Denovo Methods Manual

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March 7, 2008

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Chapter 1

Introduction

Denovo is an S_N code package. The KBA package provides a code that solves the discrete ordinates form of the transport equation on a 3D orthogonal structured mesh in parallel using the KBA algorithm.

1.1 Basic Transport Definitions

The principal unknown in radiation transport calculations is the *angular flux*,

$$\psi \equiv \psi(\mathbf{r}, \mathbf{\Omega}, E, t) \,, \tag{1.1}$$

which, in 3D, is a function of 7-independent variables, (x, y, z) in space, (θ, φ) in angle, E in energy, and t in time. The zeroth angular moment of the angular flux is the *scalar flux*,

$$\phi(\mathbf{r}, E, t) = \int_{4\pi} \psi(\mathbf{r}, \mathbf{\Omega}, E, t) \, d\mathbf{\Omega} \,. \tag{1.2}$$

The first angular moment of the angular flux is the *current*,

$$\mathbf{J}(\mathbf{r}, E, t) = \int_{4\pi} \hat{\mathbf{\Omega}} \psi(\mathbf{r}, \mathbf{\Omega}, E, t) \, d\mathbf{\Omega} \,. \tag{1.3}$$

Chapter 2

Transport Discretizations

The steady-state Boltzmann transport equation solved in Denovo is

$$\begin{aligned}\hat{\mathbf{\Omega}} \cdot \nabla\psi(\mathbf{r},\mathbf{\Omega},E) + \sigma(\mathbf{r},E)\psi(\mathbf{r},\mathbf{\Omega},E) \\ = \int_0^\infty \int_{4\pi} \sigma_\mathrm{s}(\mathbf{r},\mathbf{\Omega}'\rightarrow\mathbf{\Omega},E'\rightarrow E)\psi(\mathbf{r},\mathbf{\Omega}',E')\,d\mathbf{\Omega}'dE' + q_e(\mathbf{r},\mathbf{\Omega},E)\,. \quad (2.1)\end{aligned}$$

Here, the state is defined by the angular flux ψ and the independent variables are $\mathbf{r} = (x, y, z)$ in cm, $\mathbf{\Omega} = (\theta, \varphi)$ in str, and E in MeV representing space, angle, and energy respectively. The angles are illustrated in Fig. 2.1. The unit vector of particle direction, $\hat{\mathbf{\Omega}}$, is defined in this coordinate system,

$$\hat{\mathbf{\Omega}} = \mu\hat{\mathbf{e}}_x + \eta\hat{\mathbf{e}}_y + \xi\hat{\mathbf{e}}_z\,, \quad (2.2)$$

where

$$\xi = \cos\theta\,, \quad (2.3a)$$
$$\mu = \sqrt{1-\xi^2}\cos\varphi\,, \quad (2.3b)$$
$$\eta = \sqrt{1-\xi^2}\sin\varphi\,. \quad (2.3c)$$

The normalization of $\mathbf{\Omega}$ in Denovo is such that

$$\int_{4\pi} d\mathbf{\Omega} = \int_0^{2\pi}\int_0^{\pi} \sin\theta\, d\theta d\varphi = \int_0^{2\pi}\int_{-1}^{1} d\xi d\varphi = 4\pi\,. \quad (2.4)$$

The right-hand side of Eq. (2.1) represents a source that is comprised of external sources and scattering:

$$\begin{aligned}Q(\mathbf{r},\mathbf{\Omega},E) &= q_s(\mathbf{r},\mathbf{\Omega},E) + q_e(\mathbf{r},\mathbf{\Omega},E) \\ &= \int_0^\infty \int_{4\pi} \sigma_\mathrm{s}(\mathbf{r},\mathbf{\Omega}'\rightarrow\mathbf{\Omega},E'\rightarrow E)\psi(\mathbf{r},\mathbf{\Omega}',E')\,d\mathbf{\Omega}'dE' + q_e(\mathbf{r},\mathbf{\Omega},E)\,.\end{aligned} \quad (2.5)$$

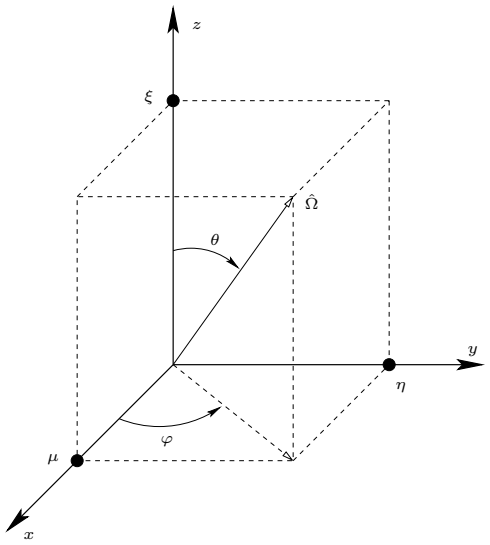

Figure 2.1: Coordinate system used in Denovo.

For the problems considered by Denovo, the scattering is only a function of the cosine of the angle between the incoming rays, and Q can be rewritten

$$Q(\mathbf{r}, \mathbf{\Omega}, E) = \int_{4\pi} \sigma_{\mathrm{s}}(\mathbf{r}, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E')\psi(\mathbf{r}, \mathbf{\Omega}', E')\, d\mathbf{\Omega}' dE' + q_e(\mathbf{r}, \mathbf{\Omega}, E)\,. \tag{2.6}$$

In operator form, we can write

$$\mathbf{L}\psi = Q\,. \tag{2.7}$$

In 3D Cartesian space, we use Eq. (2.2) to define the transport operator,

$$\mathbf{L} = \mu\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial y} + \xi\frac{\partial}{\partial z} + \sigma\,. \tag{2.8}$$

2.1 Multigroup Approximation

To begin the multigroup energy approximation we first write the transport equation (2.1) while suppressing dependencies on $\mathbf{r}$ and $\mathbf{\Omega}$,

$$\hat{\mathbf{\Omega}} \cdot \nabla\psi(E) + \sigma(E)\psi(E) = \int_0^\infty \sigma_{\mathrm{s}}(E' \rightarrow E)\psi(E')\, dE' + q_e(E')\,. \tag{2.9}$$

First, we define a discrete energy grid as shown in Fig. 2.2. Now we expand ψ as follows:

$$\psi(E) = \sum_{k=0}^{G} \psi_k B_k(E)\,, \tag{2.10}$$

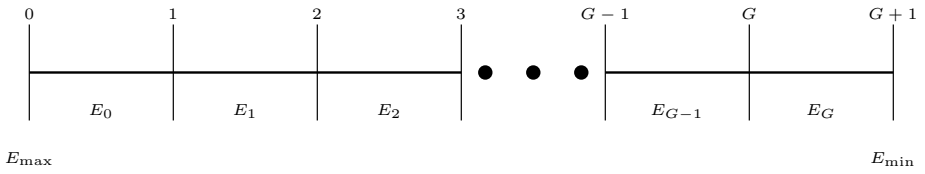

Figure 2.2: Multigroup energy grid used in Denovo.

