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Modeling Electron Transport in the Presence of Electric and Magnetic Fields

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Abstract

This report describes the theoretical background on modeling electron transport in the presence of electric and magnetic fields by incorporating the effects of the Lorentz force on electron motion into the Boltzmann transport equation. Electromagnetic fields alter the electron energy and trajectory continuously, and these effects can be characterized mathematically by differential operators in terms of electron energy and direction. Numerical solution techniques, based on the discrete-ordinates and finite-element methods, are developed and implemented in an existing radiation transport code, SCEPTRE.

Acknowledgements

We would like to thank Len Lorence for his guidance, enthusiasm and support throughout the course of this research.

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1. Introduction

In many radiation-effect studies, one critical assumption is typically made by treating electron transport totally independent from the electric field created by the deposited charge, which become invalid if the field strength is large enough to affect electron motion. An example of this is spacecraft charging due to the accumulation of low-energy electrons on the outside surface of a satellite which can cause electrical arcing, breakdown of dielectrics, and eventually lead to the destruction of electronics and failure of mission capability. With frequent buildup of potentials on the order of 10 kV on spacecraft surfaces, the effect of the high-flux, trapped electrons in the 1-100 keV range could be significant. Current modeling tools for charging predictions oversimplify the relevant physics, such as the dynamic interaction between incident electrons and electric fields generated by deposited charge, and lead to inaccurate predictions and large safety margins are often imposed due to the significant uncertainty.

To model electron transport in materials in the presence of electromagnetic (EM) fields, additional terms can be incorporated into the Boltzmann transport equation to represent the effects of the Lorentz force on particle motion and to describe how the EM fields alter the particle energy and direction continuously between collisions. These terms are significantly different from the other physical processes typically handled by the radiation transport codes. In traditional radiation transport, particles travel freely between interaction events following a straight-line path, and then undergo collision to a different streaming path with different energy. In the presence of electric and/or magnetic fields this paradigm is no longer valid, as particles travel in curved paths between collision sites and their energy changes continuously, consequently impairing many traditional solution methods.

There are production, radiation transport codes, such as ITS [1] and PENELOPE [2], which can model electron transport in the presence of electromagnetic fields. These are Monte-Carlo codes based on the condensed-history algorithms and are limited to electric field in vacuum or weak field strength in material region so that the interaction properties of electrons (stopping power) are not substantially altered within a predetermined step. Moreover, Monte-Carlo codes are restricted to problems where limited information is sought and are difficult to interface with other finite-element-based electromagnetic code used in radiation effect analysis.

In the early 1980’s, Bruce Wienke [3] demonstrated the feasibility of applying the multigroup, discrete-ordinates method to solve the one-dimensional, electron transport problem with fields. The energy redistribution term due to the electric field resembles the slowing–down operator and was treated with a multigroup-based differencing scheme. The angular redistribution terms due to the electric and magnetic fields were treated by using the spherical-harmonics expansion of the angular flux and cast into forms similar to the traditional collision and scattering operators. Our approach is an extension of his work to multi-dimensional geometries but includes discontinuous finite-element methods to treat the streaming operator and the energy-redistribution term from the electric field.

In the following sections, we describe the Boltzmann transport equation including operators representing the effects on electron motion from the Lorentz force. Detailed derivations are given to transform these operators from the velocity space to the energy-angle space common to the traditional radiation transport. We then apply the discrete-ordinates method to discretize the angular redistribution terms and demonstrate how to convert them into a form similar to the within-group scattering and suitable for implementation into an existing discrete-ordinates code. Finally, we discuss the finite-element methods to treat the entire phase space including spatial, energy and angular dependence. Discussions on coupling to the electromagnetic solver and numerical results are provided in a companion SAND report.

2. Bololtzmann Transport Equation with Lorentz Force

In the presence of external forces, the Boltzmann transport equation can be written as:

$$\frac{\partial N}{\partial t} + \mathbf{\nabla} \cdot \vec{v}N + \mathbf{\nabla}_v \cdot \vec{a}N + \sigma v N = S$$
$$\frac{\partial N}{\partial t} + \vec{v} \cdot \mathbf{\nabla} N + \vec{a} \cdot \mathbf{\nabla}_v N + (\mathbf{\nabla}_v \cdot \vec{a})N + \sigma v N = S \qquad (1)$$

where

$$N = \text{particle angular density } = N(\vec{r}, E, \vec{\Omega}, t)$$

$$\vec{r} = \text{position vector} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$$

$$\vec{\Omega} = \text{direction of particle motion} = \mu\mathbf{i} + \eta\mathbf{j} + \xi\mathbf{k}$$

$$\vec{v} = \text{particle velocity} = v\vec{\Omega} = v_x\mathbf{i} + v_y\mathbf{j} + v_z\mathbf{k}$$

$$\mathbf{\nabla} = \text{gradient operator in space} = \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}$$

$$\vec{a} = \text{acceleration} = a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}$$

$$\mathbf{\nabla}_v = \text{gradient operator in velocity space} = \mathbf{i}\frac{\partial}{\partial v_x} + \mathbf{j}\frac{\partial}{\partial v_y} + \mathbf{k}\frac{\partial}{\partial v_z}$$

$$S = \text{ the scattering and external sources}$$

with the vector components expressed in the Cartesian-coordinate system. The components of the velocity vector and the direction vector are related such that

$$\vec{v} = v_x\mathbf{i} + v_y\mathbf{j} + v_z\mathbf{k} = v(\mu\mathbf{i} + \eta\mathbf{j} + \xi\mathbf{k})$$

$$\vec{\Omega} = \mu\mathbf{i} + \eta\mathbf{j} + \xi\mathbf{k} = \frac{v_x}{v}\mathbf{i} + \frac{v_y}{v}\mathbf{j} + \frac{v_z}{v}\mathbf{k}$$

with $v = \left(v_x^2 + v_y^2 + v_z^2\right)^{\frac{1}{2}}$ and $\mu^2 + \eta^2 + \xi^2 = 1$.

The streaming operator in Eq. (1) is

$$\vec{v}\cdot\boldsymbol{\nabla}N = v\vec{\Omega}\cdot\boldsymbol{\nabla}N = v\left(\mu\frac{\partial N}{\partial x}+\eta\frac{\partial N}{\partial y}+\xi\frac{\partial N}{\partial z}\right) \tag{2}$$

The gradient operator in the velocity space is

$$\boldsymbol{\nabla}_v N = \mathbf{i}\frac{\partial N}{\partial v_x}+\mathbf{j}\frac{\partial N}{\partial v_y}+\mathbf{k}\frac{\partial N}{\partial v_z} \tag{3}$$

which can be expressed in terms of the polar angle (θ) and the azimuthal angle (φ) in the spherical coordinates:

$$\mu = \cos\theta \qquad \eta = \sin\theta\cos\varphi \qquad \xi = \sin\theta\sin\varphi \tag{4a}$$

$$v_x = v\mu = v\cos\theta \qquad v_y = v\eta = v\sin\theta\cos\varphi \qquad v_z = v\xi = v\sin\theta\sin\varphi \tag{4b}$$

Applying the chain rule of partial differentiation, we have

$$\begin{bmatrix}\frac{\partial N}{\partial v}\\ \frac{\partial N}{\partial \mu}\\ \frac{\partial N}{\partial \varphi}\end{bmatrix} = \begin{bmatrix}\frac{\partial v_x}{\partial v} & \frac{\partial v_y}{\partial v} & \frac{\partial v_z}{\partial v}\\ \frac{\partial v_x}{\partial \mu} & \frac{\partial v_y}{\partial \mu} & \frac{\partial v_z}{\partial \mu}\\ \frac{\partial v_x}{\partial \varphi} & \frac{\partial v_y}{\partial \varphi} & \frac{\partial v_z}{\partial \varphi}\end{bmatrix}\begin{bmatrix}\frac{\partial N}{\partial v_x}\\ \frac{\partial N}{\partial v_y}\\ \frac{\partial N}{\partial v_z}\end{bmatrix} = \begin{bmatrix}\mu & \sqrt{1-\mu^2}\cos\varphi & \sqrt{1-\mu^2}\sin\varphi\\ v & -\frac{v\mu\cos\varphi}{\sqrt{1-\mu^2}} & -\frac{v\mu\sin\varphi}{\sqrt{1-\mu^2}}\\ 0 & -v\sqrt{1-\mu^2}\sin\varphi & v\sqrt{1-\mu^2}\cos\varphi\end{bmatrix}\begin{bmatrix}\frac{\partial N}{\partial v_x}\\ \frac{\partial N}{\partial v_y}\\ \frac{\partial N}{\partial v_z}\end{bmatrix} \tag{5}$$

$$\begin{aligned}\begin{bmatrix}\frac{\partial N}{\partial v_x}\\ \frac{\partial N}{\partial v_y}\\ \frac{\partial N}{\partial v_z}\end{bmatrix} &= \begin{bmatrix}\mu & \frac{1-\mu^2}{v} & 0\\ \sqrt{1-\mu^2}\cos\varphi & -\frac{\mu\sqrt{1-\mu^2}}{v}\cos\varphi & -\frac{\sin\varphi}{v\sqrt{1-\mu^2}}\\ \sqrt{1-\mu^2}\sin\varphi & -\frac{\mu\sqrt{1-\mu^2}}{v}\sin\varphi & \frac{\cos\varphi}{v\sqrt{1-\mu^2}}\end{bmatrix}\begin{bmatrix}\frac{\partial N}{\partial v}\\ \frac{\partial N}{\partial \mu}\\ \frac{\partial N}{\partial \varphi}\end{bmatrix}\\ &= \begin{bmatrix}\mu & \frac{1-\mu^2}{v} & 0\\ \eta & -\frac{\mu\eta}{v} & -\frac{\xi}{v(1-\mu^2)}\\ \xi & -\frac{\mu\xi}{v} & \frac{\eta}{v(1-\mu^2)}\end{bmatrix}\begin{bmatrix}\frac{\partial N}{\partial v}\\ \frac{\partial N}{\partial \mu}\\ \frac{\partial N}{\partial \varphi}\end{bmatrix}\end{aligned} \tag{6}$$

The gradient operator $\boldsymbol{\nabla}_v$ becomes

$$\begin{aligned}\boldsymbol{\nabla}_v N &= \mathbf{i}\frac{\partial N}{\partial v_x} + \mathbf{j}\frac{\partial N}{\partial v_y} + \mathbf{k}\frac{\partial N}{\partial v_z} \\ &= \vec{\Omega}\frac{\partial N}{\partial v} + \mathbf{i}\left[\frac{1-\mu^2}{v}\frac{\partial N}{\partial \mu}\right] - \mathbf{j}\left[\frac{\mu\eta}{v}\frac{\partial N}{\partial \mu} + \frac{\xi}{v(1-\mu^2)}\frac{\partial N}{\partial \varphi}\right] - \mathbf{k}\left[\frac{\mu\xi}{v}\frac{\partial N}{\partial \mu} - \frac{\eta}{v(1-\mu^2)}\frac{\partial N}{\partial \varphi}\right]\end{aligned} \tag{7}$$

$$\begin{aligned}&\vec{a}\cdot\boldsymbol{\nabla}_v N \\ &= \left(\vec{a}\cdot\vec{\Omega}\right)\frac{\partial N}{\partial v} + \frac{1}{v}\left[a_x(1-\mu^2) - a_y\mu\eta - a_z\mu\xi\right]\frac{\partial N}{\partial \mu} - \frac{1}{v(1-\mu^2)}\left[a_y\xi - a_z\eta\right]\frac{\partial N}{\partial \varphi} \\ &= \left(\vec{a}\cdot\vec{\Omega}\right)\frac{\partial N}{\partial v} + \frac{1}{v}\left[a_x - \mu\left(\vec{a}\cdot\vec{\Omega}\right)\right]\frac{\partial N}{\partial \mu} + \frac{1}{v(1-\mu^2)}\left(\vec{\Omega}\times\vec{a}\right)_x\frac{\partial N}{\partial \varphi}\end{aligned} \tag{8}$$

Similarly, the term $\boldsymbol{\nabla}_v\cdot\vec{a}$ can be written as

$$\begin{aligned}&\boldsymbol{\nabla}_v\cdot\vec{a} \\ &= \frac{\partial a_x}{\partial v_x} + \frac{\partial a_y}{\partial v_y} + \frac{\partial a_z}{\partial v_z} \\ &= \frac{\partial}{\partial v}\left(\vec{a}\cdot\vec{\Omega}\right) + \frac{1}{v}(1-\mu^2)\frac{\partial a_x}{\partial \mu} \\ &\quad -\frac{1}{v}\left[\mu\eta\frac{\partial a_y}{\partial \mu} + \frac{\xi}{(1-\mu^2)}\frac{\partial a_y}{\partial \varphi}\right] - \frac{1}{v}\left[\mu\xi\frac{\partial a_z}{\partial \mu} - \frac{\eta}{(1-\mu^2)}\frac{\partial a_z}{\partial \varphi}\right]\end{aligned} \tag{9}$$

The particle angular flux is defined by

$$\psi\left(\vec{r},E,\vec{\Omega},t\right) \equiv vN\left(\vec{r},E,\vec{\Omega},t\right) \tag{10}$$

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial t}\left(\frac{\psi}{v}\right) = \frac{1}{v}\frac{\partial \psi}{\partial t}$$

$$\vec{v}\cdot\boldsymbol{\nabla}N = v\vec{\Omega}\cdot\boldsymbol{\nabla}N = \vec{\Omega}\cdot\boldsymbol{\nabla}\psi$$

$$\sigma vN = \sigma\psi$$

$$\frac{\partial N}{\partial v} = \frac{\partial}{\partial v}\left(\frac{\psi}{v}\right) = \frac{1}{v}\frac{\partial \psi}{\partial v} - \frac{\psi}{v^2}$$

The transport equation for the angular flux is then

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \vec{\Omega}\cdot\nabla\psi + \sigma\psi + \frac{\vec{a}\cdot\vec{\Omega}}{v}\left(\frac{\partial\psi}{\partial v} - \frac{1}{v}\psi\right) + \frac{1}{v^2}\left[a_x - \mu(\vec{a}\cdot\vec{\Omega})\right]\frac{\partial\psi}{\partial\mu} + \frac{1}{v^2(1-\mu^2)}\left(\vec{\Omega}\times\vec{a}\right)_x\frac{\partial\psi}{\partial\varphi} + (\nabla_v\cdot\vec{a})\frac{\psi}{v} = S \quad (11)$$

Acceleration due to External Force

The following derivations of the relationship between force and acceleration are taken from Reference [4]. In *classic physics* the Newton's second law of mechanics is given as follows:

$$\vec{F} = \frac{d\vec{p}}{dt} = m_o\frac{d\vec{v}}{dt} = m_o\vec{a} \quad (12)$$

indicating that the acceleration $\vec{a}$ is parallel to the force $\vec{F}$, and the mass of the particle m_o is constant.

In *relativistic physics* the acceleration $\vec{a}$ is not parallel to the force $\vec{F}$ at large velocities because the mass of the particle becomes a function of velocity so that the speed of the particle cannot exceed the speed of light in vacuum.

$$\vec{F} = \frac{d\vec{p}}{dt} = m\frac{d\vec{v}}{dt} + \frac{dm}{dt}\vec{v} \quad (13)$$

where the mass of the particle *m* is given by the Einstein expression

$$m = \mathrm{m}(v) = \gamma m_o \quad (14)$$

$$m_o = \text{rest mass of the particle}$$

$$\gamma = \frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \frac{1}{\sqrt{1-\beta^2}}$$

$$\beta = \text{particle speed normalized to speed of light} = \frac{v}{c}$$

$$c = \text{speed of light in vacuum}$$

Substituting Eq. (14) into Eq. (13) gives

$$\vec{F} = \gamma m_o \frac{d\vec{v}}{dt} + m_o \frac{d\gamma}{dt}\vec{v} = \gamma m_o \frac{d\vec{v}}{dt} + m_o \frac{\gamma^3 v}{c^2}\frac{dv}{dt}\vec{v} \tag{15}$$

The acceleration, $\vec{a} = \frac{d\vec{v}}{dt}$, can be determined by taking the dot product between the force $\vec{F}$ and the velocity $\vec{v}$

$$\begin{aligned} &\vec{F}\cdot\vec{v} \\ &= \gamma m_o \left(\frac{d\vec{v}}{dt}\cdot\vec{v}\right) + m_o \frac{\gamma^3 v}{c^2}\frac{dv}{dt}(\vec{v}\cdot\vec{v}) \\ &= \gamma m_o \left[\left(v\frac{d\vec{\Omega}}{dt} + \frac{dv}{dt}\vec{\Omega}\right)\cdot v\vec{\Omega}\right] + m_o \frac{\gamma^3 v^3}{c^2}\frac{dv}{dt} \\ &= \gamma m_o v\frac{dv}{dt} + m_o \frac{\gamma^3 v^3}{c^2}\frac{dv}{dt} \\ &= \gamma m_o (1+\gamma^2\beta^2) v\frac{dv}{dt} = \gamma^3 m_o v\frac{dv}{dt} \end{aligned} \tag{16}$$

Solving the last equation for $v\frac{dv}{dt}$

$$v\frac{dv}{dt} = \frac{\vec{F}\cdot\vec{v}}{\gamma^3 m_o} \tag{17}$$

and substituting the result into Eq. (15), we have

$$\vec{F} = \gamma m_o \frac{d\vec{v}}{dt} + \frac{m_o\gamma^3}{c^2}\frac{\vec{F}\cdot\vec{v}}{\gamma^3 m_o}\vec{v} = \gamma m_o \frac{d\vec{v}}{dt} + \beta^2\left(\vec{F}\cdot\vec{\Omega}\right)\vec{\Omega} \tag{18}$$

Solving $\frac{d\vec{v}}{dt}$ from this equation we obtain the relativistic relation between the force $\vec{F}$ and the acceleration $\vec{a}$

$$\vec{a} = \frac{1}{\gamma m_o}\left[\vec{F} - \beta^2\left(\vec{F}\cdot\vec{\Omega}\right)\vec{\Omega}\right] \tag{19}$$

For non-relativistic motion, $\beta \to 0$ and $\gamma \to 1$, we obtain the classic expression $\vec{a} = \frac{\vec{F}}{m_o}$

