + [M_\alpha][\tilde{\Sigma}_\alpha][D_\alpha][W]^{-1}\right], \tag{90}$$

where

$[\Sigma_\alpha]$ = a $N_m^\alpha \times N_m^\alpha$ diagonal matrix containing the scattering cross sections

$[\tilde{\Sigma}_\alpha]$ = a $N_m^\alpha \times N_m^\alpha$ diagonal matrix

$$= diag\left[\frac{\sigma_0(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_0(\boldsymbol{r})} \; \frac{\sigma_1(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_1(\boldsymbol{r})} \; \cdots \; \frac{\sigma_L(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_L(\boldsymbol{r})}\right]$$

and $M_{nk}^a = Y_{lm}^c(\Omega_n)$ or $Y_{lm}^s(\Omega_n)$ for $1 \le k \le N_m^a$, $1 \le n \le N_d$. Subsets of spherical harmonics selected to construct the moment-to-discrete matrices are given in Table 4 for two- and three-dimensional geometries. The shaded entries are the additional spherical harmonics to make the moment-to-discrete matrix invertible.

Table 4. Subsets of Spherical Harmonics Used to Construct the Moment-to-Discrete Matrix for the EOP Equation.

Two-Dimensional Geometry							
Even-Parity Flux				Odd-Parity Flux			
$Y^c_{lm}(\Omega)$		$Y^s_{lm}(\Omega)$		$Y^c_{lm}(\Omega)$		$Y^s_{lm}(\Omega)$	
l	m	l	m	l	m	l	m
$[0, N-2]$ even l	$[0, l]$ even m	$[2, N-2]$ even l	$[0, l]$ even m	$[1, N-1]$ odd l	$[1, l]$ odd m	$[1, N-1]$ odd l	$[1, l]$ odd m
---	---	N	$[2, N]$ even m	---	---	---	---

Three-Dimensional Geometry							
Even-Parity Flux				Odd-Parity Flux			
$Y^c_{lm}(\Omega)$		$Y^s_{lm}(\Omega)$		$Y^c_{lm}(\Omega)$		$Y^s_{lm}(\Omega)$	
l	m	l	m	l	m	l	m
$[0, N-2]$ even l	$[0, l]$	$[2, N-2]$ even l	$[1, l]$	$[1, N-1]$ odd l	$[1, l]$	$[1, N-1]$ odd l	$[1, l]$
N	$[1, N]$ odd m	N	$[1, N]$	---	---	$N+1$	$[2, N]$ even m

* The symbol [a, b] indicates the index ranges from a to b with the footnote indicating the restricted values.

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5. Summary

We have applied the discrete ordinates approximation to the second-order transport equations and demonstrated that they can be cast into a unified form with properly defined matrix operators. This common representation can be applied to either the SAAF equation or the EOP equations. The components of these matrix operators are itemized in detail for both the standard quadrature set and the Galerkin quadrature method. Finally, these formulations allow us to derive and program the corresponding finite-element equations in a common setting which are the foundations of the CEPTRE code.

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Appendix A. Properties of Spherical Harmonics

The normalized spherical harmonics, $Y_{lm}(\Omega)$, are defined by

$$Y_{lm}(\Omega) = Y_{lm}(\mu, \varphi) = \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\mu)e^{im\varphi} \tag{A-1}$$

for $l = 0 \ldots \infty$ and $m = -l, l$, where Ω is an unit vector represented by a polar angle θ and an azimuthal angle φ as shown in Figure A-1,

$$\mu = \cos\theta, \tag{A-2}$$

and $P_l^m(\mu)$ is the associated Legendre function of order l and degree m.