where $B_k(E)$ obeys the following properties

$$B_k(E) = 0 \quad \forall \quad E \notin [E_{k+1}, E_k] \,, \tag{2.11}$$

$$\int_{E_{k+1}}^{E_k} B_k(E)\, dE = 1 \,. \tag{2.12}$$

Integrating Eq. (2.10) over group g gives

$$\begin{aligned} \int_{E_{g+1}}^{E_g} \psi(E)\, dE &= \sum_{k=0}^{G} \psi_k \int_{E_{g+1}}^{E_g} B_k(E)\, dE \\ &= \psi_g \,. \end{aligned} \tag{2.13}$$

The weight-function for each group is defined

$$W_g(E) = \begin{cases} 0 & E \notin [E_{g+1}, E_g] \,, \\ 1 & E \in [E_{g+1}, E_g] \,. \end{cases} \tag{2.14}$$

Now, expand $\psi(E)$ in Eq. (2.9),

$$\begin{aligned} &\hat{\mathbf{\Omega}} \cdot \nabla\Big(\sum_{k=0}^{G} \psi_k B_k(E)\Big) + \sigma(E)\Big(\sum_{k=0}^{G} \psi_k B_k(E)\Big) \\ &\qquad = \int_0^\infty \sigma_{\mathrm{s}}(E' \to E)\Big(\sum_{g'=0}^{G} \psi_{g'} B_{g'}(E')\Big)\, dE' + \Big(\sum_{k=0}^{G} q_{ek} B_k(E)\Big) \,. \end{aligned} \tag{2.15}$$

Next, weighted-residual expression of the transport equation is obtained by multiplying by $W_g(E)$ and integrating over all energies:

$$\begin{aligned} &\int_0^\infty W_g(E)\hat{\mathbf{\Omega}} \cdot \nabla\Big(\sum_{k=0}^{G} \psi_k B_k(E)\Big)\, dE + \int_0^\infty W_g(E)\sigma(E)\Big(\sum_{k=0}^{G} \psi_k B_k(E)\Big)\, dE \\ &\qquad = \int_0^\infty W_g(E) \int_0^\infty \sigma_{\mathrm{s}}(E' \to E)\Big(\sum_{g'=0}^{G} \psi_{g'} B_{g'}(E')\Big)\, dE' dE \\ &\qquad\quad + \int_0^\infty W_g(E)\Big(\sum_{k=0}^{G} q_{ek} B_k(E)\Big)\, dE \,. \end{aligned} \tag{2.16}$$

The definition of the weight function, W_g, converts integrals over all energies into integrals over group g,

$$\int_0^\infty W_g(E)\,dE = \int_{E_{g+1}}^{E_g} dE\,. \tag{2.17}$$

Applying this expression, we proceed to evaluate each term in Eq. (2.16).

Rearranging the sum and integral operators, the streaming term in Eq. (2.16) is

$$\hat{\mathbf{\Omega}}\cdot\nabla\Big(\sum_{k=0}^{G}\psi_k\int_{E_{g+1}}^{E_g}B_k(E)\,dE\Big) = \hat{\mathbf{\Omega}}\cdot\nabla\psi_g\,, \tag{2.18}$$

where the group flux, ψ_g, is defined in Eq. (2.13). Similarly, the source term can be evaluated

$$\sum_{k=0}^{G}q_{ek}\int_{E_{g+1}}^{E_g}B_k(E)\,dE = q_{eg}\,. \tag{2.19}$$

The collision term is becomes

$$\sum_{k=0}^{G}\psi_k\int_{E_{g+1}}^{E_g}\sigma(E)B_k(E)\,dE = \sigma_g\psi_g\,, \tag{2.20}$$

where

$$\sigma_g = \int_{E_{g+1}}^{E_g}\sigma(E)B_g(E)\,dE\,. \tag{2.21}$$

The scattering term is slightly more complicated. Rearranging terms gives

$$\begin{aligned}\sum_{g'=0}^{G}\psi_{g'}\int_{E_{g+1}}^{E_g}\int_0^\infty\sigma_{\mathrm{s}}(E'\to E)B_{g'}(E')\,dE'dE&\\ = \sum_{g'=0}^{G}\psi_{g'}\int_{E_{g+1}}^{E_g}\int_{E_{g'+1}}^{E_{g'}}\sigma_{\mathrm{s}}(E'\to E)B_{g'}(E')\,dE'dE\,,&\end{aligned} \tag{2.22}$$

where we have utilized the definition of $B_g(E)$ to recognize that the integral over all energies, E', will be zero everywhere except in group g'. The scattering integral becomes

$$\sum_{g'=0}^{G}\psi_{g'}\int_{E_{g+1}}^{E_g}\int_{E_{g'+1}}^{E_{g'}}\sigma_{\mathrm{s}}(E'\to E)B_{g'}(E')\,dE'dE = \sum_{g'=0}^{G}\sigma_{\mathrm{s}gg'}\psi_{g'}\,, \tag{2.23}$$

where

$$\sigma_{\mathrm{s}\,g'\to g} = \sigma_{\mathrm{s}gg'} = \int_{E_{g+1}}^{E_g}\int_{E_{g'+1}}^{E_{g'}}\sigma_{\mathrm{s}}(E'\to E)B_{g'}(E')\,dE'dE\,. \tag{2.24}$$

Putting everything together and including space/angle dependencies, the multigroup transport equation is

$$\hat{\mathbf{\Omega}} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) + \sigma^g(\mathbf{r}) \psi^g(\mathbf{r}, \mathbf{\Omega}) = \sum_{g'=0}^{G} \int_{4\pi} \sigma_{\mathrm{s}}^{gg'}(\mathbf{r}, \mathbf{\Omega}' \cdot \mathbf{\Omega}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}') \, d\mathbf{\Omega}' + q_e^g(\mathbf{r}, \mathbf{\Omega}) \,, \quad (2.25)$$

where we have written the group indices as superscripts to provide additional clarity when we perform discretizations in angle and space. As an additional note, the energy-integrated angular flux is defined in the multigroup approximation,

$$\psi = \int_0^\infty \psi(E) \, dE = \sum_{g=0}^{G} \psi_g \int_0^\infty B_g(E) \, dE = \sum_{g=0}^{G} \psi_g \,. \quad (2.26)$$

2.2 Scattering Discretization

Equation (2.25) is still an integro-differential equation in which the principal unknown, ψ, is present in the scattering integral. Additionally, the multigroup scattering cross section is a function of angle. Accordingly, we need some method for dealing with the angular dependence of the scattering source. We tackle this problem by recognizing that σ_{s} is only a function of the cosine between the incoming and outgoing angles (the polar scattering angle assuming azimuthal symmetry). Therefore, we can expand the scattering cross section in Legendre polynomials,

$$\sigma_{\mathrm{s}}^{gg'}(\mathbf{\Omega}' \cdot \mathbf{\Omega}) = \sum_{l=0}^{N} \frac{2l+1}{4\pi} P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \sigma_{\mathrm{s}\,l}^{gg'} \,. \quad (2.27)$$

Integrating over all angles we calculate the total scattering cross section as follows:

$$\begin{aligned} \sigma_{\mathrm{s}}^{gg'} &= \int_{4\pi} \sigma_{\mathrm{s}}^{gg'}(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \, d\mathbf{\Omega} \equiv 2\pi \int_{-1}^{1} \sigma_{\mathrm{s}}^{gg'}(\mu_o) \, d\mu_o \\ &= \sum_{l=0}^{N} \frac{2l+1}{2} \sigma_{\mathrm{s}\,l}^{gg'} \int_{-1}^{1} P_0(\mu_o) P_l(\mu_o) \, d\mu_o \\ &= \sigma_{\mathrm{s}\,0}^{gg'} \,, \end{aligned} \quad (2.28)$$

where we have used the orthogonality of Legendre polynomials listed in § 4.2.