Lorentz Force

The Lorentz force [5] on a point charge due to electromagnetic fields is given by

$$\vec{F} = q\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) \tag{20}$$

where

$$q = \text{electric charge of the point charge}$$

$$\vec{\mathcal{E}} = \text{electric field } = \vec{\mathcal{E}}(\vec{r}, t)$$

$$\vec{\mathcal{B}} = \text{magnetic field } = \vec{\mathcal{B}}(\vec{r}, t)$$

Acceleration on the point charge including the relativistic effects is then

$$\begin{aligned}
\vec{a} &= \frac{1}{\gamma m_o}\left\{q\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) - \beta^2\left[q\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) \cdot \vec{\Omega}\right]\vec{\Omega}\right\} \\
&= \frac{q}{\gamma m_o}\left\{\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) - \left[\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) \cdot \frac{\vec{v}}{\mathrm{c}}\right]\frac{\vec{v}}{\mathrm{c}}\right\} \\
&= \frac{q}{\gamma m_o}\left[\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}} - \frac{\vec{\mathcal{E}} \cdot \vec{v}}{\mathrm{c}}\frac{\vec{v}}{\mathrm{c}}\right] \\
&= \frac{q}{\gamma m_o}\left[\vec{\mathcal{E}} + v\vec{\Omega} \times \vec{\mathcal{B}} - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\vec{\Omega}\right]
\end{aligned} \tag{21}$$

$$\vec{a} \cdot \vec{\Omega} = \frac{q}{\gamma m_o}\left[\vec{\mathcal{E}} + v\vec{\Omega} \times \vec{\mathcal{B}} - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\vec{\Omega}\right] \cdot \vec{\Omega} = \frac{q}{\gamma^3 m_o}\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right) \tag{22}$$

$$a_x = \frac{q}{\gamma m_o}\left[\mathcal{E}_x + v\left(\vec{\Omega} \times \vec{\mathcal{B}}\right)_x - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\mu\right] \tag{23a}$$

$$a_y = \frac{q}{\gamma m_o}\left[\mathcal{E}_y + v\left(\vec{\Omega} \times \vec{\mathcal{B}}\right)_y - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\eta\right] \tag{23b}$$

$$a_z = \frac{q}{\gamma m_o}\left[\mathcal{E}_z + v\left(\vec{\Omega} \times \vec{\mathcal{B}}\right)_z - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\xi\right] \tag{23c}$$

The components of $\vec{\Omega} \times \vec{\mathcal{B}}$ are

$$\vec{\Omega} \times \vec{\mathcal{B}} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \mu & \eta & \xi \\ \mathcal{B}_x & \mathcal{B}_y & \mathcal{B}_z \end{vmatrix} = \left(\eta \mathcal{B}_z - \xi \mathcal{B}_y\right)\mathbf{i} + (\xi \mathcal{B}_x - \mu \mathcal{B}_z)\mathbf{j} + (\mu \mathcal{B}_y - \eta \mathcal{B}_x)\mathbf{k} \tag{24}$$

$$a_x = \frac{q}{\gamma m_o}\left[\mathcal{E}_x + v\left(\eta \mathcal{B}_z - \xi \mathcal{B}_y\right) - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\mu\right] \tag{25a}$$

$$a_y = \frac{q}{\gamma m_o}\left[\mathcal{E}_y + v(\xi \mathcal{B}_x - \mu \mathcal{B}_z) - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\eta\right] \tag{25b}$$

$$a_z = \frac{q}{\gamma m_o}\left[\mathcal{E}_z + v(\mu \mathcal{B}_y - \eta \mathcal{B}_x) - \beta^2\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)\xi\right] \tag{25c}$$

For non-relativistic particles, $\beta \to 0$ and $\gamma \to 1$, the acceleration due to the Lorentz force is

$$\vec{a} = \frac{q}{m_o}\left(\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}}\right) \tag{26}$$

$$\vec{a} \cdot \vec{\Omega} = \frac{q}{m_o}\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right) \tag{27}$$

$$a_x = \frac{q}{m_o}\left[\mathcal{E}_x + v\left(\eta \mathcal{B}_z - \xi \mathcal{B}_y\right)\right] \tag{28a}$$

$$a_y = \frac{q}{m_o}\left[\mathcal{E}_y + v(\xi \mathcal{B}_x - \mu \mathcal{B}_z)\right] \tag{28b}$$

$$a_z = \frac{q}{m_o}\left[\mathcal{E}_z + v(\mu \mathcal{B}_y - \eta \mathcal{B}_x)\right] \tag{28c}$$

$\frac{\vec{a}\cdot\vec{\Omega}}{v}\frac{\partial\psi}{\partial v}$

The term $\frac{\vec{a}\cdot\vec{\Omega}}{v}\frac{\partial\psi}{\partial v}$ in Eq. (11) involves the partial derivative of the angular flux with respect to the particle speed which can be converted to a more desirable form in terms of the kinetic energy (*E*). The total energy of a particle is the sum of the kinetic energy and the rest energy, or

The term $\frac{\vec{a}\cdot\vec{\Omega}}{v}\frac{\partial\psi}{\partial v}$ in Eq. (11) involves the partial derivative of the angular flux with respect to the particle speed which can be converted to a more desirable form in terms of the kinetic energy (*E*). The total energy of a particle is the sum of the kinetic energy and the rest energy, or

$$mc^2 = E + m_o c^2 \quad \Longrightarrow \quad E = mc^2 - m_o c^2 = (\gamma - 1) m_o c^2 \tag{29}$$

Taking the derivative of the last expression with respect to *v* leads to

$$\frac{dE}{dv} = m_o c^2 \frac{d\gamma}{dv} = \frac{m_o v}{\left(1 - \frac{v^2}{c^2}\right)^{3/2}} = m_o \gamma^3 v \quad \Longrightarrow \quad dE = m_o \gamma^3 v \, dv \tag{30}$$

Thus,

$$\frac{\vec{a}\cdot\vec{\Omega}}{v}\frac{\partial\psi}{\partial v} = m_o \gamma^3 \left(\vec{a}\cdot\vec{\Omega}\right)\frac{\partial\psi}{\partial E} \tag{31}$$

Substituting Eq. (22) into Eq. (31), it can be shown that the electric field can alter the particle energy through an operator similar to the CSD operator,

$$\frac{\vec{a}\cdot\vec{\Omega}}{v}\frac{\partial\psi}{\partial v} = q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\frac{\partial\psi}{\partial E} \tag{32}$$

$\left(\vec{a}\cdot\vec{\Omega}\right)\frac{\psi}{v^2}$

It can be shown that

$$(pc)^2 = (mc^2)^2 - (m_o c^2)^2 \tag{33}$$

$$v^2 = \frac{(mc^2)^2 - (m_o c^2)^2}{(mc)^2} = \frac{(E + 2m_o c^2)E}{m(E + m_o c^2)} = \frac{c^2 E(E + 2m_o c^2)}{(E + m_o c^2)^2} = c^2\beta^2(E) \tag{34}$$

$$v = \frac{c\sqrt{E(E + 2m_o c^2)}}{E + m_o c^2} = c\sqrt{\beta^2(E)} = c\beta(E) \tag{35}$$

where

$$\beta(E) \equiv \frac{v}{c} = \sqrt{\frac{E(E + 2m_o c^2)}{(E + m_o c^2)^2}} \quad \text{and} \quad \beta^2(E) = \frac{E(E + 2m_o c^2)}{(E + m_o c^2)^2} \tag{36a}$$

and $\beta^2(E) \to \frac{2E}{m_o c^2}$ for $E \ll m_o c^2$. Hereafter, the symbol $\beta^2(E)$ will be used to represent the term $\frac{E\left(E+2m_o c^2\right)}{(E+m_o c^2)^2}$ explicitly and β^2 is still used for $\left(\frac{v}{c}\right)^2$. Furthermore,

$$\gamma = \frac{1}{\sqrt{1 - \left(\frac{v}{c}\right)^2}} = \frac{1}{\sqrt{1 - \beta^2(E)}} \tag{36b}$$

$$\frac{1}{\gamma} = \sqrt{1 - \beta^2(E)} = \frac{m_o c^2}{E + m_o c^2} = \frac{m_o c^2}{\mathcal{T}(E)} \tag{36c}$$

$$\mathcal{T}(E) = E + m_o c^2 \tag{36d}$$

The term $\frac{\psi}{v^2}$ in Eq. (11) can then be written as

$$\frac{\psi}{v^2} = \frac{\psi}{c^2\beta^2(E)} \tag{37}$$

From Eq. (22),

$$\vec{a} \cdot \vec{\Omega} = \frac{q}{\gamma^3 m_o}\left(\vec{\mathcal{E}} \cdot \vec{\Omega}\right)$$

$$\left(\vec{a}\cdot\vec{\Omega}\right)\frac{\psi}{v^2}=\frac{q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)}{\gamma^3 m_o c^2\beta^2(E)}\psi=\frac{q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)}{\mathcal{T}(E)}\frac{1-\beta^2(E)}{\beta^2(E)}\psi \quad (38)$$

$(\boldsymbol{\nabla}_v\cdot\vec{\boldsymbol{a}})\frac{\boldsymbol{\psi}}{\boldsymbol{v}}$

For non-relativistic motion,

$$\vec{a}=\frac{q}{m_o}\left(\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}\right)$$

and

$$\boldsymbol{\nabla}_v\cdot\vec{a}=\frac{q}{m_o}\left[\boldsymbol{\nabla}_v\cdot\vec{\mathcal{E}}+\boldsymbol{\nabla}_v\cdot\left(\vec{v}\times\vec{\mathcal{B}}\right)\right]=0 \quad (39)$$

For relativistic case,

$$\vec{a}=\frac{q}{\gamma m_o}\left[\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}-\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]$$

$$\begin{aligned}
\boldsymbol{\nabla}_v\cdot\vec{a}&=\boldsymbol{\nabla}_v\cdot\left\{\frac{q}{\gamma m_o}\left[\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}-\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]\right\}\\
&=\frac{q}{\gamma m_o}\boldsymbol{\nabla}_v\cdot\left[\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}-\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]+\frac{q}{m_o}\left(\boldsymbol{\nabla}_v\frac{1}{\gamma}\right)\cdot\left[\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}-\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]\\
&=-\frac{q}{\gamma m_o}\boldsymbol{\nabla}_v\cdot\left[\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]+\frac{q}{m_o}\left(\boldsymbol{\nabla}_v\frac{1}{\gamma}\right)\cdot\left[\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}-\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]\\
&=-\frac{q}{\gamma m_o c^2}\boldsymbol{\nabla}_v\cdot\left(\vec{\mathcal{E}}\cdot\vec{v}\right)\vec{v}+\frac{q}{m_o}\left(\boldsymbol{\nabla}_v\frac{1}{\gamma}\right)\cdot\left[\vec{\mathcal{E}}+\vec{v}\times\vec{\mathcal{B}}-\beta^2\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\vec{\Omega}\right]
\end{aligned}$$

$$\boldsymbol{\nabla}_v\frac{1}{\gamma}=\left(\frac{\partial}{\partial v}\frac{1}{\gamma}\right)\vec{\Omega}=-\frac{v\gamma}{c^2}\vec{\Omega}$$

$$
\begin{aligned}
&\boldsymbol{\nabla}_v \cdot (\vec{\mathcal{E}} \cdot \vec{v})\vec{v} \\
&= \frac{\partial}{\partial v_x}\left(v_x(\vec{\mathcal{E}} \cdot \vec{v})\right) + \frac{\partial}{\partial v_y}\left(v_y(\vec{\mathcal{E}} \cdot \vec{v})\right) + \frac{\partial}{\partial v_z}\left(v_z(\vec{\mathcal{E}} \cdot \vec{v})\right) \\
&= 3(\vec{\mathcal{E}} \cdot \vec{v}) + v_x \frac{\partial(\vec{\mathcal{E}} \cdot \vec{v})}{\partial v_x} + v_y \frac{\partial(\vec{\mathcal{E}} \cdot \vec{v})}{\partial v_y} + v_z \frac{\partial(\vec{\mathcal{E}} \cdot \vec{v})}{\partial v_z} \\
&= 4(\vec{\mathcal{E}} \cdot \vec{v})
\end{aligned}
$$

$$
\begin{aligned}
&\boldsymbol{\nabla}_v \cdot \vec{a} \\
&= -\frac{q}{\gamma m_o c^2}\boldsymbol{\nabla}_v \cdot (\vec{\mathcal{E}} \cdot \vec{v})\vec{v} + \frac{q}{m_o}\left(\boldsymbol{\nabla}_v \frac{1}{\gamma}\right) \cdot \left[\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}} - \beta^2(\vec{\mathcal{E}} \cdot \vec{\Omega})\vec{\Omega}\right] \\
&= -\frac{4q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v}) - \frac{q}{m_o}\left(\frac{v\gamma}{c^2}\vec{\Omega}\right) \cdot \left[\vec{\mathcal{E}} + \vec{v} \times \vec{\mathcal{B}} - \beta^2(\vec{\mathcal{E}} \cdot \vec{\Omega})\vec{\Omega}\right] \\
&= -\frac{4q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v}) - \frac{q}{m_o}\left(\frac{v\gamma}{c^2}\right)\left[(\vec{\mathcal{E}} \cdot \vec{\Omega}) - \beta^2(\vec{\mathcal{E}} \cdot \vec{\Omega})\right] \\
&= -\frac{4q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v}) - \frac{q}{m_o c^2} v\gamma(1-\beta^2)(\vec{\mathcal{E}} \cdot \vec{\Omega}) \qquad (40) \\
&= -\frac{4q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v}) - \frac{q}{m_o c^2} \gamma(1-\beta^2)(\vec{\mathcal{E}} \cdot \vec{v}) \\
&= -\frac{4q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v}) - \frac{q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v}) \\
&= -\frac{5q}{\gamma m_o c^2}(\vec{\mathcal{E}} \cdot \vec{v})
\end{aligned}
$$

$$
(\boldsymbol{\nabla}_v \cdot \vec{a})\frac{\psi}{v} = -\frac{5q(\vec{\mathcal{E}} \cdot \vec{\Omega})}{\gamma m_o c^2}\psi = -\frac{5q(\vec{\mathcal{E}} \cdot \vec{\Omega})}{E + m_o c^2}\,\psi = -\frac{5q(\vec{\mathcal{E}} \cdot \vec{\Omega})}{\mathcal{T}(\mathrm{E})}\,\psi \qquad (41)
$$

$$
\boldsymbol{\mathcal{K}\psi = \frac{1}{v^2}\left[a_x - \mu(\vec{a} \cdot \vec{\Omega})\right]\frac{\partial\psi}{\partial\mu} + \frac{1}{v^2(1-\mu^2)}(\vec{\Omega} \times \vec{a})_x \frac{\partial\psi}{\partial\varphi}}
$$

The acceleration due to the Lorentz force is given in Eq. (21):

$$
\vec{a} = \frac{q}{\gamma m_o}\left[\vec{\mathcal{E}} + v\vec{\Omega} \times \vec{\mathcal{B}} - \beta^2(\vec{\mathcal{E}} \cdot \vec{\Omega})\vec{\Omega}\right]
$$

Substituting the third term containing β^2 of $\vec{a}$ into $\mathcal{K}\psi$ leads to

$$a_x - \mu(\vec{a}\cdot\vec{\Omega}) \;\Rightarrow\; \frac{q}{\gamma m_o}\left[-\beta^2(\vec{\mathcal{E}}\cdot\vec{\Omega})\mu + \beta^2(\vec{\mathcal{E}}\cdot\vec{\Omega})\mu\right] = 0$$

and

$$\vec{\Omega}\times\vec{a} \;\Rightarrow\; \vec{\Omega}\times\left[\beta^2(\vec{\mathcal{E}}\cdot\vec{\Omega})\vec{\Omega}\right] = \beta^2(\vec{\mathcal{E}}\cdot\vec{\Omega})\vec{\Omega}\times\vec{\Omega} = 0$$

The relativistic terms in particle acceleration have *no* contribution to $\mathcal{K}\psi$ since those terms represent acceleration along the particle direction. Next, using the expressions of v^2 and v

$$\frac{1}{\gamma m_o v^2} = \frac{1}{\gamma m_o c^2 \beta^2(E)} = \frac{1}{(E + m_o c^2)\beta^2(E)} = \frac{1}{\mathcal{T}(\mathrm{E})\beta^2(E)}$$

$$v = c\beta(E)$$

we can rewrite $\mathcal{K}\psi$ to the following

$$\begin{aligned} &\frac{1}{v^2}\left[a_x - \mu(\vec{a}\cdot\vec{\Omega})\right]\frac{\partial\psi}{\partial\mu} + \frac{1}{v^2(1-\mu^2)}\left(\vec{\Omega}\times\vec{a}\right)_x\frac{\partial\psi}{\partial\varphi} \\ &= \left[\tilde{a}_x - \mu(\tilde{\boldsymbol{a}}\cdot\vec{\Omega})\right]\frac{\partial\psi}{\partial\mu} + \frac{1}{(1-\mu^2)}\left(\vec{\Omega}\times\tilde{\boldsymbol{a}}\right)_x\frac{\partial\psi}{\partial\varphi} \end{aligned} \tag{42}$$

with

$$\tilde{\boldsymbol{a}} \equiv \frac{q}{\mathcal{D}(E)}\left[\vec{\mathcal{E}} + c\beta(E)\left(\vec{\Omega}\times\vec{\mathcal{B}}\right)\right] \tag{43}$$

$$\mathcal{D}(E) \equiv \mathcal{T}(E)\beta^2(E) = \frac{E(E + 2m_o c^2)}{E + m_o c^2} \tag{44}$$