The spherical harmonics are orthonormal in that

$$\int_{4\pi} Y^*_{l'm'}(\Omega)Y_{lm}(\Omega)d\Omega = \int_0^{2\pi}\int_{-1}^{1} Y^*_{l'm'}(\mu, \varphi)Y_{lm}(\mu, \varphi)d\mu d\varphi = \delta_{ll'}\delta_{mm'}, \tag{A-3}$$

where $Y^*_{lm}(\mu, \varphi)$ is the complex conjugate of $Y_{lm}(\mu, \varphi)$, and

$$Y^*_{lm}(\mu, \varphi) = (-1)^m Y_{l,-m}(\mu, \varphi). \tag{A-4}$$

The spherical harmonics satisfy the important *addition theorem*. Consider two vectors, Ω and Ω', which have the coordinates (μ, φ) and (μ', φ'). Let θ_0 be the angle between the vectors Ω and Ω', then

$$\mu_0 \equiv \Omega \cdot \Omega' = \cos\theta_0 = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi'). \tag{A-5}$$

The addition theorem states that

$$P_l(\mu_0) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}(\mu, \varphi)Y^*_{lm}(\mu', \varphi'), \tag{A-6}$$

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Appendix C. Symmetry and Positive Definiteness of the Transport Operators

In this appendix, we will show that the operators R, R^{-1}, and T_S defined in Section 3 for the SAAF equation are symmetric and positive definite. An operator L is symmetric if

$$\langle v, Lu \rangle = \langle Lv, u \rangle, \tag{C-1}$$

and is strictly positive definite if

$$\langle u, Lu \rangle > 0 \tag{C-2}$$

for all non-zero functions u and v. The symbol $\langle u, v \rangle$ denotes the inner product between two functions:

$$\langle u, v \rangle = \int_V \int_{4\pi} u(\boldsymbol{r}, \Omega) v(\boldsymbol{r}, \Omega) d\Omega dV. \tag{C-3}$$

Furthermore, the following boundary conditions are imposed on the functions under consideration:

$$u(\boldsymbol{r}_b, \Omega) = f(\Omega) \qquad \text{for } \Omega \cdot \boldsymbol{n}_b < 0, \tag{C-4}$$

$$\Omega \cdot \nabla u(\boldsymbol{r}_b, \Omega) + R u(\boldsymbol{r}_b, \Omega) = 0 \qquad \text{for } \Omega \cdot \boldsymbol{n}_b > 0, \tag{C-5}$$

where $\boldsymbol{r}_b$ and $\boldsymbol{n}_b$ are the position vector and outward normal on the external boundary, respectively.

C.1 Removal Operator

The removal operator R in the one-group transport equation is defined in Eq. (22) and can be written as

$$Ru(\boldsymbol{r}, \Omega) = \sigma(\boldsymbol{r})u(\boldsymbol{r}, \Omega) - \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)u(\boldsymbol{r}, \Omega')d\Omega' \tag{C-6}$$

where the scattering cross section only depends on the cosine of the scattering angle between the incoming and outgoing directions. The removal operator $\boldsymbol{R}$ can be shown to be symmetric by substituting the last equation into Eq. (C-1):

$$\begin{aligned}
&\langle v, Ru\rangle \\
&= \int_V \int_{4\pi} v(\boldsymbol{r}, \Omega)\left[\sigma(\boldsymbol{r})u(\boldsymbol{r}, \Omega) - \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)u(\boldsymbol{r}, \Omega')d\Omega'\right]d\Omega dV \\
&= \int_V \int_{4\pi} u(\boldsymbol{r}, \Omega)\left[\sigma(\boldsymbol{r})v(\boldsymbol{r}, \Omega) - \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega \cdot \Omega')v(\boldsymbol{r}, \Omega')d\Omega'\right]d\Omega dV \\
&= \langle Rv, u\rangle
\end{aligned} \tag{C-7}$$

where we obtain the second expression by interchanging the variables and order of integration over angles.