Applying Eq. (2.27) in Eq. (2.25) gives a scattering source defined by

$$q_s^g(\mathbf{\Omega}) = \sum_{g'=0}^{G} \int_{4\pi} \sum_{l=0}^{N} \frac{2l+1}{4\pi} P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega}) \sigma_{\mathrm{s}\,l}^{gg'} \psi^{g'}(\mathbf{\Omega}') \, d\mathbf{\Omega}' \,, \quad (2.29)$$

where we have suppressed the spatial dependence, $\mathbf{r}$. The addition theorem of Spherical Harmonics can be used to evaluate the Legendre function, $P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega})$,

$$P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\mathbf{\Omega}) Y_{lm}^*(\mathbf{\Omega}') \,, \tag{2.30}$$

where the Y_{lm} are defined in Eq. (13). The scattering must be real; therefore, we can follow a methodology similar to the techniques described in § 4.2 that shows how to expand a real-valued function using complex Spherical Harmonics. First, the expansion is split into positive and negative components of m,

$$P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega}) = \frac{4\pi}{2l+1} \Big[Y_{l0}(\mathbf{\Omega}) Y_{l0}(\mathbf{\Omega}') + \sum_{m=1}^{l} \big(Y_{lm}(\mathbf{\Omega}) Y_{lm}^*(\mathbf{\Omega}') + Y_{l-m}(\mathbf{\Omega}) Y_{l-m}^*(\mathbf{\Omega}') \big) \Big] \,. \tag{2.31}$$

Examining the $m = 0$ term gives the following result

$$Y_{l0} = \sqrt{\frac{2l+1}{4\pi}} \, P_{l0} = Y_{l0}^e \,, \tag{2.32}$$

where the Y_e are defined in Eq. (31).

Expanding the Spherical Harmonics into real and imaginary components as shown in Eq. (26), the sum over $m > 0$ becomes

$$\sum_{m=1}^{l} \Big(\hat{Y}_{lm}^e(\mathbf{\Omega}) \hat{Y}_{lm}^e(\mathbf{\Omega}') + \hat{Y}_{lm}^o(\mathbf{\Omega}) \hat{Y}_{lm}^o(\mathbf{\Omega}') + \hat{Y}_{l-m}^e(\mathbf{\Omega}) \hat{Y}_{l-m}^e(\mathbf{\Omega}') + \hat{Y}_{l-m}^o(\mathbf{\Omega}) \hat{Y}_{l-m}^o(\mathbf{\Omega}') \Big) \,, \tag{2.33}$$

where the imaginary terms have been set to zero because the scattering must be real. Using Eqs. (47) and (48), the summation becomes

$$\sum_{m=1}^{l} \Big(2\hat{Y}_{lm}^e(\mathbf{\Omega}) \hat{Y}_{lm}^e(\mathbf{\Omega}') + 2\hat{Y}_{lm}^o(\mathbf{\Omega}) \hat{Y}_{lm}^o(\mathbf{\Omega}') \Big) \tag{2.34}$$

Comparing Eqs. (24) and (25) with Eqs. (31) and (32) leads to the following relationships,

$$\hat{Y}_{lm}^e = \frac{1}{\sqrt{2}} Y_{lm}^e \,, \quad \hat{Y}_{lm}^o = \frac{1}{\sqrt{2}} Y_{lm}^o \,. \tag{2.35}$$

After applying these equations in the $m > 0$ terms and combining with the $m = 0$ term described above, the expression for $P_l(\mathbf{\Omega} \cdot \mathbf{\Omega}')$ is

$$P_l(\mathbf{\Omega}' \cdot \mathbf{\Omega}) = \frac{4\pi}{2l+1} \Big[Y_{l0}^e(\mathbf{\Omega}) Y_{l0}^e(\mathbf{\Omega}') + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}) Y_{lm}^e(\mathbf{\Omega}') + Y_{lm}^o(\mathbf{\Omega}) Y_{lm}^o(\mathbf{\Omega}') \big) \Big] \,, \tag{2.36}$$

where, as shown in § 4.2, the Y^e and Y^o form an orthonormal basis.

Returning to the scattering source defined in Eq. (2.29), Eq. (2.36) provides the Legendre polynomial for the cosine of the scattering angle, and

$$q_s^g(\mathbf{\Omega}) = \sum_{g'=0}^{G} \int_{4\pi} \sum_{l=0}^{N} \Big[Y_{l0}^e(\mathbf{\Omega}) Y_{l0}^e(\mathbf{\Omega}') + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}) Y_{lm}^e(\mathbf{\Omega}') + Y_{lm}^o(\mathbf{\Omega}) Y_{lm}^o(\mathbf{\Omega}') \big) \Big] \sigma_{\mathrm{s}\,l}^{gg'} \psi^{g'}(\mathbf{\Omega}')\, d\mathbf{\Omega}' \,. \tag{2.37}$$

Rearranging terms and defining

$$\phi_{lm}^g = \int_{4\pi} Y_{lm}^e(\mathbf{\Omega}) \psi^g(\mathbf{\Omega})\, d\mathbf{\Omega} \,, \quad m \geq 0 \,, \tag{2.38}$$

$$\vartheta_{lm}^g = \int_{4\pi} Y_{lm}^o(\mathbf{\Omega}) \psi^g(\mathbf{\Omega})\, d\mathbf{\Omega} \,, \quad m > 0 \,, \tag{2.39}$$

which follows directly from Eqs. (39) and (40), the scattering source becomes

$$q_s^g(\mathbf{r}, \mathbf{\Omega}) = \sum_{g'=0}^{G} \sum_{l=0}^{N} \sigma_{\mathrm{s}\,l}^{gg'}(\mathbf{r}) \Big[Y_{l0}^e(\mathbf{\Omega}) \phi_{l0}^{g'}(\mathbf{r}) + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}) \phi_{lm}^{g'}(\mathbf{r}) + Y_{lm}^o(\mathbf{\Omega}) \vartheta_{lm}^{g'}(\mathbf{r}) \big) \Big] \,. \tag{2.40}$$

Equation (2.40) is the multigroup anisotropic scattering source that is defined by the order of the Legendre expansion, P_N, of the scattering. For a given P_N order, $(N+1)^2$ moments are required to integrate the scattering operator. The moments in Eqs. (2.38) and (2.39) are the *angular flux moments* or, simply, flux moments.

The scalar flux is defined in Eq.(1.2) as the zeroth moment of the angular flux. Therefore, we have

$$\phi^g = \int_{4\pi} \psi^g\, d\mathbf{\Omega} = \sqrt{4\pi} \int_{4\pi} Y_{00}^e \psi^g\, d\mathbf{\Omega} = \sqrt{4\pi} \phi_{00}^g \,. \tag{2.41}$$

The current is defined

$$\begin{aligned} \mathbf{J}^g &= \int_{4\pi} \Big[\mu \psi^g \hat{\mathbf{e}}_x + \eta \psi^g \hat{\mathbf{e}}_y + \xi \psi^g \hat{\mathbf{e}}_z \Big]\, d\mathbf{\Omega} \\ &= -\sqrt{\frac{4\pi}{3}} \phi_{11}^g \hat{\mathbf{e}}_x - \sqrt{\frac{4\pi}{3}} \vartheta_{11}^g \hat{\mathbf{e}}_y + \sqrt{\frac{4\pi}{3}} \phi_{10}^g \hat{\mathbf{e}}_z \,. \end{aligned} \tag{2.42}$$

More concisely,

$$J_x^g = -\sqrt{\frac{4\pi}{3}} \phi_{11}^g \,, \quad J_y^g = -\sqrt{\frac{4\pi}{3}} \vartheta_{11}^g \,, \quad J_z^g = \sqrt{\frac{4\pi}{3}} \phi_{10}^g \,, \tag{2.43}$$

for $\mathbf{J} = J_x \hat{\mathbf{e}}_x + J_y \hat{\mathbf{e}}_y + J_z \hat{\mathbf{e}}_z$.