One can further simplify Eq. (42) by considering the following

$$\tilde{\boldsymbol{a}}\cdot\vec{\Omega} = \frac{q}{\mathcal{D}(E)}\left[\vec{\mathcal{E}} + c\beta(E)\left(\vec{\Omega}\times\vec{\mathcal{B}}\right)\right]\cdot\vec{\Omega} = \frac{q}{\mathcal{D}(E)}(\vec{\mathcal{E}}\cdot\vec{\Omega})$$

$$\tilde{a}_x - \mu(\tilde{\boldsymbol{a}} \cdot \vec{\Omega}) = \frac{q}{\mathcal{D}(E)}\left[\mathcal{E}_x - (\vec{\mathcal{E}} \cdot \vec{\Omega})\mu + c\beta(E)(\vec{\Omega} \times \vec{\mathcal{B}})_x\right]$$
$$= \frac{q}{\mathcal{D}(E)}\left[\mathcal{E}_x(1-\mu^2) - \mathcal{E}_y\mu\eta - \mathcal{E}_z\mu\xi + c\beta(E)(\mathcal{B}_z\eta - \mathcal{B}_y\xi)\right] \tag{45}$$

$$\begin{aligned}
&(\vec{\Omega} \times \tilde{\boldsymbol{a}})_x \\
&= \frac{q}{\mathcal{D}(E)}\left(\vec{\Omega} \times [\vec{\mathcal{E}} + c\beta(E)\,\vec{\Omega} \times \vec{\mathcal{B}}]\right)_x \\
&= \frac{q}{\mathcal{D}(E)}\left[\vec{\Omega} \times \vec{\mathcal{E}} + c\beta(E)\,\vec{\Omega} \times \vec{\Omega} \times \vec{\mathcal{B}}\right]_x \\
&= \frac{q}{\mathcal{D}(E)}\left[\vec{\Omega} \times \vec{\mathcal{E}} + c\beta(E)[\vec{\Omega}(\vec{\Omega} \cdot \vec{\mathcal{B}}) - \vec{\mathcal{B}}(\vec{\Omega} \cdot \vec{\Omega})]\right]_x \\
&= \frac{q}{\mathcal{D}(E)}\left[(\vec{\Omega} \times \vec{\mathcal{E}})_x + c\beta(E)[(\vec{\Omega} \cdot \vec{\mathcal{B}})\mu - \mathcal{B}_x]\right] \\
&= \frac{q}{\mathcal{D}(E)}\left[\mathcal{E}_z\eta - \mathcal{E}_y\xi + c\beta(E)[\mathcal{B}_y\mu\eta + \mathcal{B}_z\mu\xi - \mathcal{B}_x(1-\mu^2)]\right]
\end{aligned} \tag{46}$$

Substituting Eqs. (32), (38), (41), (45) and (46) into Eq. (11)

$$\begin{aligned}
&\frac{1}{c\beta(E)}\frac{\partial\psi}{\partial t} + \vec{\Omega} \cdot \boldsymbol{\nabla}\psi + \sigma\psi \\
&+q(\vec{\mathcal{E}} \cdot \vec{\Omega})\left[\frac{\partial\psi}{\partial E} - \frac{1+4\beta^2(E)}{\mathcal{D}(E)}\psi\right] \\
&+ \frac{q}{\mathcal{D}(E)}\left[\mathcal{E}_x(1-\mu^2) - \mathcal{E}_y\mu\eta - \mathcal{E}_z\mu\xi + c\beta(E)(\mathcal{B}_z\eta - \mathcal{B}_y\xi)\right]\frac{\partial\psi}{\partial\mu} \\
&+ \frac{q}{\mathcal{D}(E)(1-\mu^2)}\left[\mathcal{E}_z\eta - \mathcal{E}_y\xi + c\beta(E)[\mathcal{B}_y\mu\eta + \mathcal{B}_z\mu\xi - \mathcal{B}_x(1-\mu^2)]\right]\frac{\partial\psi}{\partial\varphi} = S
\end{aligned} \tag{47}$$

$$\mu = \cos\theta \qquad \eta = \sqrt{1-\mu^2}\cos\varphi \qquad \xi = \sqrt{1-\mu^2}\sin\varphi$$

$$\mathcal{T}(E) = E + m_o c^2$$

$$\beta^2(E) = \frac{E(E + 2m_o c^2)}{(E + m_o c^2)^2}$$

$$\mathcal{D}(E) = \mathcal{T}(E)\beta^2(E) = \frac{E(E + 2m_o c^2)}{E + m_o c^2}$$

	$E \ll m_o c^2$	$E \gg m_o c^2$
$\mathcal{T}(E)$	$m_o c^2$	E
$\beta^2(E)$	$\frac{2E}{m_o c^2}$	1
$\mathcal{D}(E)$	$2E$	E
$\frac{1}{\mathcal{D}(E)}$	$\frac{1}{2E}$	$\frac{1}{E}$
$\frac{1+4\beta^2(E)}{\mathcal{D}(E)}$	$\frac{1}{2E}$	$\frac{5}{E}$
$\frac{\beta(E)}{\mathcal{D}(E)}$	$\frac{1}{\sqrt{2E m_o c^2}}$	$\frac{1}{E}$

From Eq. (47),

$$\begin{gathered}\frac{1}{c\beta(E)}\frac{\partial\psi}{\partial t}+\vec{\Omega}\cdot\nabla\psi+\sigma\psi\\ +q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\left[\frac{\partial\psi}{\partial E}-\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\psi\right]\\ +\frac{q}{\mathcal{D}(E)}\left\{\mathcal{E}_x(1-\mu^2)\frac{\partial\psi}{\partial\mu}-\mathcal{E}_y\left[\mu\eta\frac{\partial\psi}{\partial\mu}+\frac{\xi}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right]-\mathcal{E}_z\left[\mu\xi\frac{\partial\psi}{\partial\mu}-\frac{\eta}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right]\right\}\\ +\frac{qc\beta(E)}{\mathcal{D}(E)}\left\{-\mathcal{B}_x\frac{\partial\psi}{\partial\varphi}-\mathcal{B}_y\left[\xi\frac{\partial\psi}{\partial\mu}-\frac{\mu\eta}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right]+\mathcal{B}_z\left[\eta\frac{\partial\psi}{\partial\mu}+\frac{\mu\xi}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right]\right\}=\mathrm{S}\end{gathered} \tag{47a}$$

$$\mu=\cos\theta \qquad \eta=\sqrt{1-\mu^2}\cos\varphi \qquad \xi=\sqrt{1-\mu^2}\sin\varphi$$

$$\beta^2(E)=\frac{E(E+2m_o c^2)}{(E+m_o c^2)^2}$$

$$\mathcal{D}(E)=\mathcal{T}(E)\beta^2(E)=\frac{E(E+2m_o c^2)}{E+m_o c^2}$$

For non-relativistic electrons,

$$\begin{aligned}
&\frac{1}{v}\frac{\partial\psi}{\partial t} + \vec{\Omega}\cdot\nabla\psi + \sigma\psi \\
&+q(\vec{\mathcal{E}}\cdot\vec{\Omega})\left[\frac{\partial\psi}{\partial E} - \frac{1}{2E}\psi\right] \\
&+\frac{q}{2E}\left\{\mathcal{E}_x(1-\mu^2)\frac{\partial\psi}{\partial\mu} - \mathcal{E}_y\left[\mu\eta\frac{\partial\psi}{\partial\mu} + \frac{\xi}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right] - \mathcal{E}_z\left[\mu\xi\frac{\partial\psi}{\partial\mu} - \frac{\eta}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right]\right\} \\
&+\frac{qv}{2E}\left\{-\mathcal{B}_x\frac{\partial\psi}{\partial\varphi} - \mathcal{B}_y\left[\xi\frac{\partial\psi}{\partial\mu} - \frac{\mu\eta}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right] + \mathcal{B}_z\left[\eta\frac{\partial\psi}{\partial\mu} + \frac{\mu\xi}{(1-\mu^2)}\frac{\partial\psi}{\partial\varphi}\right]\right\} = \mathrm{S}
\end{aligned} \tag{47b}$$

$$v = \sqrt{\frac{2E}{m_o}} \qquad \beta = 0 \qquad D(E) = 2E$$

It is noted that Eq. (47) is the consequence from including two additional terms describing the change in velocity due to the Lorentz force, $\vec{a}\cdot\nabla_v N + (\nabla_v\cdot\vec{a})N$, to the Boltzmann transport equation. One can obtain a similar result by considering the effects in the momentum space. The only difference is in the energy redistribution term such that the coefficient $1 + 4\beta^2(E)$ should be replaced by $1 - \beta^2(E)$.

3. Discrete-Ordinates Method

In the discrete-ordinates approximation [6], the angular flux is determined at a set of discrete directions such that $\psi(\Omega) \rightarrow \psi(\Omega_\mathrm{n})$ for $\{\Omega_\mathrm{n}\}$. To evaluate the scattering source, the angular flux is often represented by a finite expansion in terms of spherical harmonics as

$$\psi(\Omega) = \sum_{l=0}^{L} \sum_{m=0}^{l} [Y_{lm}^{c}(\Omega)\phi_{lm}^{c} + Y_{lm}^{s}(\Omega)\phi_{lm}^{s}] \tag{48}$$

The real and imaginary parts of the spherical harmonics are defined by

$$Y_{lm}^{c}(\Omega) = Y_{lm}^{c}(\mu,\varphi) = C_{lm}P_{l}^{m}(\mu)\cos m\varphi \tag{49a}$$

$$Y_{lm}^{s}(\Omega) = Y_{lm}^{s}(\mu,\varphi) = C_{lm}P_{l}^{m}(\mu)\sin m\varphi \tag{49b}$$

where $P_l^m(\mu)$ is the associated Legendre polynomial of order *l* and degree *m*,

$$P_l^m(\mu) = (-1)^\mathrm{m}(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_l(\mu) \tag{49c}$$

$$C_{lm} = \left[\frac{2l+1}{4\pi}(2-\delta_{m0})\frac{(l-m)!}{(l+m)!}\right]^{1/2} \tag{49d}$$

Using the expansion Eq. (48), one can represent the angular derivatives $\frac{\partial\psi}{\partial\mu}$ and $\frac{\partial\psi}{\partial\phi}$ in terms of the angular moments (see Appendix A for details)

$$\begin{aligned}\frac{\partial\psi}{\partial\mu} &= \frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}\left\{\left[\tilde{C}_{lm}Y_{lm}^{c}(\Omega) - l\mu Y_{lm}^{c}(\Omega)\right]\phi_{lm}^{c} + \left[\tilde{C}_{lm}Y_{lm}^{s}(\Omega) - l\mu Y_{lm}^{s}(\Omega)\right]\phi_{lm}^{s}\right\} \\ &= \frac{1}{\sqrt{1-\mu^2}}\sum_{l=1}^{L}\sum_{m=0}^{l}\left\{\left[\tilde{C}_{lm}\tilde{Y}_{lm}^{c}(\Omega) - l\mu\tilde{Y}_{lm}^{c}(\Omega)\right]\phi_{lm}^{c} + \left[\tilde{C}_{lm}\tilde{Y}_{lm}^{s}(\Omega) - l\mu\tilde{Y}_{lm}^{s}(\Omega)\right]\phi_{lm}^{s}\right\}\end{aligned} \tag{50}$$

$$\frac{\partial\psi}{\partial\varphi} = -\sum_{l=1}^{L}\sum_{m=0}^{l} m[Y_{lm}^{s}(\Omega)\phi_{lm}^{c} - Y_{lm}^{c}(\Omega)\phi_{lm}^{s}] \tag{51}$$

where the modified spherical harmonics are defined as

$$\tilde{Y}_{lm}^{c}(\Omega) \equiv \frac{Y_{lm}^{c}(\Omega)}{\sqrt{1-\mu^2}} \tag{52a}$$

$$\tilde{Y}_{\mathrm{lm}}^{\mathrm{s}}(\Omega) \equiv \frac{\mathrm{Y}_{\mathrm{lm}}^{\mathrm{s}}(\Omega)}{\sqrt{1-\mu^2}} \tag{52b}$$

$$\tilde{Y}_{lm}^{c}(\Omega) = \tilde{Y}_{lm}^{s}(\Omega) = 0 \quad \text{for } m > l \tag{52c}$$

$$\tilde{C}_{lm} = \left[\frac{2l+1}{2l-1}(l-m)(l+m)\right]^{1/2} \tag{52d}$$

The angular moments can be generated from the discrete angular flux through the following:

$$\boldsymbol{\phi} = [\boldsymbol{D}]\boldsymbol{\psi} \tag{53}$$

where

$\boldsymbol{\phi}$ is a column vector containing the angular moments

$\boldsymbol{\psi}$ is a column vector containing the discrete angular flux

$[\boldsymbol{D}]$ is the discrete to moment matrix with a dimension of $N_M \times N_D$

N_M is the number of angular moments

N_D is the number of directions

The angular-moment vector is arranged in an orderly fashion

$$\boldsymbol{\phi} = [\phi_{00}^{c} \quad \phi_{10}^{c} \quad \phi_{11}^{c} \quad \phi_{20}^{c} \quad \phi_{21}^{c} \quad \phi_{22}^{c} \quad \cdots]^T \tag{54}$$

for 2D geometry, and

$$\boldsymbol{\phi} = [\phi_{00}^{c} \quad \phi_{10}^{c} \quad \phi_{11}^{c} \quad \phi_{11}^{s} \quad \phi_{20}^{c} \quad \phi_{21}^{c} \quad \phi_{21}^{s} \quad \phi_{22}^{c} \quad \phi_{22}^{s} \quad \phi_{30}^{c} \quad \phi_{31}^{c} \quad \phi_{31}^{s} \quad \cdots]^T \tag{55}$$

for 3D geometry such that there is a unique, bi-directional mapping between the indices (l, m), the cosine- and sine-component and an index n' (the location of the angular moment in $\boldsymbol{\phi}$),

$$\left(l, m, \substack{cosine \\ sine}\right) \Leftrightarrow n'$$

With these, one can cast the angular redistribution terms into matrix form similar to that of the scattering term.

$$\begin{gathered}\frac{1}{c\beta(E)}\frac{\partial \boldsymbol{\psi}}{\partial t} + \vec{\Omega}\cdot\nabla\boldsymbol{\psi} + \sigma\boldsymbol{\psi} + q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\left[\frac{\partial\boldsymbol{\psi}}{\partial E} - \frac{1+4\beta^2(E)}{\mathcal{D}(E)}\boldsymbol{\psi}\right] \\ + \frac{q}{\mathcal{D}(E)}\left\{\mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right] + \mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right] + \mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]\right\}[\boldsymbol{D}]\boldsymbol{\psi} \\ + \frac{qc\beta(E)}{\mathcal{D}(E)}\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right] + \mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right] + \mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]\right\}[\boldsymbol{D}]\boldsymbol{\psi} = \boldsymbol{S}\end{gathered} \tag{56}$$

where $[\boldsymbol{\mathcal{M}}]$ are the moment-to-discrete matrices due to the EM fields and have dimension of $N_D \times N_M$. The components of these moment-to-discrete matrices $\boldsymbol{\mathcal{M}}_{nn'}$ are given in the table below. The row index n corresponds to the discrete direction Ω_n. The column index n' is determined by the indices l, m and the phase (cosine or sine).

	$\boldsymbol{\mathcal{M}}_{nn'}$ **for** $\boldsymbol{l} > 0$ *and* $\boldsymbol{m} > 0$	
	Cosine Components	**Sine Components**
$\boldsymbol{\mathcal{E}_x}$	$\tilde{C}_{lm} Y_{l-1,m}^{c}(\Omega_n) - l\mu_n Y_{lm}^{c}(\Omega_n)$	$\tilde{C}_{lm} Y_{l-1,m}^{s}(\Omega_n) - l\mu_n Y_{lm}^{s}(\Omega_n)$
$\boldsymbol{\mathcal{E}_y}$	$-\mu_n \cos\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{c}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{c}(\Omega_n)\right]$ $+m\sin\varphi_n\, \tilde{Y}_{lm}^{s}(\Omega_n)$	$-\mu_n \cos\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{s}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{s}(\Omega_n)\right]$ $-m\sin\varphi_n\, \tilde{Y}_{lm}^{c}(\Omega_n)$
$\boldsymbol{\mathcal{E}_z}$	$-\mu_n \sin\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{c}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{c}(\Omega_n)\right]$ $-m\cos\varphi_n\, \tilde{Y}_{lm}^{s}(\Omega_n)$	$-\mu_n \sin\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{s}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{s}(\Omega_n)\right]$ $+m\cos\varphi_n\, \tilde{Y}_{lm}^{c}(\Omega_n)$
$\boldsymbol{\mathcal{B}_x}$	$mY_{lm}^{s}(\Omega_n)$	$-mY_{lm}^{c}(\Omega_n)$
$\boldsymbol{\mathcal{B}_y}$	$-\sin\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{c}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{c}(\Omega_n)\right]$ $-m\,\mu_n\cos\varphi_n\, \tilde{Y}_{lm}^{s}(\Omega_n)$	$-\sin\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{s}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{s}(\Omega_n)\right]$ $+m\,\mu_n\cos\varphi_n\, \tilde{Y}_{lm}^{c}(\Omega_n)$
$\boldsymbol{\mathcal{B}_z}$	$+\cos\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{c}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{c}(\Omega_n)\right]$ $-m\,\mu_n\sin\varphi_n\, \tilde{Y}_{lm}^{s}(\Omega_n)$	$\cos\varphi_n \left[\tilde{C}_{lm}\tilde{Y}_{l-1,m}^{s}(\Omega_n) - l\mu_n\tilde{Y}_{lm}^{s}(\Omega_n)\right]$ $+m\,\mu_n\sin\varphi_n\, \tilde{Y}_{lm}^{c}(\Omega_n)$
	$\boldsymbol{\mathcal{M}}_{nn'}$ **for** $\boldsymbol{l} = \boldsymbol{0}$	
All	0	0

For the case of $\mu_n = \pm 1$, the elements $\boldsymbol{\mathcal{M}}_{nn'}$ take on different forms (see Appendix B for details).

	$\boldsymbol{\mathcal{M}}_{nn'}$ **for** $\boldsymbol{\mu} = \pm\mathbf{1}$ **and** $\boldsymbol{m} \neq \mathbf{1}$	
	Cosine Moments	**Sine Moments**
All	0	0
	$\boldsymbol{\mathcal{M}}_{nn'}$ **for** $\boldsymbol{\mu} = \pm\mathbf{1}$ **and** $\boldsymbol{m} = \mathbf{1}$	
	Cosine Moments	**Sine Moments**
$\boldsymbol{\mathcal{E}_x}$	0	0
$\boldsymbol{\mathcal{E}_y}$	$-\mu C_l^*(\mu)$	0
$\boldsymbol{\mathcal{E}_z}$	0	$-\mu C_l^*(\mu)$
$\boldsymbol{\mathcal{B}_x}$	0	0
$\boldsymbol{\mathcal{B}_y}$	0	$-C_l^*(\mu)$
$\boldsymbol{\mathcal{B}_z}$	$C_l^*(\mu)$	0

$$C_l^*(1) = \frac{1}{2} l(l+1) C_{l1} = \left[\frac{l(l+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}$$

$$C_l^*(-1) = \frac{1}{2} (-1)^l l(l+1) C_{l1} = (-1)^l \left[\frac{l(l+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}$$

For the first-order transport (sweep) solver one can rewrite Eq. (56) for each direction $\vec{\Omega}_n$

$$\frac{1}{c\beta(E)}\frac{\partial\psi_n}{\partial t}+\vec{\Omega}_n\cdot\boldsymbol{\nabla}\psi_n+\sigma\psi_n+q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}_n\right)\left[\frac{\partial\psi_n}{\partial E}-\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\psi_n\right]$$
$$=S_n-\frac{q}{\mathcal{D}(E)}\left\{\mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right]_n+\mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]_n+\mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]_n\right\}\boldsymbol{\phi}$$
$$-\frac{qc\beta(E)}{\mathcal{D}(E)}\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right]_n+\mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]_n+\mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]_n\right\}\boldsymbol{\phi} \tag{57}$$

where $\psi_n=\psi\left(\vec{r},E,\vec{\Omega}_n,t\right)$, $\boldsymbol{\phi}$ is a column vector containing the angular moments, $[\boldsymbol{\mathcal{M}}]_n$ is the *n*th row of the moment-to-discrete matrix $[\boldsymbol{\mathcal{M}}]$, and S_n contains the within-group scattering source, the between-group scattering source and the external source for the direction $\vec{\Omega}_n$.