The positive definite condition follows from an application of the Cauchy-Schwartz inequality:

$$\langle u, v\rangle \le \sqrt{\langle u, u\rangle}\sqrt{\langle v, v\rangle}\,. \tag{C-8}$$

$$\begin{aligned}
&\langle u, Ru\rangle \\
&= \int_V \int_{4\pi} u(\boldsymbol{r}, \Omega)\left[\sigma(\boldsymbol{r})u(\boldsymbol{r}, \Omega) - \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)u(\boldsymbol{r}, \Omega')d\Omega'\right]d\Omega dV \\
&= \int_V \int_{4\pi} \sigma(\boldsymbol{r})u^2(\boldsymbol{r}, \Omega)d\Omega dV - \int_V \int_{4\pi} \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)u(\boldsymbol{r}, \Omega)u(\boldsymbol{r}, \Omega')d\Omega' d\Omega dV \\
&= \int_V \int_{4\pi} \sigma(\boldsymbol{r})u^2(\boldsymbol{r}, \Omega)d\Omega dV \\
&\quad - \int_V \int_{4\pi} \int_{4\pi} \sqrt{\sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)}u(\boldsymbol{r}, \Omega)\sqrt{\sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)}u(\boldsymbol{r}, \Omega')d\Omega' d\Omega dV \\
&\ge \int_V \int_{4\pi} \sigma(\boldsymbol{r})u^2(\boldsymbol{r}, \Omega)d\Omega dV \\
&\quad - \sqrt{\int_V \int_{4\pi} \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)u^2(\boldsymbol{r}, \Omega)d\Omega' d\Omega dV}\sqrt{\int_V \int_{4\pi} \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega)u^2(\boldsymbol{r}, \Omega')d\Omega' d\Omega dV}
\end{aligned} \tag{C-9}$$

Interchanging the variables and order of integration in the first square root leads to

$$\int_V \int_{4\pi} \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega) u^2(\boldsymbol{r}, \Omega) d\Omega' d\Omega dV = \int_V \int_{4\pi} \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega) u^2(\boldsymbol{r}, \Omega') d\Omega' d\Omega dV$$

and

$$\langle u, Ru \rangle \geq \int_V \int_{4\pi} \left[\sigma(\boldsymbol{r}) - \int_{4\pi} \sigma_s(\boldsymbol{r}, \Omega' \cdot \Omega) d\Omega' \right] u^2(\boldsymbol{r}, \Omega) d\Omega dV > 0 . \qquad \text{(C-10)}$$

This inequality is justified if the total cross section is greater than the scattering cross section. Hence the removal operator is symmetric and positive definite.

C.2 Inverse Removal Operator

The inverse removal operator R^{-1} in the SAAF equation is given in Eq. (42) and can be written as

$$R^{-1} u(\boldsymbol{r}, \Omega) = \frac{1}{\sigma(\boldsymbol{r})} \left[u(\boldsymbol{r}, \Omega) + \int_{4\pi} \tilde{\sigma}_s(\boldsymbol{r}, \Omega' \cdot \Omega) u(\boldsymbol{r}, \Omega') d\Omega' \right], \qquad \text{(C-11)}$$

where

$$\tilde{\sigma}_s(\boldsymbol{r}, \Omega' \cdot \Omega) = \sum_{l=0}^{L} \frac{\sigma_l(\boldsymbol{r})}{\sigma(\boldsymbol{r}) - \sigma_l(\boldsymbol{r})} \sum_{m=-l}^{l} Y_{lm}(\Omega) Y^*_{lm}(\Omega') . \qquad \text{(C-12)}$$

Comparing Eq. (C-11) with (C-6), it can be readily shown that the operator R^{-1} is symmetric. To prove positive definiteness, consider a function $u = Rw$ and

$$\langle u, R^{-1} u \rangle = \langle Rw, w \rangle > 0 . \qquad \text{(C-13)}$$

Hence the inverse removal operator is also symmetric and positive definite.