2.3 External Source Discretization

The external source gets expanded in Spherical Harmonics to be consistent with the scattering. Equation (38) gives the Spherical Harmonics expansion of a real-valued function. Applying the same methodology gives the expansion of the external source

$$q_e^g(\mathbf{\Omega}) = \sum_{l=0}^{N} \Big[Y_{l0}^e(\mathbf{\Omega}) q_{l0}^g + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}) q_{lm}^g + Y_{lm}^o(\mathbf{\Omega}) s_{lm}^g \big) \Big] , \tag{2.44}$$

where the spatial dependence has been suppressed. The even and odd source moments are defined

$$q_{lm}^g = \int_{4\pi} Y_{lm}^e(\mathbf{\Omega}) q_e^g(\mathbf{\Omega})\, d\mathbf{\Omega} , \quad m \geq 0 , \tag{2.45}$$

$$s_{lm}^g = \int_{4\pi} Y_{lm}^o(\mathbf{\Omega}) q_e^g(\mathbf{\Omega})\, d\mathbf{\Omega} , \quad m > 0 . \tag{2.46}$$

Now, using Eqs.(2.40) and (2.44), we write the entire source as

$$\begin{aligned} Q^g(\mathbf{r}, \mathbf{\Omega}) &= q_s^g(\mathbf{r}, \mathbf{\Omega}) + q_e^g(\mathbf{r}, \mathbf{\Omega}) \\ &= \sum_{g'=0}^{G} \sum_{l=0}^{N} \sigma_{\mathrm{s}\,l}^{gg'}(\mathbf{r}) \Big[Y_{l0}^e(\mathbf{\Omega}) \phi_{l0}^{g'}(\mathbf{r}) + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}) \phi_{lm}^{g'}(\mathbf{r}) + Y_{lm}^o(\mathbf{\Omega}) \vartheta_{lm}^{g'}(\mathbf{r}) \big) \Big] \\ &\quad + \sum_{l=0}^{N} \Big[Y_{l0}^e(\mathbf{\Omega}) q_{l0}^g(\mathbf{r}) + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}) q_{lm}^g(\mathbf{r}) + Y_{lm}^o(\mathbf{\Omega}) s_{lm}^g(\mathbf{r}) \big) \Big] . \end{aligned} \tag{2.47}$$

2.4 Angular Discretization

Combining Eqs. (2.25) and (2.47) gives the multigroup transport equation with the scattering and external source expanded in Spherical Harmonics,

$$\hat{\mathbf{\Omega}} \cdot \nabla \psi^g(\mathbf{\Omega}) + \sigma^g \psi^g(\mathbf{\Omega}) = Q^g(\mathbf{\Omega}) \tag{2.48}$$

where the spatial dependence has been suppressed. While Spherical Harmonics have been used to expand the scattering and external sources, we still have a dependence on $\mathbf{\Omega}$ that needs to be resolved. We apply the discrete ordinates (S_N) approximation, which is a collocation method in angle. Solving Eq. (2.48) at discrete angular locations requires the following equation,

$$\begin{aligned} \hat{\mathbf{\Omega}}_a \cdot \nabla \psi_a^g + \sigma^g \psi_a^g &= \sum_{g'=0}^{G} \sum_{l=0}^{N} \sigma_{\mathrm{s}\,l}^{gg'} \Big[Y_{l0}^e(\mathbf{\Omega}_a) \phi_{l0}^{g'} + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}_a) \phi_{lm}^{g'} + Y_{lm}^o(\mathbf{\Omega}_a) \vartheta_{lm}^{g'} \big) \Big] \\ &\quad + \sum_{l=0}^{N} \Big[Y_{l0}^e(\mathbf{\Omega}_a) q_{l0}^g + \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}_a)) q_{lm}^g + Y_{lm}^o(\mathbf{\Omega}_a) s_{lm}^g \big) \Big] , \end{aligned} \tag{2.49}$$

where $\psi_a^g \equiv \psi^g(\mathbf{\Omega}_a)$. The angles are integrated by a quadrature rule such that

$$\int_{4\pi} d\mathbf{\Omega} = \sum_{a=1}^{n} w_a = 4\pi \ , \tag{2.50}$$

where w_a are the quadrature weights, and n is the total number of angles. Different quadrature sets have different numbers of unknowns. The Level-Symmetric quadrature set has $n = N(N+2)$ unknowns for an S_N approximation.

Given that many angles result from even low-order S_N approximations, we see why the external source has been expanded in Spherical Harmonics. Consider, an S_8 calculation has 80 angles per unknown location per group. For a P_3 expansion 16 moments are required to define the source, a factor of 5 reduction in memory storage. An S_{16} calculation could be used for more accuracy with a P_3 calculation resulting in a factor of 18 savings in memory.

Using the quadrature integration rule the flux moments in Eqs. (2.38) and (2.39) are evaluated using

$$\phi_{lm}^g = \sum_{a=1}^{n} Y_{lm}^e(\mathbf{\Omega}_a)\psi_a^g w_a \ , \tag{2.51}$$

$$\vartheta_{lm}^g = \sum_{a=1}^{n} Y_{lm}^o(\mathbf{\Omega}_a)\psi_a^g w_a \ . \tag{2.52}$$

Similarly, the source moments in Eqs. (2.45) and (2.46) are calculated using

$$q_{lm}^g = \sum_{a=1}^{n} Y_{lm}^e(\mathbf{\Omega}_a) q_e^g(\mathbf{\Omega}_a) w_a \ , \tag{2.53}$$

$$s_{lm}^g = \sum_{a=1}^{n} Y_{lm}^o(\mathbf{\Omega}_a) q_e^g(\mathbf{\Omega}_a) w_a \ . \tag{2.54}$$

The S_N method will be conservative if the quadrature set effectively integrates the even and odd Spherical Harmonics. If the orthogonality conditions in Eqs. (34) and (35) are preserved, then integrating the anisotropic scattering should yield,

$$\int_{4\pi} q_s^g(\mathbf{\Omega})\, d\mathbf{\Omega} = \sum_{a=1}^{n} q_s^g(\mathbf{\Omega}_a) w_a = \sqrt{4\pi}\sigma_{\mathrm{s}\,0}^{gg'}\,\phi_{00}^{g'} = \sigma_s^{gg'}\phi^{g'} \ , \tag{2.55}$$

which will yield a conservative particle balance equation.