For the second-order solvers Eq. (56) may be the preferable form with all the angular flux cast in a vector form:

$$\frac{1}{c\beta(E)}\frac{\partial\boldsymbol{\psi}}{\partial t}+\vec{\Omega}\cdot\boldsymbol{\nabla}\boldsymbol{\psi}+\sigma\boldsymbol{\psi}+q\left(\vec{\mathcal{E}}\cdot\vec{\Omega}\right)\left[\frac{\partial\boldsymbol{\psi}}{\partial E}-\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\boldsymbol{\psi}\right]$$
$$+\frac{q}{\mathcal{D}(E)}\left\{\mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right]+\mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]+\mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]\right\}[\boldsymbol{D}]\boldsymbol{\psi}$$
$$+\frac{qc\beta(E)}{\mathcal{D}(E)}\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right]+\mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]+\mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]\right\}[\boldsymbol{D}]\boldsymbol{\psi}=\boldsymbol{S} \tag{56}$$

4. Discontinuous Finite-Element Methods in Energy and Space

We have applied the discrete-ordinates method to treat the angular redistribution from the EM fields. The other discretization schemes employed are

- Discontinuous finite-element method (DFEM) in space
- Discontinuous finite-element method in energy

More details of these discrization schemes can be found in References 7 and 8. We will first ignore the time dependence and concentrate on the angularly discretized equations for the first-order solver.

$$\begin{aligned}
&\vec{\Omega}_n \cdot \boldsymbol{\nabla}\psi_n + \sigma\psi_n + q\left(\vec{\mathcal{E}} \cdot \vec{\Omega}_n\right)\left[\frac{\partial \psi_n}{\partial E} - \frac{1 + 4\beta^2(E)}{\mathcal{D}(E)}\psi_n\right] \\
&= S_n - \frac{q}{\mathcal{D}(E)}\left\{ \mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right]_n + \mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]_n + \mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]_n\right\}\boldsymbol{\phi} \\
&\quad - \frac{qc\beta(E)}{\mathcal{D}(E)}\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right]_n + \mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]_n + \mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]_n\right\}\boldsymbol{\phi}
\end{aligned} \tag{57}$$

$$\psi_n = \psi_n(\vec{r}, E)$$

$$\boldsymbol{\phi} = \boldsymbol{\phi}(\vec{r}, E)$$

$$S_n = S_n(\vec{r}, E)$$

Expand the angular flux as

$$\psi_n(\vec{r}, E) = \sum_{i=1}^{I} H_i\,(\vec{r}\,) \sum_{j=1}^{J} G_j(\,E)\psi_{ij}\left(\vec{\Omega}_n\right) \tag{58}$$

where $H_i(\vec{r}\,)$ is the *i*th basis function in space, $G_j(\,E)$ is the *j*th basis function in energy, and $\psi_{ij}\left(\vec{\Omega}_n\right)$ are the expansion coefficients. To derive the DFEM equations, we start by substituting the expansion Eq. (58) into Eq. (57), multiplying the result by $H_i(\vec{r}\,)G_j(\,E)$ and integrating the result over an elemental volume V_e and an energy bin $[E_g, E_{g-1}]$. The integrals involving the gradient terms ($\vec{\Omega}_n \cdot \boldsymbol{\nabla}\psi_n$ and $\frac{\partial \psi_n}{\partial E}$) are separated into a surface integral and a volume integral, which allow the angular flux at the surface to be different from the interior angular flux within an element. Details of DFEM formulation are given in Appendix D.

For a given pair of element-group the angular fluxes (a total of *IJ* unknowns) can be arranged into a column vector:

$$\mathbf{\Psi} = \begin{bmatrix} \mathbf{\Psi}_1 \\ \mathbf{\Psi}_2 \\ \vdots \\ \mathbf{\Psi}_J \end{bmatrix} \tag{59}$$

$$\mathbf{\Psi}_j = \begin{bmatrix} \psi_{1j}(\vec{\Omega}) \\ \psi_{2j}(\vec{\Omega}) \\ \vdots \\ \psi_{Ij}(\vec{\Omega}) \end{bmatrix} \tag{60}$$

For example, a piecewise linear differencing in energy with tetrahedral element will lead to 8 angular unknowns.

The DFEM formulation leads to the following system for **$\mathbf{\Psi}$:**

$$[\boldsymbol{\mathcal{L}}]\mathbf{\Psi} + [\boldsymbol{\mathcal{C}}]\mathbf{\Psi} + [\boldsymbol{\mathcal{P}}]\mathbf{\Psi} - [\boldsymbol{\mathcal{Q}}]\mathbf{\Psi} = \boldsymbol{\mathcal{S}} - \boldsymbol{\mathcal{R}}_{\boldsymbol{\mathcal{E}}} - \boldsymbol{\mathcal{R}}_{\boldsymbol{\mathcal{B}}} \tag{61}$$

The vectors $\boldsymbol{\mathcal{S}}, \boldsymbol{\mathcal{R}}_{\boldsymbol{\mathcal{E}}}$ and $\boldsymbol{\mathcal{R}}_{\boldsymbol{\mathcal{B}}}$ are arranged in the order as $\mathbf{\Psi}$.

Streaming Term

$$[\boldsymbol{\mathcal{L}}]\mathbf{\Psi} = \sum_{\boldsymbol{k=1}}^{N_k} [\boldsymbol{\mathcal{L}}_{A_k}]\mathbf{\Psi} - [\boldsymbol{\mathcal{L}}_V]\mathbf{\Psi} \tag{62}$$

$$[\boldsymbol{\mathcal{L}}_{A_k}]\mathbf{\Psi} = \vec{\Omega} \cdot \begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{H}}_{A_k} & \mathcal{G}_{12}\boldsymbol{\mathcal{H}}_{A_k} & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{H}}_{A_k} \\ \mathcal{G}_{21}\boldsymbol{\mathcal{H}}_{A_k} & \mathcal{G}_{22}\boldsymbol{\mathcal{H}}_{A_k} & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{H}}_{A_k} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{H}}_{A_k} & \mathcal{G}_{J2}\boldsymbol{\mathcal{H}}_{A_k} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{H}}_{A_k} \end{bmatrix} \begin{bmatrix} \mathbf{\Psi}_1 \\ \mathbf{\Psi}_2 \\ \vdots \\ \mathbf{\Psi}_J \end{bmatrix} \tag{62a}$$

$$[\boldsymbol{\mathcal{L}}_V]\mathbf{\Psi} = \vec{\Omega} \cdot \begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{H}}_V & \mathcal{G}_{12}\boldsymbol{\mathcal{H}}_V & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{H}}_V \\ \mathcal{G}_{21}\boldsymbol{\mathcal{H}}_V & \mathcal{G}_{22}\boldsymbol{\mathcal{H}}_V & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{H}}_V \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{H}}_V & \mathcal{G}_{J2}\boldsymbol{\mathcal{H}}_V & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{H}}_V \end{bmatrix} \begin{bmatrix} \mathbf{\Psi}_1 \\ \mathbf{\Psi}_2 \\ \vdots \\ \mathbf{\Psi}_J \end{bmatrix} \tag{62b}$$

$$\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} = \text{an } I \times I \text{ matrix of vectors } = \left[\vec{\mathcal{H}}_{A_k ii'}\right] \tag{62c}$$

$$\vec{\mathcal{H}}_{A_k ii'} = \int_{A_k} dA \vec{n}_k H_i(\vec{r}\,) H_{\boldsymbol{i}'}(\vec{r}\,) \tag{62d}$$

$$\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} = \text{an } I \times I \text{ matrix of vectors } = \left[\vec{\mathcal{H}}_{Vii'}\right] \tag{62e}$$

$$\vec{\mathcal{H}}_{Vii'} = \int_{V_e} dV [\boldsymbol{\nabla} H_i(\vec{r}\,)] H_{\boldsymbol{i}'}(\vec{r}\,) \tag{62f}$$

$$\mathcal{G}_{jj'} = \int_{E_g}^{E_{g-1}} dE\, G_j(\,E) G_{j'}(\,E) \tag{62g}$$

where N_k is the number of faces and A_k is the kth face of an element. It is noted that the term $\left[\boldsymbol{\mathcal{L}}_{\boldsymbol{A_k}}\right]\boldsymbol{\Psi}$ consists of the angular fluxes on the surfaces and will be moved to RHS for $\vec{n}_k \cdot \vec{\Omega} < 0$.

Collision Term

$$[\boldsymbol{\mathcal{C}}]\boldsymbol{\Psi} = \begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{H}} & \mathcal{G}_{12}\boldsymbol{\mathcal{H}} & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{H}} \\ \mathcal{G}_{21}\boldsymbol{\mathcal{H}} & \mathcal{G}_{22}\boldsymbol{\mathcal{H}} & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{H}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{H}} & \mathcal{G}_{J2}\boldsymbol{\mathcal{H}} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{H}} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J \end{bmatrix} \tag{63}$$

$$\boldsymbol{\mathcal{H}} = \text{an } I \times I \text{ matrix } = [\mathcal{H}_{ii'}] \tag{63a}$$

$$\mathcal{H}_{ii'} = \int_{V_e} dV H_i(\vec{r}\,) H_{\boldsymbol{i}'}(\vec{r}\,) \tag{63b}$$

Energy Redistribution from Electric Field $\left[\frac{\partial \psi}{\partial E}\right]$

$$[\boldsymbol{\mathcal{P}}]\boldsymbol{\Psi} = \left[\boldsymbol{\mathcal{P}}_{\boldsymbol{g-1}}\right]\boldsymbol{\Psi} - \left[\boldsymbol{\mathcal{P}}_{\boldsymbol{g}}\right]\boldsymbol{\Psi} - \left[\widetilde{\boldsymbol{\mathcal{P}}}\right]\boldsymbol{\Psi} \tag{64}$$

$$[\boldsymbol{\mathcal{P}}_{\boldsymbol{g}}]\boldsymbol{\Psi} = q\vec{\Omega}\cdot\begin{bmatrix}\mathcal{P}_{11}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{P}_{12}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{P}_{1J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \mathcal{P}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{P}_{22}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{P}_{2J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{P}_{J1}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{P}_{J2}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{P}_{JJ}\boldsymbol{\mathcal{H}}_{\mathcal{E}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \quad \text{at } E_g \tag{64a}$$

$$\mathcal{P}_{jj'}(E) = G_j(E)G_{j'}(E) \tag{64b}$$

$$\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} = \text{an } I \times I \text{ matrix of vectors } = [\vec{\mathcal{H}}_{\mathcal{E}ii'}] \tag{64c}$$

$$\vec{\mathcal{H}}_{\mathcal{E}ii'} = \int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})H_{\boldsymbol{i'}}(\vec{r}) \tag{64d}$$

$$[\tilde{\boldsymbol{\mathcal{P}}}]\boldsymbol{\Psi} = \vec{\Omega}\cdot\begin{bmatrix}\tilde{\mathcal{P}}_{11}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \tilde{\mathcal{P}}_{12}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \tilde{\mathcal{P}}_{1J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \tilde{\mathcal{P}}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \tilde{\mathcal{P}}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \tilde{\mathcal{P}}_{2J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\mathcal{P}}_{J1}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \tilde{\mathcal{P}}_{J2}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \tilde{\mathcal{P}}_{JJ}\boldsymbol{\mathcal{H}}_{\mathcal{E}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \tag{64e}$$

$$\tilde{\mathcal{P}}_{jj'} = \int_{E_g}^{E_{g-1}} dE\left[\frac{\partial}{\partial E}G_j(E)\right]G_{j'}(E) \tag{64f}$$

It is noted that the terms $[\boldsymbol{\mathcal{P}}_{\boldsymbol{g-1}}]\boldsymbol{\Psi}$ and $[\boldsymbol{\mathcal{P}}_{\boldsymbol{g}}]\boldsymbol{\Psi}$ consist of the angular fluxes on the energy-bin boundaries and may be moved to RHS depending on the sign of $\vec{\Omega}\cdot\vec{\mathcal{E}}$ and the direction of sweep in energy.

Energy Redistribution from Electric Field $\left[\frac{\mathbf{1+4}\boldsymbol{\beta}^{\mathbf{2}}(\boldsymbol{E})}{\boldsymbol{\mathcal{D}}(\boldsymbol{E})}\boldsymbol{\psi}\right]$

$$[\boldsymbol{Q}]\boldsymbol{\Psi} = q\vec{\Omega}\cdot\begin{bmatrix}\mathcal{Q}_{11}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{Q}_{12}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{Q}_{1J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \mathcal{Q}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{Q}_{22}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{Q}_{2J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{Q}_{J1}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{Q}_{J2}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{Q}_{JJ}\boldsymbol{\mathcal{H}}_{\mathcal{E}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \tag{65}$$

$$\mathcal{Q}_{jj'} = \int_{E_g}^{E_{g-1}} dE \frac{1+4\beta^2(E)}{\mathcal{D}(E)} G_j(E) G_{j'}(E) \quad (65a)$$

Angular Redistribution due to Electric Field

For a specific direction $\vec{\Omega}_n$, the angular redistribution term for the *i*th spatial basis function and the *j*th basis function in energy is

$$\boldsymbol{\mathcal{R}}_{\mathcal{E}} = \boldsymbol{\mathcal{R}}_{\mathcal{E}_x} + \boldsymbol{\mathcal{R}}_{\mathcal{E}_y} + \boldsymbol{\mathcal{R}}_{\mathcal{E}_z} \quad (66)$$

$$\mathcal{R}_{\mathcal{E}nij} = q \sum_{i'=1}^{I} \left(\mathcal{H}_{\mathcal{E}_x ii'} \left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right]_n + \mathcal{H}_{\mathcal{E}_y ii'} \left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]_n + \mathcal{H}_{\mathcal{E}_z ii'} \left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]_n \right) \left[\sum_{j'=1}^{J} \tilde{\mathcal{G}}_{jj'} \boldsymbol{\phi}_{i'j'} \right] \quad (66a)$$

$$\mathcal{H}_{\mathcal{E}ii'} = \int_{V_e} dV \mathcal{E} H_i(\vec{r}) H_{\boldsymbol{i'}}(\vec{r}) \quad (66b)$$

$$\tilde{\mathcal{G}}_{jj'} = \int_{E_g}^{E_{g-1}} dE \frac{1}{\mathcal{D}(E)} G_j(E) G_{j'}(E) \quad (66c)$$

where the symbol $\mathcal{E}$ is used to denote one of the three components of the electric field $(\mathcal{E}_x, \mathcal{E}_y, \mathcal{E}_z)$, $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n$ is the *n*th row of the moment-to-discrete matrix $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]$ defined previously and $\boldsymbol{\phi}_{ij}$ is a column vector containing the expansion coefficients of the angular moments corresponding to the *i*th basis function in space and the *j*th basis function in energy.

Angular Redistribution due to Magnetic Field

For a specific direction $\vec{\Omega}_n$, the angular redistribution term for the *i*th spatial basis function and the *j*th basis function in energy is

$$\boldsymbol{\mathcal{R}}_{\mathcal{B}} = \boldsymbol{\mathcal{R}}_{\mathcal{B}_x} + \boldsymbol{\mathcal{R}}_{\mathcal{B}_y} + \boldsymbol{\mathcal{R}}_{\mathcal{B}_z} \quad (67)$$

$$\mathcal{R}_{\mathcal{B}nij} = q \sum_{i'=1}^{I} \left(\mathcal{H}_{\mathcal{B}_x ii'} \left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right]_n + \mathcal{H}_{\mathcal{B}_y ii'} \left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]_n + \mathcal{H}_{\mathcal{B}_z ii'} \left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]_n \right) \left[\sum_{j'=1}^{J} \mathcal{G}_{jj'}^{*} \boldsymbol{\phi}_{i'j'} \right] \quad (67a)$$

$$\mathcal{R}_{\mathcal{B}nij} = \sum_{i=1}^{I} \mathcal{H}_{\mathcal{B}ii'} \sum_{j=1}^{J} \mathcal{G}_{jj'}^{*} [\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n \boldsymbol{\phi}_{i'j'} \tag{67b}$$

$$\mathcal{H}_{\mathcal{B}ii'} = \int_{V_e} dV \mathcal{B} H_i(\vec{r}\,) H_{\boldsymbol{i'}}(\vec{r}\,) \tag{67c}$$

$$\mathcal{G}_{jj'}^{*} = c \int_{E_g}^{E_{g-1}} dE \frac{\beta(E)}{\mathcal{D}(E)} G_j(\,E) G_{j'}(\,E) \tag{67b}$$

where the symbol $\mathcal{B}$ is used to denote one of the three components of the magnetic field $(\mathcal{B}_x, \mathcal{B}_y, \mathcal{B}_z)$ and $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n$ is the *n*th row of the moment-to-discrete matrix $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]$ as given previously.

5. Finite-Element Methods in Angle

Finite-element methods have also been applied to the angular variable, but to a less extent than to the spatial and energy variables. In this work, we have applied both continuous and discontinuous finite-element methods to treat the angular dependence of the EM terms.

Expand the angular flux as

$$\psi(\vec{r}, E, \vec{\Omega}) = \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E) \sum_{k=1}^{K} W_k(\vec{\Omega}) \psi_{ijk} \tag{68}$$

where $H_i(\vec{r})$ is the *i*th basis function in space, $G_j(E)$ is the *j*th basis function in energy, $W_k(\vec{\Omega})$ is the kth basis function in angle, and ψ_{ijk} are the expansion coefficients to be solved.

Elemental equations for the expansion coefficients can be derived by applying the Galerkin method similar to that outlines in the previous section. Detailed descriptions of these can be found in References 9 and 10.