C.3 Second-Order Transport Operator

The transport operator in the SAAF equation is defined as

$$T_S u(\boldsymbol{r}, \Omega) = -\Omega \cdot \nabla\left[R^{-1}\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)\right] + Ru(\boldsymbol{r}, \Omega). \tag{C-14}$$

Applying the identity

$$v(\boldsymbol{r}, \Omega)\Omega \cdot \nabla u(\boldsymbol{r}, \Omega) = \nabla \cdot [\Omega v(\boldsymbol{r}, \Omega)u(\boldsymbol{r}, \Omega)] - u(\boldsymbol{r}, \Omega)\Omega \cdot \nabla v(\boldsymbol{r}, \Omega). \tag{C-15}$$

and the divergence theorem, we have

$$\begin{aligned}
&\langle v, T_S u\rangle \\
&= -\int_V\int_{4\pi} v(\boldsymbol{r}, \Omega)\left(\Omega \cdot \nabla\left[R^{-1}\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)\right]\right)d\Omega dV + \langle v, \boldsymbol{R}u\rangle \\
&= \int_V\int_{4\pi}\left[\Omega \cdot \nabla v(\boldsymbol{r}, \Omega)\right]\left[R^{-1}\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)\right]d\Omega dV \\
&\quad -\int_V\int_{4\pi}\Omega \cdot \nabla\left[v(\boldsymbol{r}, \Omega)R^{-1}\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)\right]d\Omega dV + \langle v, \boldsymbol{R}u\rangle \\
&= \langle \Omega \cdot \nabla v, \boldsymbol{R}^{-1}\Omega \cdot \nabla u\rangle + \langle v, \boldsymbol{R}u\rangle - \int_A\int_{4\pi}(\Omega \cdot \boldsymbol{n})\left[v(\boldsymbol{r}, \Omega)\boldsymbol{R}^{-1}\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)\right]d\Omega dA \\
&= \langle \boldsymbol{R}^{-1}\Omega \cdot \nabla v, \Omega \cdot \nabla u\rangle + \langle \boldsymbol{R}v, u\rangle - \int_A\int_{4\pi}(\Omega \cdot \boldsymbol{n})\left[u(\boldsymbol{r}, \Omega)\boldsymbol{R}^{-1}\Omega \cdot \nabla v(\boldsymbol{r}, \Omega)\right]d\Omega dA \\
&= \int_V\int_{4\pi}\left[\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)\right]\left[R^{-1}\Omega \cdot \nabla v(\boldsymbol{r}, \Omega)\right]d\Omega dV \\
&\quad -\int_V\int_{4\pi}\Omega \cdot \nabla\left[u(\boldsymbol{r}, \Omega)\boldsymbol{R}^{-1}\Omega \cdot \nabla v(\boldsymbol{r}, \Omega)\right]d\Omega dV + \langle \boldsymbol{R}v, u\rangle \\
&= -\int_V\int_{4\pi}\left(\Omega \cdot \nabla\left[R^{-1}\Omega \cdot \nabla v(\boldsymbol{r}, \Omega)\right]\right)u(\boldsymbol{r}, \Omega)d\Omega dV + \langle v, \boldsymbol{R}u\rangle \\
&= \langle T_S v, u\rangle
\end{aligned} \tag{C-16}$$

where we have made use of the boundary conditions given in Eqs. (C-3) and (C-4). To prove the positive definite condition, we can manipulate the intermediate results given in Eq. (C-16):

$$\begin{aligned}
&\langle u, T_S u\rangle \\
&= \langle \Omega \cdot \nabla u, R^{-1}\Omega \cdot \nabla u\rangle + \langle u, Ru\rangle - \int_A \int_{4\pi} (\Omega \cdot \boldsymbol{n})[u(\boldsymbol{r}, \Omega)R^{-1}\Omega \cdot \nabla u(\boldsymbol{r}, \Omega)]d\Omega dA \\
&= \langle \Omega \cdot \nabla u, R^{-1}\Omega \cdot \nabla u\rangle + \langle u, Ru\rangle + \int_A \int_{4\pi} |\Omega \cdot \boldsymbol{n}| u^2(\boldsymbol{r}, \Omega) d\Omega dA
\end{aligned} \tag{C-17}$$

which is always positive since both R and R^{-1} are positive definite and the surface integral is also positive.

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