2.5 Operator Form of the Discrete Ordinates Equation

The multigroup discrete ordinates, or S_N, equation is (see Eq.(2.48))

$$\begin{aligned}\hat{\mathbf{\Omega}}_a \cdot \nabla \psi_a^g(\mathbf{r}) + \sigma^g(\mathbf{r})\psi_a^g(\mathbf{r}) \\ = \sum_{g'=0}^{G}\sum_{l=0}^{N} \sigma_{s\,l}^{gg'}(\mathbf{r})\Big[Y_{l0}^e(\mathbf{\Omega}_a)\phi_{l0}^{g'}(\mathbf{r}) + \sum_{m=1}^{l}\big(Y_{lm}^e(\mathbf{\Omega}_a)\phi_{lm}^{g'}(\mathbf{r}) + Y_{lm}^o(\mathbf{\Omega}_a)\vartheta_{lm}^{g'}(\mathbf{r})\big)\Big] \\ + \sum_{l=0}^{N}\Big[Y_{l0}^e(\mathbf{\Omega}_a)q_{l0}^g(\mathbf{r}) + \sum_{m=1}^{l}\big(Y_{lm}^e(\mathbf{\Omega}_a))q_{lm}^g(\mathbf{r}) + Y_{lm}^o(\mathbf{\Omega}_a)s_{lm}^g(\mathbf{r})\big)\Big] \,. \quad (2.56)\end{aligned}$$

We defer the spatial treatment of Eq. (2.56) until § 2.6. This equation can be written using a concise operator notation that helps illuminate numerical solution techniques. The operator form of Eq. (2.56) is

$$\mathbf{L}\psi = \mathbf{MS}\phi + \mathbf{M}q_e \,, \quad (2.57)$$

where

$$Q = \mathbf{MS}\phi + \mathbf{M}q_e \,. \quad (2.58)$$

Here we use the convention that bold letters represent discrete operators or matrices and script symbols and letters represent vectors.

The sizes of the operators in Eq. (2.57) are determined from the following dimensions:

$$\begin{aligned} N_g &= \text{number of groups} \,, \\ t &= \text{number of moments} \,, \\ n &= \text{number of angles} \,, \\ N &= P_N \text{ order} \,, \\ N_c &= \text{number of cells} \,, \\ N_e &= \text{number of unknowns per cell} \,. \end{aligned} \quad (2.59)$$

Now, we define

$$a = N_g \times n \times N_c \times N_e \,, \quad (2.60)$$

$$f = N_g \times t \times N_c \times N_e \,. \quad (2.61)$$

Equation (2.57) can then be defined in terms of the sizes of the operators,

$$(a \times a)(a \times 1) = (a \times f)(f \times f)(f \times 1) + (a \times f)(f \times 1) \,. \quad (2.62)$$

More specifically, with the groups defined over the range $g \in [0, G]$, at each spatial unknown

we can write

$$\mathbf{L}\begin{pmatrix}[\psi]_0\\[\psi]_1\\[\psi]_2\\\vdots\\[\psi]_G\end{pmatrix} = \begin{pmatrix}[\mathbf{M}]_{00} & 0 & 0 & 0 & 0\\ 0 & [\mathbf{M}]_{11} & 0 & 0 & 0\\ 0 & 0 & [\mathbf{M}]_{22} & 0 & 0\\ 0 & 0 & 0 & \ddots & 0\\ 0 & 0 & 0 & 0 & [\mathbf{M}]_{GG}\end{pmatrix}\begin{pmatrix}[\mathbf{S}]_{00} & [\mathbf{S}]_{01} & [\mathbf{S}]_{02} & \cdots & [\mathbf{S}]_{0G}\\ [\mathbf{S}]_{10} & [\mathbf{S}]_{11} & [\mathbf{S}]_{12} & \cdots & [\mathbf{S}]_{1G}\\ [\mathbf{S}]_{20} & [\mathbf{S}]_{21} & [\mathbf{S}]_{22} & \cdots & [\mathbf{S}]_{2G}\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ [\mathbf{S}]_{G0} & [\mathbf{S}]_{G1} & [\mathbf{S}]_{G2} & \cdots & [\mathbf{S}]_{GG}\end{pmatrix} \times \begin{pmatrix}[\phi]_0\\[\phi]_1\\[\phi]_2\\\vdots\\[\phi]_G\end{pmatrix} + \begin{pmatrix}[\mathbf{M}]_{00} & 0 & 0 & 0 & 0\\ 0 & [\mathbf{M}]_{11} & 0 & 0 & 0\\ 0 & 0 & [\mathbf{M}]_{22} & 0 & 0\\ 0 & 0 & 0 & \ddots & 0\\ 0 & 0 & 0 & 0 & [\mathbf{M}]_{GG}\end{pmatrix}\begin{pmatrix}[q_e]_0\\[q_e]_1\\[q_e]_2\\\vdots\\[q_e]_G\end{pmatrix}, \quad (2.63)$$

where the notation $[\cdot]_g$ indicates a block matrix over all unknowns for a single group. Accordingly, we define

$$[\psi]_g = \begin{pmatrix}\psi_1^g & \psi_2^g & \psi_3^g & \cdots \psi_n^g\end{pmatrix}^T . \quad (2.64)$$

The operator $\mathbf{M}$ is the moment-to-discrete matrix. It is used to convert harmonic moments into discrete angles, and it is defined

$$[\mathbf{M}]_{gg} = \begin{pmatrix}Y_{00}^e(\mathbf{\Omega}_1) & Y_{10}^e(\mathbf{\Omega}_1) & Y_{11}^o(\mathbf{\Omega}_1) & Y_{11}^e(\mathbf{\Omega}_1) & Y_{20}^e(\mathbf{\Omega}_1) & \cdots & Y_{NN}^o(\mathbf{\Omega}_1) & Y_{NN}^e(\mathbf{\Omega}_1)\\ Y_{00}^e(\mathbf{\Omega}_2) & Y_{10}^e(\mathbf{\Omega}_2) & Y_{11}^o(\mathbf{\Omega}_2) & Y_{11}^e(\mathbf{\Omega}_2) & Y_{20}^e(\mathbf{\Omega}_2) & \cdots & Y_{NN}^o(\mathbf{\Omega}_2) & Y_{NN}^e(\mathbf{\Omega}_2)\\ Y_{00}^e(\mathbf{\Omega}_3) & Y_{10}^e(\mathbf{\Omega}_3) & Y_{11}^o(\mathbf{\Omega}_3) & Y_{11}^e(\mathbf{\Omega}_3) & Y_{20}^e(\mathbf{\Omega}_3) & \cdots & Y_{NN}^o(\mathbf{\Omega}_3) & Y_{NN}^e(\mathbf{\Omega}_3)\\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots\\ Y_{00}^e(\mathbf{\Omega}_n) & Y_{10}^e(\mathbf{\Omega}_n) & Y_{11}^o(\mathbf{\Omega}_n) & Y_{11}^e(\mathbf{\Omega}_n) & Y_{20}^e(\mathbf{\Omega}_n) & \cdots & Y_{NN}^o(\mathbf{\Omega}_n) & Y_{NN}^e(\mathbf{\Omega}_n)\end{pmatrix}. \quad (2.65)$$

The scattering cross sections are defined

$$[\mathbf{S}]_{gg'} = \begin{pmatrix}\sigma_{\mathrm{s}\,0}^{gg'} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & \sigma_{\mathrm{s}\,1}^{gg'} & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & \sigma_{\mathrm{s}\,1}^{gg'} & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & \sigma_{\mathrm{s}\,1}^{gg'} & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & \sigma_{\mathrm{s}\,2}^{gg'} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & \ddots & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{\mathrm{s}\,N}^{gg'} & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{\mathrm{s}\,N}^{gg'}\end{pmatrix}. \quad (2.66)$$

Here the block-matrix $[\mathbf{S}]_{gg'}$ defines scattering cross sections for particles that scatter from group g' into group g. The lower triangular part of $\mathbf{S}$ represents down-scattering, the diagonal represents in-group scattering, and the upper diagonal is up-scattering.