Conclusions

We have developed a mathematical model, by including the effects of Lorentz force in the Boltzmann transport equation, for electron transport with electromagnetic fields. Two deterministic, numerical techniques are developed to treat the energy- and angular-redistribution due to the electromagnetic fields.

In the first approach, we apply the traditional discrete-ordinates method to discretize the differential, angular redistribution terms with the spatial- and energy-dependence are treated with discontinuous finite-element methods. The discrete system can be arranged into a form very similar to that encountered in standard radiation transport. More specifically, the energy- and angular-redistribution operators are transformed into a series of scattering matrices. However, convergence of this approach is highly problematic when applying the source iteration. In the second approach, we apply the discontinuous finite-element methods to the entire phase space in which the angular flux is represented by a triple-product of basis functions in space, energy and angle. Despite of its complexity, this approach offers two advantages: convergence of the source iteration is less problematic and improved accuracy in angular flux.

We have also demonstrated full coupling between the transport and electromagnetic solvers via a staggered time advancing scheme on a problem involving propagation of an electron beam over a diode. There are significant discrepancies between our results and EMPHASI-PIC calculation which require further investigations.

The finite-element methods and the software components developed in this research project should be productized and incorporated into the existing radiation transport capability at Sandia. In particular,

1. Finite-element in angle can improve accuracy and mitigate the notorious ray-effects associated with the discrete-ordinates method for problems involving localized source,
2. Finite-element in energy can be extended to the continuous slowing-down (CSD) approximation in electron transport and eliminate the numerical straggling associated with the finite-differencing scheme commonly applied to the Boltzmann-CSD equation.

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Appendix A. Modified Spherical Harmonics

In SCEPTRE, the angular flux is represented by a finite expansion in terms of spherical harmonics as

$$\Psi(\Omega) = \sum_{l=0}^{L} \sum_{m=0}^{l} [Y_{lm}^{c}(\Omega)\phi_{lm}^{c} + Y_{lm}^{s}(\Omega)\phi_{lm}^{s}] \quad \text{(A1)}$$

The real and imaginary parts of the spherical harmonics are defined by

$$Y_{lm}^{c}(\Omega) = Y_{lm}^{c}(\mu,\varphi) = C_{lm} P_{l}^{m}(\mu) \cos m\varphi \quad \text{(A2)}$$

$$Y_{lm}^{s}(\Omega) = Y_{lm}^{s}(\mu,\varphi) = C_{lm} P_{l}^{m}(\mu) \sin m\varphi \quad \text{(A3)}$$

where $P_l^m(\mu)$ is the associated Legendre polynomial of order *l* and degree *m*,

$$P_{l}^{m}(\mu) = (-1)^{\mathrm{m}}(1-\mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu) \quad \text{(A4)}$$

$$C_{lm} = \left[\frac{2l+1}{4\pi}(2-\delta_{m0})\frac{(l-m)!}{(l+m)!}\right]^{1/2} \quad \text{(A5)}$$

$$\begin{aligned}\frac{\partial\psi}{\partial\mu} &= \frac{\partial}{\partial\mu}\sum_{l=0}^{L}\sum_{m=0}^{l}[C_{lm}P_l^m(\mu)\cos m\varphi\,\phi_{lm}^{c} + C_{lm}P_l^m(\mu)\sin m\varphi\phi_{lm}^{s}] \\ &= \sum_{l=1}^{L}\sum_{m=0}^{l}[C_{lm}\cos m\varphi\phi_{lm}^{c} + C_{lm}\sin m\varphi\,\phi_{lm}^{s}]\frac{\partial}{\partial\mu}P_l^m(\mu)\end{aligned}$$

From Wolfran's Mathworld (http://mathworld.wolfram.com/LegendrePolynomial.html)

$$(1-\mu^2)\frac{\partial}{\partial\mu}P_l^m(\mu) = (l+m)P_{l-1}^m(\mu) - l\mu P_l^m(\mu) \quad \text{for } l > 0 \text{ and } m < l \quad \text{(A6)}$$

$$(1-\mu^2)\frac{\partial}{\partial\mu}P_l^l(\mu) = -l\mu P_l^l(\mu) \quad \text{for } l > 0 \quad \text{(A7)}$$

$$P_l^m(\mu) = 0 \quad \text{for } m > l \quad \text{(A8)}$$

$$\begin{aligned}\frac{\partial\psi}{\partial\mu} &= \frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}[C_{lm}\cos m\varphi\phi_{lm}^c + C_{lm}\sin m\varphi\phi_{lm}^s]\,[(l+m)P_{l-1}^m(\mu) - l\mu P_l^m(\mu)] \\ &= \frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}(l+m)[C_{lm}P_{l-1}^m(\mu)\cos m\varphi\,\phi_{lm}^c + C_{lm}\,P_{l-1}^m(\mu)\sin m\varphi\phi_{lm}^s] \\ &\quad -\frac{\mu}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l} l[C_{lm}P_l^m(\mu)\cos m\varphi\,\phi_{lm}^c + C_{lm}\,P_l^m(\mu)\sin m\varphi\phi_{lm}^s]\end{aligned} \tag{A9}$$

From Eq. (A5), it can be shown that

$$\frac{C_{lm}}{C_{l-1,m}} = \frac{\left[\frac{2l+1}{4\pi}(2-\delta_{m0})\frac{(l-m)!}{(l+m)!}\right]^{1/2}}{\left[\frac{2l-1}{4\pi}(2-\delta_{m0})\frac{(l-m-1)!}{(l+m-1)!}\right]^{1/2}} = \left[\frac{2l+1}{2l-1}\frac{l-m}{l+m}\right]^{1/2}$$

$$\begin{aligned}\frac{\partial\psi}{\partial\mu} &= \frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}\left[\frac{2l+1}{2l-1}(l-m)(l+m)\right]^{1/2}[Y_{l-1,m}^c(\Omega)\phi_{lm}^c + Y_{l-1,m}^s(\Omega)\phi_{lm}^s] \\ &\quad -\frac{\mu}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l} l[Y_{lm}^c(\Omega)\phi_{lm}^c + Y_{lm}^s(\Omega)\phi_{lm}^s] \\ &= \frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}\left\{\left[\frac{2l+1}{2l-1}(l-m)(l+m)\right]^{1/2} Y_{l-1,m}^c(\Omega) - l\mu Y_{lm}^c(\Omega)\right\}\phi_{lm}^c \\ &\quad +\frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}\left\{\left[\frac{2l+1}{2l-1}(l-m)(l+m)\right]^{1/2} Y_{l-1,m}^s(\Omega) - l\mu Y_{lm}^s(\Omega)\right\}\phi_{lm}^s\end{aligned} \tag{A10}$$

Define the modified spherical harmonics as

$$\tilde{Y}_{lm}^c(\Omega) = \frac{Y_{lm}^c}{\sqrt{1-\mu^2}} \tag{A11}$$

$$\tilde{Y}_{lm}^s(\Omega) = \frac{Y_{lm}^S}{\sqrt{1-\mu^2}} \tag{A12}$$

$$\tilde{Y}_{lm}^c(\Omega) = \tilde{Y}_{lm}^s(\Omega) = 0 \quad \text{for } m > l \tag{A13}$$

$$\tilde{C}_{lm} = \left[\frac{2l+1}{2l-1}(l-m)(l+m)\right]^{1/2} \tag{A14}$$

$$\begin{aligned}\frac{\partial\psi}{\partial\mu} &= \frac{1}{1-\mu^2}\sum_{l=1}^{L}\sum_{m=0}^{l}\left\{\left[\tilde{C}_{lm}Y_{lm}^{c}(\Omega) - l\mu Y_{lm}^{c}(\Omega)\right]\phi_{lm}^{c} + \left[\tilde{C}_{lm}Y_{lm}^{s}(\Omega) - l\mu Y_{lm}^{s}(\Omega)\right]\phi_{lm}^{s}\right\} \\ &= \frac{1}{\sqrt{1-\mu^2}}\sum_{l=1}^{L}\sum_{m=0}^{l}\left\{\left[\tilde{C}_{lm}\tilde{Y}_{lm}^{c}(\Omega) - l\mu \tilde{Y}_{lm}^{c}(\Omega)\right]\phi_{lm}^{c} + \left[\tilde{C}_{lm}\tilde{Y}_{lm}^{s}(\Omega) - l\mu \tilde{Y}_{lm}^{s}(\Omega)\right]\phi_{lm}^{s}\right\}\end{aligned} \tag{A15}$$

$$\begin{aligned}\frac{\partial\psi}{\partial\varphi} &= \frac{\partial}{\partial\varphi}\sum_{l=0}^{L}\sum_{m=0}^{l}\left[\phi_{lm}^{c}C_{lm}P_l^m(\mu)\cos m\varphi + \phi_{lm}^{s}C_{lm}P_l^m(\mu)\sin m\varphi\right] \\ &= \sum_{l=1}^{L}\sum_{m=0}^{l} m\left[\phi_{lm}^{s}C_{lm}P_l^m(\mu)\cos m\varphi - \phi_{lm}^{c}C_{lm}P_l^m(\mu)\sin m\varphi\right] \\ &= -\sum_{l=1}^{L}\sum_{m=0}^{l} m\left[Y_{lm}^{s}(\Omega)\phi_{lm}^{c} - Y_{lm}^{c}(\Omega)\phi_{lm}^{s}\right]\end{aligned} \tag{A16}$$

More on Modified Spherical Harmonics

The modified spherical harmonics are defined by

$$\tilde{Y}_{lm}^{c}(\Omega) = \frac{Y_{lm}^{c}}{\sqrt{1-\mu^2}} = C_{lm}\frac{P_l^m(\mu)}{\sqrt{1-\mu^2}}\cos m\varphi = C_{lm}\tilde{P}_l^m(\mu)\cos m\varphi \tag{A17}$$

$$\tilde{Y}_{lm}^{s}(\Omega) = \frac{Y_{lm}^{s}}{\sqrt{1-\mu^2}} = C_{lm}\frac{P_l^m(\mu)}{\sqrt{1-\mu^2}}\sin m\varphi = C_{lm}\tilde{P}_l^m(\mu)\sin m\varphi \tag{A18}$$

where $\tilde{P}_l^m(\mu)$ is the modified, associated Legendre polynomial,

$$\tilde{P}_l^m(\mu) = (-1)^{\mathrm{m}}(1-\mu^2)^{(m-1)/2}\frac{d^m}{d\mu^m}P_l(\mu) \tag{A19}$$

It can be easily shown that for $m > 1$

$$\lim_{\mu\to\pm1}\tilde{P}_l^m(\mu) = 0 \tag{A20}$$

For $m = 1$, $\tilde{P}_l^1(\mu) = -\frac{d}{d\mu}P_l(\mu)$

$$\lim_{\mu \to 1} \tilde{P}_l^1(\mu) = -\lim_{\mu \to 1} \frac{d}{d\mu} P_l(\mu) = -\frac{1}{2} l(l+1) \tag{A21}$$

$$\lim_{\mu \to -1} \tilde{P}_l^1(\mu) = -\lim_{\mu \to -1} \frac{d}{d\mu} P_l(\mu) = \frac{1}{2} (-1)^l l(l+1) \tag{A22}$$

Appendix B. Moment-To-Discrete Matrices for $\boldsymbol{\mu = \pm 1}$

Here we consider the limits of the elements in the moment-to-discrete matrices in the case of $\mu = \pm 1$. Since these elements consist of either the associated Legendre $P_l^m(\mu)$

$$P_l^m(\mu) = (-1)^{\mathrm{m}}(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_l(\mu) \tag{B1}$$

or the modified, associated Legendre $\tilde{P}_l^m(\mu)$

$$\tilde{P}_l^m(\mu) = (-1)^{\mathrm{m}}(1-\mu^2)^{(m-1)/2}\frac{d^m}{d\mu^m}P_l(\mu) \tag{B2}$$

and these polynomials vanish for the case $\mu = \pm 1$ for $m \geq 2$,

$$\boldsymbol{\mathcal{M}_{nn'}} = 0 \quad \text{for } m \geq 2 \tag{B3}$$

For $l > 0$ and $m = 0$, we only need to examine terms consists of $\tilde{C}_{lm}\tilde{Y}_{l-1,m}^c(\Omega_n) - l\mu_n\tilde{Y}_{lm}^c(\Omega_n)$ since all other terms vanish for $\mu = \pm 1$

$$\begin{aligned}
\boldsymbol{\mathcal{M}_{nn'}} &\propto \left(\frac{2l+1}{2l-1}\right)^{\frac{1}{2}} l\tilde{Y}_{l-1,0}^c(\Omega) - l\mu\tilde{Y}_{l0}^c(\Omega) \\
&\propto\ l\left(\frac{2l+1}{2l-1}\right)^{\frac{1}{2}}\sqrt{2l-1}\tilde{P}_{l-1}(\mu) - l\mu\sqrt{2l+1}\tilde{P}_l(\mu) \\
&\propto l\sqrt{2l+1}\frac{P_{l-1}(\mu) - \mu P_l(\mu)}{\sqrt{1-\mu^2}}
\end{aligned}$$

$$\lim_{\mu\to 1}\boldsymbol{\mathcal{M}_{nn'}} \propto \lim_{\mu\to 1}\frac{P_{l-1}(\mu) - \mu P_l(\mu)}{\sqrt{1-\mu^2}} = \lim_{\mu\to 1}\frac{1-\mu}{\sqrt{1-\mu^2}} = \lim_{\mu\to 1}\sqrt{\frac{1-\mu}{1+\mu}} = 0 \tag{B4}$$

$$\begin{aligned}
\lim_{\mu\to -1}\boldsymbol{\mathcal{M}_{nn'}} &\propto \lim_{\mu\to -1}\frac{P_{l-1}(\mu) - \mu P_l(\mu)}{\sqrt{1-\mu^2}} \\
&= (-1)^{l-1}\lim_{\mu\to -1}\frac{1+\mu}{\sqrt{1-\mu^2}} = (-1)^{l-1}\lim_{\mu\to -1}\sqrt{\frac{1+\mu}{1-\mu}} = 0
\end{aligned} \tag{B5}$$

For $m = 1$, $\frac{\partial\psi}{\partial\mu}$ becomes (from Eq. (63))

$$\frac{\partial\psi}{\partial\mu} = \frac{1}{1-\mu^2}\sum_{l=1}^{L} C_{l1}[(l+1)P_{l-1}^{1}(\mu) - l\mu P_l^1(\mu)](\cos\varphi\phi_{l1}^{c} + \sin\varphi\phi_{l1}^{s})$$

Since

$$P_l^1(\mu) = -(1-\mu^2)^{1/2}\frac{d}{d\mu}P_l(\mu)$$

the last expression of $\frac{\partial\psi}{\partial\mu}$ can be written as

$$\frac{\partial\psi}{\partial\mu} = \frac{1}{\sqrt{1-\mu^2}}\sum_{l=1}^{L} C_{l1}\left[l\mu\frac{d}{d\mu}P_l(\mu) - (l+1)\frac{d}{d\mu}P_{l-1}(\mu)\right](\cos\varphi\phi_{l1}^{c} + \sin\varphi\phi_{l1}^{s})$$

Using the recurrence relation

$$\frac{d}{d\mu}P_{l-1}(\mu) = \mu\frac{d}{d\mu}P_l(\mu) - lP_l(\mu)$$

$$\frac{\partial\psi}{\partial\mu} = \frac{1}{\sqrt{1-\mu^2}}\sum_{l=1}^{L} C_{l1}\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right](cos\,\varphi\phi_{l1}^{c} + sin\,\varphi\phi_{l1}^{s}) \tag{B7}$$

For $m = 1$, $\frac{\partial\psi}{\partial\varphi}$ becomes (from Eq. (64))

$$\frac{\partial\psi}{\partial\varphi} = -\sum_{l=1}^{L}[Y_{l1}^{s}(\Omega)\phi_{lm}^{c} - Y_{l1}^{c}(\Omega)\phi_{lm}^{s}] = \sqrt{1-\mu^2}\sum_{l=1}^{L} C_{l1}\frac{d}{d\mu}P_l(\mu)(\sin\varphi\,\phi_{l1}^{c} - \cos\varphi\,\phi_{l1}^{s}) \tag{B8}$$

We will examine $\boldsymbol{\mathcal{M}_{nn'}}$ for each EM field component individually using (B7) and (B8).