Finally, the flux and source moment vectors are defined

$$[\phi]_g = \begin{pmatrix}\phi_{00}^g & \phi_{10}^g & \vartheta_{11}^g & \phi_{11}^g & \phi_{20}^g & \cdots & \vartheta_{NN}^g & \phi_{NN}^g\end{pmatrix}^T , \quad (2.67)$$

$$[q_e]_g = \begin{pmatrix}q_{00}^g & q_{10}^g & s_{11}^g & q_{11}^g & q_{20}^g & \cdots & s_{NN}^g & q_{NN}^g\end{pmatrix}^T . \quad (2.68)$$

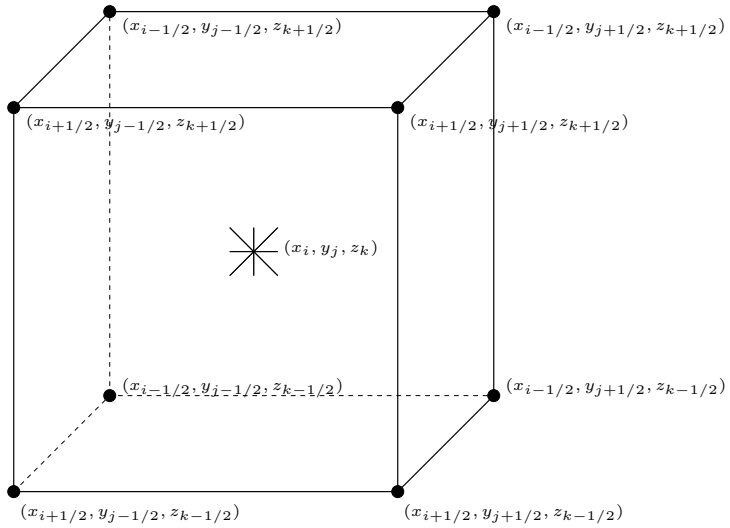

Figure 2.3: Mesh cell from the orthogonal, (x, y, z) mesh used in Denovo.

Multiplying the matrices in Eq. (2.63) gives the following series of equations,

$$\begin{aligned}
\mathbf{L}[\psi]_0 &= [\mathbf{M}]\big([\mathbf{S}]_{00}[\phi]_0 + [\mathbf{S}]_{01}[\phi]_1 + \ldots + [\mathbf{S}]_{0G}[\phi]_G\big) + [\mathbf{M}][q_e]_0 \,, \\
\mathbf{L}[\psi]_1 &= [\mathbf{M}]\big([\mathbf{S}]_{10}[\phi]_0 + [\mathbf{S}]_{11}[\phi]_1 + \ldots + [\mathbf{S}]_{1G}[\phi]_G\big) + [\mathbf{M}][q_e]_1 \,, \\
&\vdots \\
\mathbf{L}[\psi]_G &= [\mathbf{M}]\big([\mathbf{S}]_{G0}[\phi]_0 + [\mathbf{S}]_{G1}[\phi]_1 + \ldots + [\mathbf{S}]_{GG}[\phi]_G\big) + [\mathbf{M}][q_e]_G \,,
\end{aligned} \tag{2.69}$$

where $[\mathbf{M}]_{00} = [\mathbf{M}]_{11} = \ldots = [\mathbf{M}]_{GG} = [\mathbf{M}]$. Therefore, the discrete ordinates equations can be decomposed into a series of single-group equations. We will use this property in Chapter 3 when solution methods are discussed.

2.6 Spatial Discretizations

Multiple spatial discretization schemes have been studied and developed to solve Eq. (2.56). We will investigate spatial schemes that solve the following form of the transport equation,

$$\hat{\mathbf{\Omega}} \cdot \psi(\mathbf{r}) + \sigma(\mathbf{r})\psi(\mathbf{r}) = Q(\mathbf{r}) \,, \tag{2.70}$$

where we have dropped the angular and energy-group subscripts for clarity. Equation (2.70) is general for any non-spatially coupled source. We will confine our discussions to an orthogonal, (x, y, z) mesh illustrated in Fig. 2.3. In this geometry, the transport operator has the following form

$$\mathbf{L} = \mu\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial y} + \xi\frac{\partial}{\partial z} + \sigma \,. \tag{2.71}$$

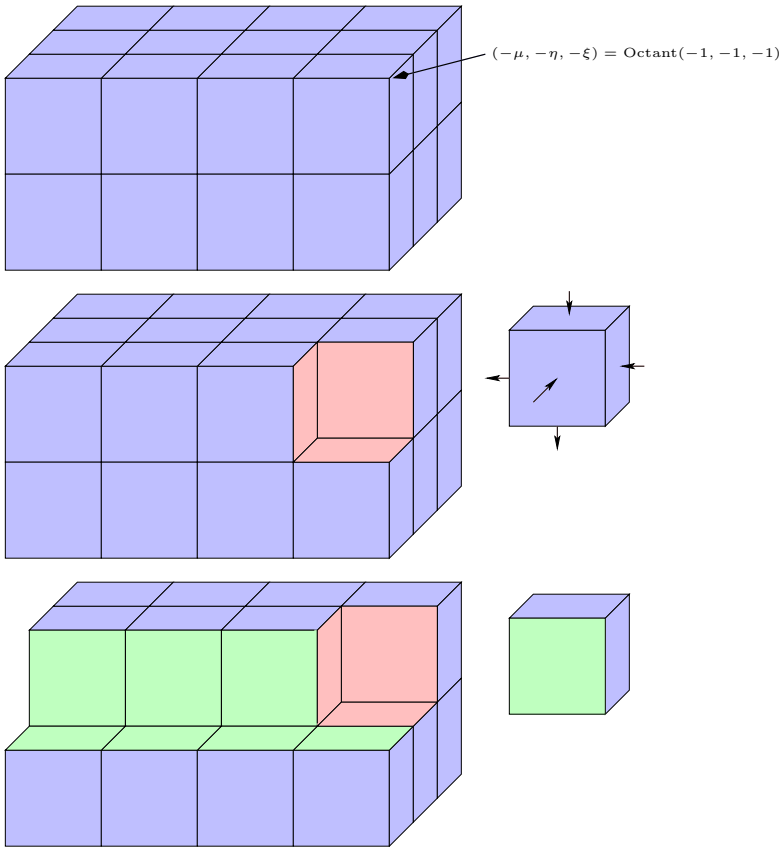

Figure 2.4: Transport sweep strategy on an orthogonal (x, y, z) mesh. The illustrated sweep direction is in Octant$(-1, -1, -1)$. The blue sides represent angular fluxes known from boundary conditions. Red sides indicate unknown fluxes before upwinding. Green sides represent "upwinded" angular fluxes.

All of the spatial schemes that are used in Denovo can be converted into a lower-triangular system that can be solved by a single pass through the mesh in the direction of particle travel (although this is not generally true for unstructured meshes). This technique is referred to as a transport *sweep*, and it is the method applied to invert $\mathbf{L}$ in Denovo.