$\boldsymbol{\mathcal{E}_x}$

$$\begin{aligned}(1-\mu^2)&\frac{\partial\psi}{\partial\mu}\\ &= (1-\mu^2)^{1/2}\sum_{l=1}^{L} C_{l1}\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right](cos\,\varphi\phi_{l1}^{c} + sin\,\varphi\phi_{l1}^{s})\\ &\longrightarrow 0 \quad as\;\; \mu \longrightarrow \pm 1\end{aligned} \tag{B9}$$

$\boldsymbol{\varepsilon_y}$

$$
\begin{aligned}
&-\mu\eta\frac{\partial\psi}{\partial\mu}-\frac{\xi}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\\
&=-\mu\cos\varphi\sum_{l=1}^{L}C_{l1}\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right](cos\,\varphi\phi_{l1}^c+sin\,\varphi\phi_{l1}^s)\\
&\quad-\sin\varphi\sum_{l=1}^{L}C_{l1}\frac{d}{d\mu}P_l(\mu)(\sin\varphi\,\phi_{l1}^c-\cos\varphi\,\phi_{l1}^s)\\
&=-\sum_{l=1}^{L}C_{l1}\left\{\mu\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right]cos^2\varphi+\frac{d}{d\mu}P_l(\mu)\sin^2\varphi\right\}\phi_{l1}^c\\
&\quad-\sum_{l=1}^{L}C_{l1}\left\{\mu\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right]\cos\varphi\sin\varphi-\frac{d}{d\mu}P_l(\mu)\cos\varphi\sin\varphi\right\}\phi_{l1}^s
\end{aligned}
$$

The Legendre polynomials satisfy the differential equation

$$(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+l(l+1)y=0 \tag{B10}$$

and satisfy the following:

$$
\begin{aligned}
&\mu\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right]\\
&=(\mu^2-1)\frac{d}{d\mu}P_l(\mu)-\mu(1-\mu^2)\frac{d^2}{d\mu^2}P_l(\mu)+\frac{d}{d\mu}P_l(\mu)
\end{aligned}
$$

$$\lim_{\mu\to1}\mu\frac{d}{d\mu}P_l(\mu)=\lim_{\mu\to1}\frac{1}{2}l(l+1)P_l(\mu)=\frac{1}{2}l(l+1) \tag{B11}$$

$$\lim_{\mu\to1}\frac{d}{d\mu}P_l(\mu)=\frac{1}{2}l(l+1) \tag{B11a}$$

$$\lim_{\mu\to-1}\mu\frac{d}{d\mu}P_l(\mu)=\lim_{\mu\to-1}\frac{1}{2}l(l+1)P_l(\mu)=\frac{1}{2}(-1)^l l(l+1) \tag{B12}$$

$$\lim_{\mu\to-1}\frac{d}{d\mu}P_l(\mu)=\frac{1}{2}(-1)^{l+1}l(l+1) \tag{B12a}$$

$$\lim_{\mu\to 1}\left(-\mu\eta\frac{\partial\psi}{\partial\mu}-\frac{\xi}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\right)=-\frac{1}{2}\sum_{l=1}^{L}l(l+1)C_{l1}\,\phi_{l1}^{c} \tag{B13}$$

$$\lim_{\mu\to -1}\left(-\mu\eta\frac{\partial\psi}{\partial\mu}-\frac{\xi}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\right)=-\frac{1}{2}\sum_{l=1}^{L}(-1)^{l+1}l(l+1)C_{l1}\,\phi_{l1}^{c} \tag{B14}$$

$\boldsymbol{\mathcal{E}_z}$

$$\begin{aligned}
&-\mu\xi\frac{\partial\psi}{\partial\mu}+\frac{\eta}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\\
&=-\mu\sin\varphi\sum_{l=1}^{L}C_{l1}\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right](cos\,\varphi\phi_{l1}^{c}+sin\,\varphi\phi_{l1}^{s})\\
&\quad+\cos\varphi\sum_{l=1}^{L}C_{l1}\frac{d}{d\mu}P_l(\mu)(\sin\varphi\,\phi_{l1}^{c}-\cos\varphi\,\phi_{l1}^{s})\\
&=-\sum_{l=1}^{L}C_{l1}\left\{\mu\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right]\cos\varphi\sin\varphi-\frac{d}{d\mu}P_l(\mu)\cos\varphi\sin\varphi\right\}\phi_{l1}^{c}\\
&\quad-\sum_{l=1}^{L}C_{l1}\left\{\mu\left[l(l+1)P_l(\mu)-\mu\frac{d}{d\mu}P_l(\mu)\right]\sin^2\varphi+\frac{d}{d\mu}P_l(\mu)\,cos^2\,\varphi\right\}\phi_{l1}^{s}
\end{aligned}$$

$$\lim_{\mu\to 1}\left(-\mu\xi\frac{\partial\psi}{\partial\mu}+\frac{\eta}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\right)=-\frac{1}{2}\sum_{l=1}^{L}l(l+1)C_{l1}\,\phi_{l1}^{s} \tag{B15}$$

$$\lim_{\mu\to -1}\left(-\mu\xi\frac{\partial\psi}{\partial\mu}+\frac{\eta}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\right)=-\frac{1}{2}\sum_{l=1}^{L}(-1)^{l+1}l(l+1)C_{l1}\,\phi_{l1}^{s} \tag{B16}$$

$\boldsymbol{\mathcal{B}_z}$

$$\eta \frac{\partial \psi}{\partial \mu} + \frac{\mu \xi}{1-\mu^2}\frac{\partial \psi}{\partial \varphi}$$

$$= \cos\varphi \sum_{l=1}^{L} C_{l1}\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right](cos\,\varphi\phi_{l1}^{c} + sin\,\varphi\phi_{l1}^{s})$$

$$+\mu\sin\varphi \sum_{l=1}^{L} C_{l1}\frac{d}{d\mu}P_l(\mu)(\sin\varphi\,\phi_{l1}^{c} - \cos\varphi\,\phi_{l1}^{s})$$

$$= \sum_{l=1}^{L} C_{l1}\left\{\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right]cos^2\,\varphi + \mu\frac{d}{d\mu}P_l(\mu)\sin^2\varphi\right\}\phi_{l1}^{c}$$

$$+\sum_{l=1}^{L} C_{l1}\left\{\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right]\cos\varphi\sin\varphi - \mu\frac{d}{d\mu}P_l(\mu)\cos\varphi\sin\varphi\right\}\phi_{l1}^{s}$$

$$\lim_{\mu\to 1}\left(\eta\frac{\partial \psi}{\partial \mu} + \frac{\mu\xi}{1-\mu^2}\frac{\partial \psi}{\partial \varphi}\right) = \frac{1}{2}\sum_{l=1}^{L} l(l+1)C_{l1}\,\phi_{l1}^{c} \qquad \text{(B17)}$$

$$\lim_{\mu\to -1}\left(\eta\frac{\partial \psi}{\partial \mu} + \frac{\mu\xi}{1-\mu^2}\frac{\partial \psi}{\partial \varphi}\right) = \frac{1}{2}\sum_{l=1}^{L} (-1)^l l(l+1)C_{l1}\,\phi_{l1}^{c} \qquad \text{(B18)}$$

$\boldsymbol{\mathcal{B}_y}$

$$-\xi\frac{\partial \psi}{\partial \mu} + \frac{\mu\eta}{1-\mu^2}\frac{\partial \psi}{\partial \varphi}$$

$$= -\sin\varphi \sum_{l=1}^{L} C_{l1}\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right](\cos\varphi\phi_{l1}^{c} + \sin\varphi\phi_{l1}^{s})$$

$$+\mu\cos\varphi \sum_{l=1}^{L} C_{l1}\frac{d}{d\mu}P_l(\mu)(\sin\varphi\,\phi_{l1}^{c} - \cos\varphi\,\phi_{l1}^{s})$$

$$= -\sum_{l=1}^{L} C_{l1}\left\{\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right]\cos\varphi\sin\varphi - \mu\frac{d}{d\mu}P_l(\mu)\cos\varphi\sin\varphi\right\}\phi_{l1}^{c}$$

$$-\sum_{l=1}^{L} C_{l1}\left\{\left[l(l+1)P_l(\mu) - \mu\frac{d}{d\mu}P_l(\mu)\right]\sin^2\varphi + \mu\frac{d}{d\mu}P_l(\mu)\cos^2\varphi\right\}\phi_{l1}^{s}$$

$$\lim_{\mu\to 1}\left(-\xi\frac{\partial \psi}{\partial \mu} + \frac{\mu\eta}{1-\mu^2}\frac{\partial \psi}{\partial \varphi}\right) = -\frac{1}{2}\sum_{l=1}^{L} l(l+1)C_{l1}\,\phi_{l1}^{s} \qquad \text{(77a)}$$

$$\lim_{\mu\to-1}\left(-\xi\frac{\partial\psi}{\partial\mu}+\frac{\mu\eta}{1-\mu^2}\frac{\partial\psi}{\partial\varphi}\right)=-\frac{1}{2}\sum_{l=1}^{L}(-1)^l l(l+1)C_{l1}\,\phi_{l1}^{s} \tag{77b}$$

$\boldsymbol{\mathcal{B}_x}$

$$\frac{\partial\psi}{\partial\varphi}=\sqrt{1-\mu^2}\sum_{l=1}^{L}C_{l1}\frac{d}{d\mu}P_l(\mu)(\sin\varphi\,\phi_{l1}^{c}-\cos\varphi\,\phi_{l1}^{s})\longrightarrow 0 \quad \text{as } \mu \longrightarrow \pm 1 \tag{78}$$

	$\boldsymbol{\mathcal{M}_{nn'}}$ **for** $\boldsymbol{\mu = \pm 1}$	
	Cosine Moments	**Sine Moments**
$\boldsymbol{\mathcal{E}_x}$	0	0
$\boldsymbol{\mathcal{E}_y}$	$-\mu C_l^*(\mu)$	0
$\boldsymbol{\mathcal{E}_z}$	0	$-\mu C_l^*(\mu)$
$\boldsymbol{\mathcal{B}_x}$	0	0
$\boldsymbol{\mathcal{B}_y}$	0	$-C_l^*(\mu)$
$\boldsymbol{\mathcal{B}_z}$	$C_l^*(\mu)$	0

$$C_l^*(1)=\frac{1}{2}l(l+1)C_{l1}=\left[\frac{l(l+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}$$

$$C_l^*(-1)=\frac{1}{2}(-1)^l l(l+1)C_{l1}=(-1)^l\left[\frac{l(l+1)(2l+1)}{8\pi}\right]^{\frac{1}{2}}$$

Appendix C. Summary of Energy Dependent Quantities

The following quantities are needed to generate the moment-to-discrete matrices. For a given kinetic energy (E)

$$\tau = \frac{E}{m_o c^2}$$

	Relativistic	Non-Relativistic
$\mathcal{T}(E)$	$E + m_o c^2$	$E + m_o c^2$
$\beta(E)$	$\frac{\sqrt{\tau(\tau+2)}}{\tau+1}$	0
$\frac{1}{\mathcal{D}(E)}$	$\frac{\tau+1}{\tau+2}\frac{1}{E}$	$\frac{1}{2E}$
$\frac{c\beta(E)}{\mathcal{D}(E)}$	$\sqrt{\frac{\tau}{\tau+2}}\frac{c}{E}$	$\frac{v(E)}{\mathcal{D}(E)} = \frac{c}{\sqrt{2m_o c^2 E}}$
$\frac{1+4\beta^2(E)}{\mathcal{D}(E)}$	$\frac{1+4\beta^2(E)}{\mathcal{D}(E)}$	$\frac{1}{2E}$
$v(E)$	$c\beta(E)$	$\sqrt{\frac{2E}{m_o}} = \sqrt{\frac{2E}{m_o c^2}}\,c$

Appendix D

Derivations of Discontinuous Finite-Element Equations in Space and Energy

Expand the angular flux as

$$\psi(\vec{r}, E, \vec{\Omega}) = \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E) \psi_{ij}(\vec{\Omega}) \tag{D1}$$

where $H_i(\vec{r})$ is the *i*th basis function in space, $G_j(E)$ is the *j*th basis function in energy, and $\psi_{ij}(\vec{\Omega})$ are the expansion coefficients. We will ignore the time dependence for simplicity but will treat the time-derivative term at the end.

Substitute the expansion (D1) into the transport equation, multiply the result by $H_i(\vec{r})G_j(E)$ and integrate the resultant equation over an elemental volume V_e and an energy bin $[E_g, E_{g-1}]$ …

Collision Term

$$\begin{aligned}
&\int_{V_e} dV \int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E)\sigma(\vec{r}, E) \sum_{i'=1}^{I} H_{i'}(\vec{r}) \sum_{j'=1}^{J} G_{j'}(E)\psi_{i'j'}(\vec{\Omega}) \\
&= \sigma_g(\vec{r}_e) \int_{V_e} dV \int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E) \sum_{i'=1}^{I} H_{i'}(\vec{r}) \sum_{j'=1}^{J} G_{j'}(E)\psi_{i'j'}(\vec{\Omega}) \\
&= \sigma_g(\vec{r}_e) \sum_{i'=1}^{I} \sum_{j'=1}^{J} \int_{V_e} dV H_i(\vec{r})H_{i'}(\vec{r}) \int_{E_g}^{E_{g-1}} dE\, G_j(E)G_{j'}(E)\psi_{i'j'}(\vec{\Omega})
\end{aligned}$$

for $i = 1 \ldots I$ and $j = 1 \ldots J$. Here we have assumed that the total cross section is constant within the element and the energy bin. Other functional forms are allowed if they are available from the cross-section library. The last expression can be arranged into a block matrix form with a total number of *IJ* unknowns:

$$[\boldsymbol{\mathcal{C}}]\boldsymbol{\Psi} = \begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{H}} & \mathcal{G}_{12}\boldsymbol{\mathcal{H}} & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{H}} \\ \mathcal{G}_{21}\boldsymbol{\mathcal{H}} & \mathcal{G}_{22}\boldsymbol{\mathcal{H}} & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{H}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{H}} & \mathcal{G}_{J2}\boldsymbol{\mathcal{H}} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{H}} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J \end{bmatrix} \tag{D2}$$

$$\mathbf{\Psi}_j = \begin{bmatrix} \psi_{1j}(\vec{\Omega}) \\ \psi_{2j}(\vec{\Omega}) \\ \vdots \\ \psi_{Ij}(\vec{\Omega}) \end{bmatrix} \tag{D3}$$

$$\boldsymbol{\mathcal{H}} = \text{an } I \times I \text{ matrix } = [\mathcal{H}_{\boldsymbol{ii'}}] \tag{D4}$$

$$\mathcal{H}_{ii'} = \int_{V_e} dV H_i(\vec{r}\,) H_{\boldsymbol{i'}}(\vec{r}\,) \tag{D5}$$

$$\mathcal{G}_{jj'} = \int_{E_g}^{E_{g-1}} dE\, G_j(\,E) G_{j'}(\,E) \tag{D6}$$

Streaming Term

$$\int_{V_e} dV \int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r}\,)G_j(\,E)\left[\boldsymbol{\nabla}\cdot\vec{\Omega}\psi\left(\vec{r},E,\vec{\Omega}\right)\right]$$

$$= \int_{V_e} dV \int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\left\{\boldsymbol{\nabla}\cdot\left[\vec{\Omega}H_i(\vec{r}\,)\psi\left(\vec{r},E,\vec{\Omega}\right)\right] - \left[\boldsymbol{\nabla}\cdot\vec{\Omega}H_i(\vec{r}\,)\right]\psi\left(\vec{r},E,\vec{\Omega}\right)\right\}$$

$$= \int_{A_e} dA\left(\vec{n}\cdot\vec{\Omega}\right)H_i(\vec{r}\,)\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\psi\left(\vec{r},E,\vec{\Omega}\right)$$

$$-\vec{\Omega}\cdot\int_{V_e} dV\boldsymbol{\nabla}H_i(\vec{r}\,)\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\psi\left(\vec{r},E,\vec{\Omega}\right)$$

$$= \int_{A_e} dA\left(\vec{n}\cdot\vec{\Omega}\right)H_i(\vec{r}\,)\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\sum_{i'=1}^{I} H_{i'}\,(\vec{r}\,)\sum_{j'=1}^{J} G_{j'}(\,E)\psi_{\boldsymbol{i'}\,j'}\left(\vec{\Omega}\right)$$

$$-\ \vec{\Omega}\cdot\int_{V_e} dV\boldsymbol{\nabla}H_i(\vec{r}\,)\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\sum_{i'=1}^{I} H_{i'}\,(\vec{r}\,)\sum_{j'=1}^{J} G_{j'}(\,E)\psi_{\boldsymbol{i'}\,j'}\left(\vec{\Omega}\right)$$

$$= \sum_{k=1}^{N_k}\int_{A_k} dA\left(\vec{n}_k\cdot\vec{\Omega}\right)H_i(\vec{r}\,)\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\sum_{i'=1}^{I} H_{i'}\,(\vec{r}\,)\sum_{j'=1}^{J} G_{j'}(\,E)\psi_{\boldsymbol{i'}\,j'}\left(\vec{\Omega}\right)$$

$$-\ \vec{\Omega}\cdot\int_{V_e} dV\boldsymbol{\nabla}H_i(\vec{r}\,)\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\sum_{i'=1}^{I} H_{i'}\,(\vec{r}\,)\sum_{j'=1}^{J} G_{j'}(\,E)\psi_{\boldsymbol{i'}\,j'}\left(\vec{\Omega}\right)$$

where N_k is the number of faces and A_k is the kth face of an element.

$$[\boldsymbol{\mathcal{L}}]\boldsymbol{\Psi} = \sum_{\boldsymbol{k=1}}^{N_k}\left[\boldsymbol{\mathcal{L}}_{\boldsymbol{A_k}}\right]\boldsymbol{\Psi} - [\boldsymbol{\mathcal{L}}_{\boldsymbol{V}}]\boldsymbol{\Psi} \tag{D7}$$

$$\left[\boldsymbol{\mathcal{L}}_{\boldsymbol{A_k}}\right]\boldsymbol{\Psi} = \vec{\Omega}\cdot\begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} & \mathcal{G}_{12}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} \\ \mathcal{G}_{21}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} & \mathcal{G}_{22}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} & \mathcal{G}_{J2}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{H}}_{\boldsymbol{A_k}} \end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \tag{D8}$$

$$[\boldsymbol{\mathcal{L}}_{\boldsymbol{V}}]\boldsymbol{\Psi} = \vec{\Omega}\cdot\begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} & \mathcal{G}_{12}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} \\ \mathcal{G}_{21}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} & \mathcal{G}_{22}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} & \mathcal{G}_{J2}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} \end{bmatrix}\begin{bmatrix} \boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J \end{bmatrix} \tag{D9}$$

$$\boldsymbol{\mathcal{H}}_{\boldsymbol{A}} = \text{an } I \times I \text{ matrix of vectors } = \left[\vec{\mathcal{H}}_{A_k ii'}\right] \tag{D10}$$

$$\vec{\mathcal{H}}_{A_k ii'} = \int_{A_e} dA\vec{n}_k H_i(\vec{r}\,)H_{\boldsymbol{i'}}(\vec{r}\,) \tag{D11}$$

$$\boldsymbol{\mathcal{H}}_{\boldsymbol{V}} = \text{an } I \times I \text{ matrix of vectors } = \left[\vec{\mathcal{H}}_{Vii'}\right] \tag{D12}$$

$$\vec{\mathcal{H}}_{Vii'} = \int_{V_e} dV[\boldsymbol{\nabla} H_i(\vec{r}\,)]H_{\boldsymbol{i'}}(\vec{r}\,) \tag{D13}$$