For each discrete angle, the incoming angular fluxes in each cell are defined by

$$\hat{\mathbf{\Omega}}_a \cdot \hat{\mathbf{n}} < 0 \,, \tag{2.72}$$

where $\hat{\mathbf{n}}$ is the outgoing normal on each side of the cell. For an orthogonal mesh a further simplification is possible in that the angles can be grouped into *octants* such that every angle in an octant sweeps through the mesh in the same order. The transport sweep is illustrated in Fig. 2.4. Because the angle is in Octant$(-1, -1, -1)$ the solution marches in the $(-x, -y, -z)$ direction. Fluxes on the $(+x, +y, +z)$ side of each cell are known from boundary conditions (indicated by blue sides) or the solution from the "upwind" cell (indicated by green sides).

Application of Eq. (2.72) shows that these are the incoming faces of each cell for this octant. As shown in the figure, the outgoing fluxes are upwinded to the red faces on adjacent cells. The new incoming fluxes are represented by green faces. The sweep moves to the next cell as dictated by the octant direction and performs the next solve. This process is repeated until all cells are solved for a given angle.

2.6.1 Weighted-Diamond Difference

The weighted-diamond difference method is derived by integrating Eq. (2.70) over the spatial cell defined in Fig. 2.3. Applying $\iiint(\cdot)\,dxdydz$ gives the following balance equation in a cell,

$$\frac{\mu}{\Delta_i}(\psi_{i+1/2}-\psi_{i-1/2})+\frac{\eta}{\Delta_j}(\psi_{j+1/2}-\psi_{j-1/2})+\frac{\xi}{\Delta_k}(\psi_{k+1/2}-\psi_{k-1/2})+\sigma_{ijk}\psi_{ijk}=Q_{ijk}\,, \quad (2.73)$$

where

$$\begin{aligned}
\psi_{ijk} &= \frac{1}{\Delta_i\Delta_j\Delta_k}\iiint \psi(\mathbf{r})\,dxdydz\,,\\
Q_{ijk} &= \frac{1}{\Delta_i\Delta_j\Delta_k}\iiint Q(\mathbf{r})\,dxdydz\,,\\
\psi_{i\pm1/2} &= \frac{1}{\Delta_j\Delta_k}\iint \psi(x_{i\pm1/2},y,z)\,dydz\,,\\
\psi_{j\pm1/2} &= \frac{1}{\Delta_i\Delta_k}\iint \psi(x,y_{j\pm1/2},z)\,dxdz\,,\\
\psi_{k\pm1/2} &= \frac{1}{\Delta_i\Delta_j}\iint \psi(x,y,z_{k\pm1/2})\,dxdy\,.
\end{aligned}$$

The volume of the cell is

$$V_{ijk}=\int_{x_{i-1/2}}^{x_{i+1/2}}\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{z_{k-1/2}}^{z_{k+1/2}} dxdydz=\Delta_i\Delta_j\Delta_k\,. \quad (2.74)$$

The weighted-diamond equations are obtained by applying the following closure equations to Eq. (2.73)

$$\begin{aligned}
\psi_{ijk} &= \frac{1+\alpha_i}{2}\psi_{i+1/2}+\frac{1-\alpha_i}{2}\psi_{i-1/2}\,,\\
\psi_{ijk} &= \frac{1+\alpha_j}{2}\psi_{j+1/2}+\frac{1-\alpha_j}{2}\psi_{j-1/2}\,,\\
\psi_{ijk} &= \frac{1+\alpha_k}{2}\psi_{k+1/2}+\frac{1-\alpha_k}{2}\psi_{k-1/2}\,.
\end{aligned} \quad (2.75)$$

Equations (2.73) and (2.75) constitute the weighted-diamond difference (WDD) equations.

Solving the balance equation with the WDD closures in the direction of particle travel yields

$$\underline{\mu \gtrless 0\,,\, \eta \gtrless 0\,,\, \xi \gtrless 0}$$

$$\begin{aligned}
\psi_{ijk} &= \frac{Q_{ijk} + \frac{2}{(1\pm\alpha_i)}\frac{|\mu|}{\Delta_i}\bar{\psi}_{i\mp 1/2} + \frac{2}{(1\pm\alpha_j)}\frac{|\eta|}{\Delta_j}\bar{\psi}_{j\mp 1/2} + \frac{2}{(1\pm\alpha_k)}\frac{|\xi|}{\Delta_k}\bar{\psi}_{k\mp 1/2}}{\sigma_{ijk} + \frac{2}{(1\pm\alpha_i)}\frac{|\mu|}{\Delta_i} + \frac{2}{(1\pm\alpha_j)}\frac{|\eta|}{\Delta_j} + \frac{2}{(1\pm\alpha_k)}\frac{|\xi|}{\Delta_k}}\,, \\
\psi_{i\pm 1/2} &= \frac{2}{(1\pm\alpha_i)}\psi_{ijk} - \frac{(1\mp\alpha_i)}{(1\pm\alpha_i)}\bar{\psi}_{i\mp 1/2}\,, \\
\psi_{j\pm 1/2} &= \frac{2}{(1\pm\alpha_j)}\psi_{ijk} - \frac{(1\mp\alpha_j)}{(1\pm\alpha_j)}\bar{\psi}_{j\mp 1/2}\,, \\
\psi_{k\pm 1/2} &= \frac{2}{(1\pm\alpha_k)}\psi_{ijk} - \frac{(1\mp\alpha_k)}{(1\pm\alpha_k)}\bar{\psi}_{k\mp 1/2}\,.
\end{aligned} \tag{2.76}$$

Here, the $\bar{\psi}$ represents an incoming (known) angular flux. Thus, by sweeping in the direction of particle travel, the angular flux in each cell is solved uniquely because there are 4 equations and 4 unknowns, $\{\psi_{ijk}, \psi_{i\pm 1/2}, \psi_{j\pm 1/2}, \psi_{k\pm 1/2}\}$.

2.6.2 Linear Discontinuous

The Linear Discontinous (LD) method is a Finite Element method in which the angular flux is expanded in the function space spanned by $\{1, x, y, z\}$. We begin the derivation by developing the weak-form of Eq. (2.70) by integrating over a single element, e, and multiplying by a weighting function for the element, w_{en},

$$\int_{V_e} w_{en}(\hat{\mathbf{\Omega}}\cdot\psi + \sigma\psi)\,dV = \int_{V_e} w_{en} Q\,dV\,. \tag{2.77}$$

Here, the element is defined in Figure 2.3 yielding $dV = dxdydz$, and $n = 1,\ldots,4$ because the function space has four unknowns. Furthermore, we make the assumption that the elements in the orthogonal grid all have equal weight functions, so $w_{en} \equiv w_n$. Applying Green's Theorem to the gradient term gives

$$\oint_{\partial V_e} w_n \hat{\mathbf{n}}\cdot\hat{\mathbf{\Omega}}\psi\,dA - \int_{V_e}\hat{\mathbf{\Omega}}\cdot\nabla w_n\psi\,dV + \int_{V_e} w_n\sigma\psi\,dV_e = \int_{V_e} w_n Q\,dV\,, \quad n = 1,2,3,4\,. \tag{2.78}$$

Note that the weak-form equation has reduced the derivative-order dependence on ψ by one. Now, we expand the angular flux in the following basis,

$$\psi = \sum_{m=1}^{4} b_m(\mathbf{r})\psi_{ijk}^{(m)}\,, \quad \mathbf{r}\in\partial V_e\,. \tag{2.79}$$

Applying the Galerkin Finite Element approximation in which $w_i = b_i$, the weak-form equation becomes

$$\oint_{\partial V_e} b_n \hat{\mathbf{n}} \cdot \hat{\mathbf{\Omega}} \psi \, dA - \sum_{m=1}^{4} \int_{V_e} \hat{\mathbf{\Omega}} \cdot \nabla b_n b_m \psi_{ijk}^{(m)} \, dV + \sum_{m=1}^{4} \int_{V_e} b_n \sigma b_m \psi_{ijk}^{(m)} \, dV = \sum_{m=1}^{4} \int_{V_e} b_n b_m Q_{ijk}^{(m)} \, dV \,, \quad (2.80)$$

where the source has been expanded in the same basis as the angular flux. Also, we have not expanded the flux in the surface term, which we will deal with later.