Energy Redistribution from Electric Field $\left[\frac{\partial\psi}{\partial E}\right]$

$$q\vec{\Omega}\cdot\int_{V_e} dV\vec{\mathcal{E}}\int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E)\frac{\partial}{\partial E}\psi(\vec{r},E,\vec{\Omega})$$
$$= q\vec{\Omega}\cdot\int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})\left\{\int_{E_g}^{E_{g-1}} dE\frac{\partial}{\partial E}\left[G_j(E)\psi(\vec{r},E,\vec{\Omega})\right] - \int_{E_g}^{E_{g-1}} dE\left[\frac{\partial}{\partial E}G_j(E)\right]\psi(\vec{r},E,\vec{\Omega})\right\}$$
$$= q\vec{\Omega}\cdot\int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})\left\{G_j(E)\psi(\vec{r},E,\vec{\Omega})\Big|_{E_g}^{E_{g-1}} - \int_{E_g}^{E_{g-1}} dE\left[\frac{\partial}{\partial E}G_j(E)\right]\psi(\vec{r},E,\vec{\Omega})\right\}$$
$$= q\vec{\Omega}\cdot\sum_{i'=1}^{I}\int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})H_{i'}(\vec{r})\sum_{j'=1}^{J}\left[G_j(E)G_{j'}(E)\psi_{i'j'}(\vec{\Omega})\right]_{E_g}^{E_{g-1}}$$
$$-\; q\vec{\Omega}\cdot\sum_{i'=1}^{I}\int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})H_{i'}(\vec{r})\sum_{j'=1}^{J}\int_{E_g}^{E_{g-1}} dE\left[\frac{\partial}{\partial E}G_j(E)\right]G_{j'}(E)\psi_{i'j'}(\vec{\Omega})$$

$$[\boldsymbol{\mathcal{P}}]\boldsymbol{\Psi} = [\boldsymbol{\mathcal{P}}_{\boldsymbol{g-1}}]\boldsymbol{\Psi} - [\boldsymbol{\mathcal{P}}_{\boldsymbol{g}}]\boldsymbol{\Psi} - [\widetilde{\boldsymbol{\mathcal{P}}}]\boldsymbol{\Psi} \tag{D14}$$

$$[\boldsymbol{\mathcal{P}}_{\boldsymbol{g}}]\boldsymbol{\Psi} = q\vec{\Omega}\cdot\begin{bmatrix}\mathcal{P}_{11}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} & \mathcal{P}_{12}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} & \cdots & \mathcal{P}_{1J}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} \\ \mathcal{P}_{21}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} & \mathcal{P}_{22}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} & \cdots & \mathcal{P}_{2J}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{P}_{J1}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} & \mathcal{P}_{J2}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} & \cdots & \mathcal{P}_{JJ}\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \quad \text{at } E_g \tag{D15}$$

$$\mathcal{P}_{jj'}(E) = G_j(E)G_{j'}(E) \tag{D16}$$

$$\boldsymbol{\mathcal{H}}_{\boldsymbol{\mathcal{E}}} = \text{an } I \times I \text{ matrix of vectors } = [\vec{\mathcal{H}}_{\mathcal{E}ii'}] \tag{D17}$$

$$\vec{\mathcal{H}}_{\mathcal{E}ii'} = \int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})H_{\boldsymbol{i'}}(\vec{r}) \tag{D18}$$

$$[\tilde{\boldsymbol{\mathcal{P}}}]\boldsymbol{\Psi} = q\vec{\Omega}\cdot\begin{bmatrix}\tilde{\mathcal{P}}_{11}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \tilde{\mathcal{P}}_{12}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \tilde{\mathcal{P}}_{1J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \tilde{\mathcal{P}}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \tilde{\mathcal{P}}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \tilde{\mathcal{P}}_{2J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\mathcal{P}}_{J1}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \tilde{\mathcal{P}}_{J2}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \tilde{\mathcal{P}}_{JJ}\boldsymbol{\mathcal{H}}_{\mathcal{E}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \tag{D19}$$

$$\tilde{\mathcal{P}}_{jj'} = \int_{E_g}^{E_{g-1}} dE\left[\frac{\partial}{\partial E}G_j(E)\right]G_{j'}(E) \tag{D20}$$

Energy Redistribution from Electric Field $\left[\frac{\mathbf{1+4}\boldsymbol{\beta}^{\mathbf{2}}(\boldsymbol{E})}{\boldsymbol{\mathcal{D}}(\boldsymbol{E})}\boldsymbol{\psi}\right]$

$$\begin{aligned} & q\vec{\Omega}\cdot\int_V dV\vec{\mathcal{E}}\int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E)\left[\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\psi(\vec{r},E,\vec{\Omega})\right] \\ & = q\vec{\Omega}\cdot\int_{V_e} dV\vec{\mathcal{E}}\int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E)\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\sum_{\boldsymbol{i'=1}}^{\boldsymbol{I}} H_{\boldsymbol{i'}}(\vec{r})\sum_{j'=1}^{J} G_{j'}(E)\psi_{\boldsymbol{i'}j'}(\vec{\Omega}) \\ & = q\vec{\Omega}\cdot\sum_{i'=1}^{I}\sum_{j'=1}^{J}\int_{V_e} dV\vec{\mathcal{E}}H_i(\vec{r})H_{i'}(\vec{r})\int_{E_g}^{E_{g-1}} dE\frac{1+4\beta^2(E)}{\mathcal{D}(E)}G_j(E)G_{j'}(E)\psi_{i'j'}(\vec{\Omega}) \end{aligned} \tag{D21}$$

$$[\boldsymbol{\mathcal{Q}}]\boldsymbol{\Psi} = q\vec{\Omega}\cdot\begin{bmatrix}\mathcal{Q}_{11}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{Q}_{12}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{Q}_{1J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \mathcal{Q}_{21}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{Q}_{22}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{Q}_{2J}\boldsymbol{\mathcal{H}}_{\mathcal{E}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{Q}_{J1}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \mathcal{Q}_{J2}\boldsymbol{\mathcal{H}}_{\mathcal{E}} & \cdots & \mathcal{Q}_{JJ}\boldsymbol{\mathcal{H}}_{\mathcal{E}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \tag{D22}$$

$$\mathcal{Q}_{jj'} = \int_{E_g}^{E_{g-1}} dE\frac{1+4\beta^2(E)}{\mathcal{D}(E)}G_j(E)G_{j'}(E) \tag{D23}$$

Angular Redistribution due to Electric Field

The discrete angular redistribution from the electric field is

$$\boldsymbol{\mathcal{R}}_{\mathcal{E}}(\vec{r},E) \equiv \begin{bmatrix} \mathcal{R}_{\mathcal{E}1}(\vec{r},E) \\ \mathcal{R}_{\mathcal{E}2}(\vec{r},E) \\ \vdots \\ \mathcal{R}_{\mathcal{E}N}(\vec{r},E) \end{bmatrix} = \frac{q\mathcal{E}}{\mathcal{D}(E)}[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]\boldsymbol{\phi}(\vec{r},E) \tag{D24}$$

where the symbol $\mathcal{E}$ is used to denote one of the three components of the electric field $(\mathcal{E}_x, \mathcal{E}_y, \mathcal{E}_z)$, $\boldsymbol{\mathcal{R}}_{\mathcal{E}}(\vec{r},E)$ is a column vector containing the contribution from the electric field to all directions, $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]$ is the equivalent moment-to-discrete matrix for the electric field component $\mathcal{E}$, and $\boldsymbol{\phi}(\vec{r},E)$ is a column vector containing the angular moments. The angular moments can be represented by the same basis functions in space and energy:

$$\boldsymbol{\phi}(\vec{r},E) = \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E)\boldsymbol{\phi}_{ij} \tag{D25}$$

$\boldsymbol{\phi}_{ij}$ is a column vector containing the expansion coefficients of the angular moments corresponding to the *i*th basis function in space and the *j*th basis function in energy.

$$\boldsymbol{\mathcal{R}}_{\mathcal{E}}(\vec{r},E) = \frac{q\mathcal{E}}{\mathcal{D}(E)} \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E)[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]\boldsymbol{\phi}_{ij} \tag{D26}$$

For a specific direction $\vec{\Omega}_n$,

$$\begin{aligned} \mathcal{R}_{\mathcal{E}n}(\vec{r},E) &= \frac{q\mathcal{E}}{\mathcal{D}(E)} \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E)[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n\boldsymbol{\phi}_{ij} \\ &= [\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \frac{q\mathcal{E}}{\mathcal{D}(E)} \sum_{i=1}^{I} H_i(\vec{r}) \sum_{j=1}^{J} G_j(E)\boldsymbol{\phi}_{ij} \end{aligned} \tag{D27}$$

where $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n$ is the *n*th row of the matrix $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]$ and is independent of space or energy. Multiplying Eq. (D27) by $H_i(\vec{r})G_j(E)$ and integrating the result over an element V_e and an energy bin $[E_g, E_{g-1}]$ yield

$$\mathcal{R}_{\mathcal{E}nij} = [\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \int_V dV \int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r}\,) G_j(\,E) \frac{q\mathcal{E}}{\mathcal{D}(E)} \sum_{i'=1}^{I} H_{i'}\,(\vec{r}\,) \sum_{j'=1}^{J} G_{j'}(\,E) \boldsymbol{\phi}_{i'j'}$$
$$= q[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \sum_{i'=1}^{I} \mathcal{H}_{\mathcal{E}ii'} \sum_{j'=1}^{J} \tilde{\mathcal{G}}_{jj'} \boldsymbol{\phi}_{i'j'} \qquad \text{(D28)}$$

$$\mathcal{H}_{\mathcal{E}ii'} = \int_{V_e} dV \mathcal{E} H_i(\vec{r}\,) H_{\boldsymbol{i'}}(\vec{r}\,) \qquad \text{(D29)}$$

$$\tilde{\mathcal{G}}_{jj'} = \int_{E_g}^{E_{g-1}} dE \frac{1}{\mathcal{D}(E)} G_j(\,E) G_{j'}(\,E) \qquad \text{(D30)}$$

Angular Redistribution due to Magnetic Field

The discrete angular redistribution from the Magnetic field is

$$\boldsymbol{\mathcal{R}}_{\mathcal{B}}(\vec{r}, E) \equiv \begin{bmatrix} \mathcal{R}_{\mathcal{B}1}(\vec{r}, E) \\ \mathcal{R}_{\mathcal{B}2}(\vec{r}, E) \\ \vdots \\ \mathcal{R}_{\mathcal{B}N}(\vec{r}, E) \end{bmatrix} = \frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)} [\boldsymbol{\mathcal{M}}_{\mathcal{B}}] \boldsymbol{\phi}(\vec{r}, E) \qquad \text{(D31)}$$

where the symbol $\mathcal{B}$ is used to denote one of the three components of the magnetic field $(\mathcal{B}_x, \mathcal{B}_y, \mathcal{B}_z)$, $\boldsymbol{\mathcal{R}}_{\mathcal{B}}(\vec{r}, E)$ is a column vector containing the contribution from the magnetic field to all directions, $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]$ is the moment-to-discrete matrix due to the magnetic field component $\mathcal{B}$, and $\boldsymbol{\phi}(\vec{r}, E)$ is a column vector containing the angular moments. Using the spatial and energy expansion in Eq. (D25) we obtain

$$\boldsymbol{\mathcal{R}}_{\mathcal{B}}(\vec{r}, E) = \frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)} \sum_{i=1}^{I} H_i\,(\vec{r}\,) \sum_{j=1}^{J} G_j(\,E) [\boldsymbol{\mathcal{M}}_{\mathcal{B}}] \boldsymbol{\phi}_{ij} \qquad \text{(D32)}$$

For a specific direction $\vec{\Omega}_n$, the last expression can be written as

$$\begin{aligned}\mathcal{R}_{\mathcal{B}n}(\vec{r},E) &= \frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)}\sum_{i=1}^{I} H_i(\vec{r})\sum_{j=1}^{J} G_j(E)[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n\boldsymbol{\phi}_{ij} \\ &= \frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)}[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n\sum_{i=1}^{I} H_i(\vec{r})\sum_{j=1}^{J} G_j(E)\boldsymbol{\phi}_{ij}\end{aligned} \tag{D33}$$

where $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n$ is the nth row of the matrix $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]$. Multiplying Eq. (D33) by $H_i(\vec{r})G_j(E)$ and integrating the result over an element V_e and an energy bin $[E_g, E_{g-1}]$ yield

$$\begin{aligned}\mathcal{R}_{\mathcal{B}nij} &= [\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n\int_V dV\int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E)\frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)}\sum_{i'=1}^{I} H_{i'}(\vec{r})\sum_{j'=1}^{J} G_{j'}(E)\boldsymbol{\phi}_{i'j'} \\ &= q[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n\sum_{i'=1}^{I}\mathcal{H}_{\mathcal{B}ii'}\sum_{j'=1}^{J}\mathcal{G}^{*}_{jj'}\boldsymbol{\phi}_{i'j'}\end{aligned} \tag{D34}$$

$$\mathcal{H}_{\mathcal{B}ii'} = \int_{V_e} dV\mathcal{B}H_i(\vec{r})H_{\boldsymbol{i'}}(\vec{r}) \tag{D35}$$

$$\mathcal{G}^{*}_{jj'} = c\int_{E_g}^{E_{g-1}} dE\,\frac{\beta(E)}{\mathcal{D}(E)}G_j(E)G_{j'}(E) \tag{D36}$$

Time-Derivative Term

$$\begin{aligned}&\int_{V_e} dV\int_{E_g}^{E_{g-1}} dE\, H_i(\vec{r})G_j(E)\frac{1}{c\beta(E)}\frac{\partial}{\partial t}\sum_{i'=1}^{I} H_{i'}(\vec{r})\sum_{j'=1}^{J} G_{j'}(E)\psi_{\boldsymbol{i'}j'}(\vec{\Omega},t) \\ &= \sum_{i'=1}^{I}\sum_{j'=1}^{J}\int_{V_e} dV H_i(\vec{r})H_{i'}(\vec{r})\int_{E_g}^{E_{g-1}} dE\,\frac{1}{c\beta(E)}G_j(E)G_{j'}(E)\frac{\partial}{\partial t}\psi_{i'j'}(\vec{\Omega},t)\end{aligned} \tag{D37}$$

$$[\boldsymbol{\mathcal{T}}]\boldsymbol{\Psi} = \begin{bmatrix}\hat{\mathcal{G}}_{11}\boldsymbol{\mathcal{H}} & \hat{\mathcal{G}}_{12}\boldsymbol{\mathcal{H}} & \cdots & \hat{\mathcal{G}}_{1J}\boldsymbol{\mathcal{H}} \\ \hat{\mathcal{G}}_{21}\boldsymbol{\mathcal{H}} & \hat{\mathcal{G}}_{22}\boldsymbol{\mathcal{H}} & \cdots & \hat{\mathcal{G}}_{2J}\boldsymbol{\mathcal{H}} \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\mathcal{G}}_{J1}\boldsymbol{\mathcal{H}} & \hat{\mathcal{G}}_{J2}\boldsymbol{\mathcal{H}} & \cdots & \hat{\mathcal{G}}_{JJ}\boldsymbol{\mathcal{H}}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_2 \\ \vdots \\ \boldsymbol{\Psi}_J\end{bmatrix} \tag{D38}$$

$$\mathbf{\Psi}_j = \mathbf{\Psi}_j(\vec{\Omega}, t) = \begin{bmatrix} \psi_{1j}(\vec{\Omega}, t) \\ \psi_{2j}(\vec{\Omega}, t) \\ \vdots \\ \psi_{Ij}(\vec{\Omega}, t) \end{bmatrix} \tag{D39}$$

$$\boldsymbol{\mathcal{H}} = \text{an } I \times I \text{ matrix } = [\mathcal{H}_{ii'}] \tag{D4}$$

$$\mathcal{H}_{ii'} = \int_{V_e} dV H_i(\vec{r}\,) H_{\boldsymbol{i'}}(\vec{r}\,) \tag{D5}$$

$$\hat{\mathcal{G}}_{jj'} = \int_{E_g}^{E_{g-1}} dE \frac{1}{c\beta(E)} G_j(\,E) G_{j'}(\,E) \tag{D40}$$

Appendix E. Second-Order Discrete-Ordinates Equations with DFEM in Energy and CFEM in Space

We will start with the time-independent, angularly discretized transport equation.

$$\begin{aligned}&\vec{\Omega}_n \cdot \nabla\psi_n + \sigma\psi_n + q\left(\vec{\mathcal{E}} \cdot \vec{\Omega}_n\right)\left[\frac{\partial\psi_n}{\partial E} - \frac{1+4\beta^2(E)}{\mathcal{D}(E)}\psi_n\right] \\ &+ \frac{q}{\mathcal{D}(E)}\left\{\mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right]_n + \mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]_n + \mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]_n\right\}\boldsymbol{\phi} \\ &+ \frac{qc\beta(E)}{\mathcal{D}(E)}\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right]_n + \mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]_n + \mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]_n\right\}\boldsymbol{\phi} = S_n\end{aligned} \tag{E1}$$

$$\psi_n = \psi_n(\vec{r}, E,)$$

$$S_n = S_n(\vec{r}, E)$$

Spatial dependence in the components of EM fields

$$\boldsymbol{\phi} = \boldsymbol{\phi}(\vec{r}, E) = \begin{bmatrix} \boldsymbol{\phi}_1(\vec{r}, E) \\ \boldsymbol{\phi}_2(\vec{r}, E) \\ \vdots \\ \boldsymbol{\phi}_{N_M}(\vec{r}, E) \end{bmatrix} \tag{E2}$$

Expand the angular flux as

$$\psi_n(\vec{r}, E) = \sum_{j=1}^{J} G_j(\,E)\psi_{nj}(\vec{r}) \tag{E3}$$

$$\boldsymbol{\phi}(\vec{r}, E) = \sum_{j=1}^{J} G_j(\,E)\boldsymbol{\phi}_j(\vec{r}) \tag{E4}$$

Substitute the expansions (E3) and (E4) into (E1), multiply the result by $G_j(\,E)$ and integrate the resultant equation over an energy bin $[E_g, E_{g-1}]$ …

Streaming Term

$$
\begin{aligned}
&\int_{E_g}^{E_{g-1}} dE\, G_j(E)\left[\vec{\Omega}_n \cdot \boldsymbol{\nabla}\psi_n(\vec{r}, E)\right] \\
&= \int_{E_g}^{E_{g-1}} dE\, G_j(E) \sum_{j'=1}^{J} G_{j'}(E)\vec{\Omega}_n \cdot \boldsymbol{\nabla}\psi_{\boldsymbol{n}j'}(\vec{r}) \\
&= \sum_{j'=1}^{J} \mathcal{G}_{jj'}\vec{\Omega}_n \cdot \boldsymbol{\nabla}\psi_{\boldsymbol{n}j'}(\vec{r}) = \vec{\Omega}_n \cdot \boldsymbol{\nabla}\left[\sum_{j'=1}^{J} \mathcal{G}_{jj'}\psi_{\boldsymbol{n}j'}(\vec{r})\right]
\end{aligned}
\tag{E5}
$$

$$
\mathcal{G}_{jj'} = \int_{E_g}^{E_{g-1}} dE\, G_j(E) G_{j'}(E) \tag{E6}
$$

Collision Term

$$
\begin{aligned}
&\int_{E_g}^{E_{g-1}} dE G_j(E)\sigma(\vec{r}, E) \sum_{j'=1}^{J} G_{j'}(E)\psi_{\boldsymbol{n}j'}(\vec{r}) \\
&= \sigma_g(\vec{r}_{\mathrm{e}}) \int_{E_g}^{E_{g-1}} dE G_j(E) \sum_{j'=1}^{J} G_{j'}(E)\psi_{\boldsymbol{n}j'}(\vec{r}) \\
&= \sigma_g(\vec{r}_{\mathrm{e}}) \sum_{j'=1}^{J} \int_{E_g}^{E_{g-1}} dE\, G_j(E) G_{j'}(E)\psi_{\boldsymbol{n}j'}(\vec{r}) \\
&= \sigma_g(\vec{r}_{\mathrm{e}}) \sum_{j'=1}^{J} \mathcal{G}_{jj'}\psi_{\boldsymbol{n}j'}(\vec{r})
\end{aligned}
\tag{E7}
$$

Energy Redistribution from Electric Field $\left[\frac{\partial\psi}{\partial E}\right]$

$$
\begin{aligned}
&q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\int_{E_g}^{E_{g-1}}dE\,G_j(\,E)\frac{\partial}{\partial E}\psi_n(\vec{r},E)\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\left\{\int_{E_g}^{E_{g-1}}dE\,\frac{\partial}{\partial E}\left[G_j(\,E)\psi_n(\vec{r},E)\right]-\int_{E_g}^{E_{g-1}}dE\left[\frac{\partial}{\partial E}G_j(\,E)\right]\psi_n(\vec{r},E)\right\}\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\left\{G_j(\,E)\psi_n(\vec{r},E)\Big|_{E_g}^{E_{g-1}}-\int_{E_g}^{E_{g-1}}dE\left[\frac{\partial}{\partial E}G_j(\,E)\right]\psi_n(\vec{r},E)\right\}\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\sum_{j'=1}^{J}\left\{\left[G_j(\,E)G_{j'}(\,E)\right]_{E_g}^{E_{g-1}}-\int_{E_g}^{E_{g-1}}dE\left[\frac{\partial}{\partial E}G_j(\,E)\right]G_{j'}(\,E)\right\}\psi_{\boldsymbol{n}j'}(\vec{r})\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\sum_{j'=1}^{J}\left\{\mathcal{P}_{jj'}(E_{g-1})-\mathcal{P}_{jj'}(E_g)-\tilde{\mathcal{P}}_{jj'}\right\}\psi_{\boldsymbol{n}j'}(\vec{r})
\end{aligned}
\tag{E8}
$$

$$
\mathcal{P}_{jj'}(\mathrm{E})=G_j(\,E)G_{j'}(\,E)
\tag{E9}
$$

$$
\tilde{\mathcal{P}}_{jj'}=\int_{E_g}^{E_{g-1}}dE\left[\frac{\partial}{\partial E}G_j(\,E)\right]G_{j'}(\,E)
\tag{E10}
$$

Energy Redistribution from Electric Field $\left[\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\boldsymbol{\psi}\right]$

$$
\begin{aligned}
&q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\int_{E_g}^{E_{g-1}}dE\,G_j(\,E)\left[\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\psi_n(\vec{r},E)\right]\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\int_{E_g}^{E_{g-1}}dE\,G_j(\,E)\frac{1+4\beta^2(E)}{\mathcal{D}(E)}\sum_{j'=1}^{J}G_{j'}(\,E)\psi_{nj'}(\vec{r})\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\sum_{j'=1}^{J}\int_{E_g}^{E_{g-1}}dE\,\frac{1+4\beta^2(E)}{\mathcal{D}(E)}G_j(\,E)G_{j'}(\,E)\psi_{nj'}(\vec{r})\\
&=q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\sum_{j'=1}^{J}\mathcal{Q}_{jj'}\psi_{nj'}(\vec{r})
\end{aligned}
\tag{E11}
$$

$$\mathcal{Q}_{jj'} = \int_{E_g}^{E_{g-1}} dE \frac{1 + 4\beta^2(E)}{\mathcal{D}(E)} G_j(E) G_{j'}(E) \tag{E12}$$

Angular Redistribution due to Electric Field

For a specific direction $\vec{\Omega}_n$,

$$\mathcal{R}_{\mathcal{E}n}(\vec{r}, E) = \frac{q\mathcal{E}}{\mathcal{D}(E)} [\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \boldsymbol{\phi}(\vec{r}, E) = \frac{q\mathcal{E}}{\mathcal{D}(E)} [\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \sum_{j=1}^{J} G_j(E) \boldsymbol{\phi}_j(\vec{r}) \tag{E13}$$

where the symbol $\mathcal{E}$ is used to denote one of the three components of the electric field $(\mathcal{E}_x, \mathcal{E}_y, \mathcal{E}_z)$ and $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n$ is the *n*th row of the matrix $[\boldsymbol{\mathcal{M}}_{\mathcal{E}}]$. Multiplying Eq. (E13) by $G_j(E)$ and integrating the result over an energy bin $[E_g, E_{g-1}]$ yield

$$\begin{aligned} &\int_{E_g}^{E_{g-1}} dE\, G_j(E) \frac{q\mathcal{E}}{\mathcal{D}(E)} [\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \sum_{j'=1}^{J} G_{j'}(E) \boldsymbol{\phi}_{j'}(\vec{r}) \\ &= q\mathcal{E} [\boldsymbol{\mathcal{M}}_{\mathcal{E}}]_n \sum_{j=1}^{J} \tilde{\mathcal{G}}_{jj'} \boldsymbol{\phi}_{j'}(\vec{r}) \end{aligned} \tag{E14}$$

$$\tilde{\mathcal{G}}_{jj'} = \int_{E_g}^{E_{g-1}} dE \frac{1}{\mathcal{D}(E)} G_j(E) G_{j'}(E) \tag{E15}$$

Angular Redistribution due to Magnetic Field

For a specific direction $\vec{\Omega}_n$,

$$\mathcal{R}_{\mathcal{B}n}(\vec{r}, E) = \frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)} [\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n \boldsymbol{\phi}(\vec{r}, E) = \frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)} \sum_{j=1}^{J} G_j(E) [\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n \boldsymbol{\phi}_j(\vec{r}) \tag{E16}$$

where the symbol $\mathcal{B}$ is used to denote one of the three components of the magnetic field $(\mathcal{B}_x, \mathcal{B}_y, \mathcal{B}_z)$ and $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n$ is the *n*th row of the matrix $[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]$. Multiplying Eq. (E16) by $G_j(E)$ and integrating the result and an energy bin $[E_g, E_{g-1}]$ yield

$$\int_{E_g}^{E_{g-1}} dE\, G_j(\,E)\frac{qc\beta(E)\mathcal{B}}{\mathcal{D}(E)}\sum_{j'=1}^{J} G_{j'}(\,E)[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n \boldsymbol{\phi}_{j'}(\vec{r})$$
$$= q\mathcal{B}\sum_{j=1}^{J}\tilde{\mathcal{G}}_{jj'}[\boldsymbol{\mathcal{M}}_{\mathcal{B}}]_n \boldsymbol{\phi}_{i'j'} \tag{E17}$$

$$\mathcal{G}^{*}_{jj'} = c\int_{E_g}^{E_{g-1}} dE\,\frac{\beta(E)}{\mathcal{D}(E)}G_j(\,E)G_{j'}(\,E) \tag{E18}$$

Source Term

$$S_{nj}(\vec{r}) = \int_{E_g}^{E_{g-1}} dE\, G_j(\,E)S_n(\vec{r},E) \tag{E19}$$

Combining Eqs. (E5), (E7), (E8), (E11), (E14), (E17) and (E19), we obtain the equation for the *j*th expansion coefficient (in energy) of $\psi_{\boldsymbol{n}}(\vec{r},E)$

$$\vec{\Omega}_n\cdot\boldsymbol{\nabla}\left[\sum_{j'=1}^{J}\mathcal{G}_{jj'}\psi_{\boldsymbol{n}j'}(\vec{r})\right] + \sigma_g(\vec{r}_{\mathrm{e}})\sum_{j'=1}^{J}\mathcal{G}_{jj'}\psi_{\boldsymbol{n}j'}(\vec{r}) +$$
$$q\vec{\mathcal{E}}\cdot\vec{\Omega}_n\sum_{j'=1}^{J}\left\{\mathcal{P}_{jj'}\left(E_{g-1}\right)-\mathcal{P}_{jj'}\left(E_g\right)-\tilde{\mathcal{P}}_{jj'}+\mathcal{Q}_{jj'}\right\}\psi_{\boldsymbol{n}j'}(\vec{r}) +$$
$$q\left\{\mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right]_n+\mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]_n+\mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right]_n\right\}\sum_{j'=1}^{J}\tilde{\mathcal{G}}_{jj'}\boldsymbol{\phi}_{j'}(\vec{r}) + \tag{E20}$$
$$q\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right]_n+\mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]_n+\mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right]_n\right\}\sum_{j'=1}^{J}\mathcal{G}^{*}_{jj'}\boldsymbol{\phi}_{j'}(\vec{r})$$
$$= S_{nj}(\vec{r})$$

Define a column vector containing the expansion coefficients for all directions

$$\boldsymbol{\psi} = \text{a vector of length } N_D \times J = \begin{bmatrix} \boldsymbol{\psi}_1 \\ \boldsymbol{\psi}_2 \\ \vdots \\ \boldsymbol{\psi}_J \end{bmatrix} \tag{E21}$$

$$\boldsymbol{\psi}_j = \text{a vector of length } N_D = \begin{bmatrix} \psi_{1j}(\vec{r}) \\ \psi_{2j}(\vec{r}) \\ \vdots \\ \psi_{N_D j}(\vec{r}) \end{bmatrix} \tag{E23}$$

$$[\boldsymbol{L}_{\boldsymbol{\mu}}]\frac{\partial}{\partial x}\boldsymbol{\psi} + [\boldsymbol{L}_{\boldsymbol{\eta}}]\frac{\partial}{\partial y}\boldsymbol{\psi} + [\boldsymbol{L}_{\boldsymbol{\xi}}]\frac{\partial}{\partial z}\boldsymbol{\psi} + [\boldsymbol{\sigma}]\boldsymbol{\psi} + [\boldsymbol{P}]\boldsymbol{\psi} + [M_{\mathcal{E}}]\boldsymbol{\psi} + [M_{\mathcal{B}}]\boldsymbol{\psi} = \boldsymbol{S} \tag{E24}$$

$$[\boldsymbol{\Lambda}]\boldsymbol{\psi} + [\boldsymbol{\mathcal{T}}]\boldsymbol{\psi} = \boldsymbol{S} \tag{E24a}$$

$$[\boldsymbol{\Lambda}] = [\boldsymbol{L}_{\boldsymbol{\mu}}]\frac{\partial}{\partial x} + [\boldsymbol{L}_{\boldsymbol{\eta}}]\frac{\partial}{\partial y} + [\boldsymbol{L}_{\boldsymbol{\xi}}]\frac{\partial}{\partial z} \tag{E24b}$$

$$[\boldsymbol{\mathcal{T}}] = [\boldsymbol{\sigma}] + [\boldsymbol{P}] + [M_{\mathcal{E}}] + [M_{\mathcal{B}}] \tag{E24c}$$

where

$[\boldsymbol{L}_{\boldsymbol{\mu}}]$, $[\boldsymbol{L}_{\boldsymbol{\eta}}]$ and $[\boldsymbol{L}_{\boldsymbol{\xi}}]$ are block matrices $(J \times J)$

$$[\boldsymbol{L}_{\boldsymbol{\mu}}] = \begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} & \mathcal{G}_{12}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} & \cdots & \mathcal{G}_{1J}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} \\ \mathcal{G}_{21}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} & \mathcal{G}_{22}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} & \cdots & \mathcal{G}_{2J}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} & \mathcal{G}_{J2}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} \end{bmatrix} \tag{E25}$$

$$\boldsymbol{\mathcal{D}}_{\boldsymbol{\mu}} = diagonal[\mu_1 \quad \mu_2 \quad \cdots \quad \mu_{N_D}] \tag{E26}$$

$$[\boldsymbol{\sigma}] = \text{a } J \times J \text{ block matrix } = \begin{bmatrix} \mathcal{G}_{11}\boldsymbol{\sigma} & \mathcal{G}_{12}\boldsymbol{\sigma} & \cdots & \mathcal{G}_{1J}\boldsymbol{\sigma} \\ \mathcal{G}_{21}\boldsymbol{\sigma} & \mathcal{G}_{\mathbf{22}}\boldsymbol{\sigma} & \cdots & \mathcal{G}_{2J}\boldsymbol{\sigma} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{J1}\boldsymbol{\sigma} & \mathcal{G}_{J2}\boldsymbol{\sigma} & \cdots & \mathcal{G}_{JJ}\boldsymbol{\sigma} \end{bmatrix} \tag{E27}$$

$$\boldsymbol{\sigma} = diagonal[\mu_1 \quad \mu_2 \quad \cdots \quad \mu_{N_D}] \tag{E28}$$

$$[\boldsymbol{P}] = \text{a } J \times J \text{ block matrix } = \begin{bmatrix} P_{11}\boldsymbol{F} & P_{12}\boldsymbol{F} & \cdots & P_{1J}\boldsymbol{F} \\ P_{21}\boldsymbol{F} & P_{22}\boldsymbol{F} & \cdots & P_{2J}\boldsymbol{F} \\ \vdots & \vdots & \ddots & \vdots \\ P_{J1}\boldsymbol{F} & P_{J2}\boldsymbol{F} & \cdots & P_{JJ}\boldsymbol{F} \end{bmatrix} \tag{E29}$$

$$P_{jj'} = \mathcal{P}_{jj'}(E_{g-1}) - \mathcal{P}_{jj'}(E_g) - \tilde{\mathcal{P}}_{jj'} + \mathcal{Q}_{jj'} \tag{E30}$$

$$\boldsymbol{F} = diagonal\left[q\vec{\mathcal{E}} \cdot \vec{\Omega}_1 \quad q\vec{\mathcal{E}} \cdot \vec{\Omega}_2 \quad \cdots \quad q\vec{\mathcal{E}} \cdot \vec{\Omega}_{N_D}\right] \tag{E31}$$

$$[M_{\mathcal{E}}] = \text{a } J \times J \text{ block matrix } = \begin{bmatrix} \tilde{\mathcal{G}}_{11}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} & \tilde{\mathcal{G}}_{12}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} & \cdots & \tilde{\mathcal{G}}_{1J}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} \\ \tilde{\mathcal{G}}_{21}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} & \tilde{\mathcal{G}}_{22}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} & \cdots & \tilde{\mathcal{G}}_{2J}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\mathcal{G}}_{J1}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} & \tilde{\mathcal{G}}_{J2}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} & \cdots & \tilde{\mathcal{G}}_{JJ}\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} \end{bmatrix} \tag{E32}$$

$$\boldsymbol{D}_{\boldsymbol{\mathcal{E}}} = q\left\{\mathcal{E}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_x}\right] + \mathcal{E}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_y}\right] + \mathcal{E}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{E}_z}\right]\right\}[\boldsymbol{D}] \tag{E33}$$

$$[M_{\mathcal{B}}] = \text{a } J \times J \text{ block matrix } = \begin{bmatrix} \tilde{\mathcal{G}}_{11}\boldsymbol{D}_{\mathcal{B}} & \tilde{\mathcal{G}}_{12}\boldsymbol{D}_{\mathcal{B}} & \cdots & \tilde{\mathcal{G}}_{1J}\boldsymbol{D}_{\mathcal{B}} \\ \tilde{\mathcal{G}}_{21}\boldsymbol{D}_{\mathcal{B}} & \tilde{\mathcal{G}}_{22}\boldsymbol{D}_{\mathcal{B}} & \cdots & \tilde{\mathcal{G}}_{2J}\boldsymbol{D}_{\mathcal{B}} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\mathcal{G}}_{J1}\boldsymbol{D}_{\mathcal{B}} & \tilde{\mathcal{G}}_{J2}\boldsymbol{D}_{\mathcal{B}} & \cdots & \tilde{\mathcal{G}}_{JJ}\boldsymbol{D}_{\mathcal{B}} \end{bmatrix} \tag{E34}$$

$$\boldsymbol{D}_{\mathcal{B}} = q\left\{\mathcal{B}_x\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_x}\right] + \mathcal{B}_y\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_y}\right] + \mathcal{B}_z\left[\boldsymbol{\mathcal{M}}_{\mathcal{B}_z}\right]\right\}[\boldsymbol{D}] \tag{E35}$$

where $[\boldsymbol{D}]$ is the discrete-to-moment matrix. It is noted that part of the operator $[\boldsymbol{P}]\boldsymbol{\psi}$ will be moved to the RHS depending on the direction of energy sweep.

Least-Squares Finite Element Method (LSFEM) in Space

Expand the angular-flux vector $\boldsymbol{\psi}$ in Eq. (E21) in terms of the spatial basis function as

$$\boldsymbol{\psi}(\vec{r}) = \sum_{i=1}^{I} H_i(\vec{r})\boldsymbol{\chi}_{\boldsymbol{i}} \tag{E36}$$

with each $\boldsymbol{\chi}_{\boldsymbol{i}}$ containing $N_D \times J$ unknowns.

Applying LSFEM to Eq. (E24) leads to the following linear algebraic equations for each element:

$$[\boldsymbol{K}]\boldsymbol{\chi} = \boldsymbol{f} \tag{E37}$$

$$\boldsymbol{\chi} = \begin{bmatrix} \boldsymbol{\chi}_1 \\ \boldsymbol{\chi}_2 \\ \vdots \\ \boldsymbol{\chi}_I \end{bmatrix} \tag{E37a}$$

$$\boldsymbol{f} = \begin{bmatrix} \boldsymbol{f}_1 \\ \boldsymbol{f}_2 \\ \vdots \\ \boldsymbol{f}_I \end{bmatrix} \tag{E37b}$$

$[\boldsymbol{K}]$ is a $I \times I$ block matrix where each block has a size of $(N_D \times J) \times (N_D \times J)$

$$[\boldsymbol{K}_{\boldsymbol{ii'}}] = \int_{\boldsymbol{V_e}} ([\boldsymbol{\Lambda}]H_i + [\boldsymbol{\mathcal{T}}]H_i)^{\boldsymbol{T}}([\boldsymbol{\Lambda}]H_{\boldsymbol{i'}} + [\boldsymbol{\mathcal{T}}]H_{\boldsymbol{i'}})dV \tag{E37c}$$

$$\boldsymbol{f}_{\mathrm{i}} = \int_{\boldsymbol{V_e}} ([\boldsymbol{\Lambda}]H_i + [\boldsymbol{\mathcal{T}}]H_i)^{\boldsymbol{T}}\boldsymbol{S}dV \tag{E37d}$$

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