For the LD approximation the basis functions are defined

$$\begin{aligned} b_1 &= 1 \,, \\ b_2 &= \frac{2(x - x_{ijk})}{\Delta_i} \,, \\ b_3 &= \frac{2(y - y_{ijk})}{\Delta_j} \,, \\ b_4 &= \frac{2(z - z_{ijk})}{\Delta_k} \,. \end{aligned} \quad (2.81)$$

Also, we define

$$\psi_{ijk}^{(1)} = \psi^a \,, \quad \psi_{ijk}^{(2)} = \psi^x \,, \quad \psi_{ijk}^{(3)} = \psi^y \,, \quad \psi_{ijk}^{(4)} = \psi^z \,, \quad (2.82)$$

such that ψ^a is the average angular flux in the element and $\psi^{x|y|z}$ are the slopes in the (x, y, z)-directions. Using these conventions in Eq. (2.79), the angular flux in a cell is defined

$$\psi(x, y, z) = \psi^a + \frac{2(x - x_{ijk})}{\Delta_i} \psi^x + \frac{2(y - y_{ijk})}{\Delta_j} \psi^y + \frac{2(z - z_{ijk})}{\Delta_k} \psi^z \,. \quad (2.83)$$

In order to form discrete equations over all elements, the integrals in Eq. (2.80) must be calculated. The integrals for the removal and source have the following form:

$$\begin{aligned} \iiint b_1 b_1 \, dxdydz &= \Delta_i \Delta_j \Delta_k \,, & n = m = 1 \,, \\ \iiint b_n b_m \, dxdydz &= \frac{\delta_{nm}}{3} \Delta_i \Delta_j \Delta_k \,, & n, m > 1 \,. \end{aligned} \quad (2.84)$$

The second term in Eq. (2.80), fully expanded, is

$$\sum_{m=1}^{4} \psi^{(m)} \Big[\mu \iiint b_m \frac{\partial b_n}{\partial x} \, dxdydz + \eta \iiint b_m \frac{\partial b_n}{\partial y} \, dxdydz + \xi \iiint b_m \frac{\partial b_m}{\partial z} \, dxdydz \Big] \,. \quad (2.85)$$

The derivatives of the basis functions are

$$\begin{aligned}
&\frac{\partial b_1}{\partial x} = 0\,, \quad &&\frac{\partial b_2}{\partial y} = 0\,, \quad &&\frac{\partial b_3}{\partial z} = 0\,, \\
&\frac{\partial b_2}{\partial x} = \frac{2}{\Delta_i}\,, \quad &&\frac{\partial b_2}{\partial y} = 0\,, \quad &&\frac{\partial b_2}{\partial z} = 0\,, \\
&\frac{\partial b_3}{\partial x} = 0\,, \quad &&\frac{\partial b_3}{\partial y} = \frac{2}{\Delta_j}\,, \quad &&\frac{\partial b_3}{\partial z} = 0\,, \\
&\frac{\partial b_4}{\partial x} = 0\,, \quad &&\frac{\partial b_4}{\partial y} = 0\,, \quad &&\frac{\partial b_4}{\partial z} = \frac{2}{\Delta_k}\,.
\end{aligned} \tag{2.86}$$

Using these definitions, the only nonzero integrals are

$$\begin{aligned}
\iiint b_1 \frac{\partial b_2}{\partial x} &= 2\Delta_j\Delta_k\,, \\
\iiint b_1 \frac{\partial b_3}{\partial x} &= 2\Delta_i\Delta_k\,, \\
\iiint b_1 \frac{\partial b_4}{\partial x} &= 2\Delta_i\Delta_j\,.
\end{aligned} \tag{2.87}$$

Now, we can write the weak-form for each element as

$$\oint_{\partial V_e} b_n \hat{\mathbf{n}}\cdot\hat{\mathbf{\Omega}}\psi\, dA - \mathbb{T}\Psi + \sigma_e \mathbb{M}\Psi = \mathbb{M}S\,, \tag{2.88}$$

where

$$\mathbb{T} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 2\mu\Delta_j\Delta_k & 0 & 0 & 0 \\ 2\eta\Delta_i\Delta_k & 0 & 0 & 0 \\ 2\xi\Delta_i\Delta_j & 0 & 0 & 0 \end{pmatrix}\,, \quad \mathbb{M} = \Delta_i\Delta_j\Delta_k \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix}\,, \tag{2.89}$$

and

$$\begin{aligned}
\Psi &= \begin{pmatrix} \psi^a & \psi^x & \psi^y & \psi^z \end{pmatrix}^T\,, \\
S &= \begin{pmatrix} Q^a & Q^x & Q^y & Q^z \end{pmatrix}^T\,.
\end{aligned} \tag{2.90}$$

To complete the system of discrete equations required by the LD method, the surface term in Eq. (2.88) must be evaluated. Each element in the Denovo mesh has 6 faces, ie. $l = 1, \ldots, 6$. First, the surface integral is written as a sum over all faces of the element,

$$\hat{\mathbf{\Omega}}\cdot\sum_{l=1}^{6}\mathbf{n}_l \int_{\partial V_{el}} b_n\psi(\mathbf{r}_l)\, dA\,, \quad \mathbf{r}_l \in \partial V_{el}\,. \tag{2.91}$$

The flux can be expanded on each face using

$$\begin{aligned}
\psi(x_{i\pm 1/2}) &= \psi_{i\pm 1/2} + \frac{2(y-y_{ijk})}{\Delta_j}\psi^y_{i\pm 1/2} + \frac{2(z-z_{ijk})}{\Delta_k}\psi^z_{k\pm 1/2}\,, \\
\psi(y_{j\pm 1/2}) &= \psi_{j\pm 1/2} + \frac{2(x-x_{ijk})}{\Delta_i}\psi^x_{j\pm 1/2} + \frac{2(z-z_{ijk})}{\Delta_k}\psi^z_{j\pm 1/2}\,, \\
\psi(z_{k\pm 1/2}) &= \psi_{k\pm 1/2} + \frac{2(x-x_{ijk})}{\Delta_i}\psi^x_{k\pm 1/2} + \frac{2(y-y_{ijk})}{\Delta_j}\psi^y_{k\pm 1/2}\,.
\end{aligned} \tag{2.92}$$

Chapter 3

Solution Methods

In Chapter 2 the discrete ordinates equations were defined. Here, solution methods that are applied in Denovo will be explained. The general strategy that is pursued is a series of iterations over the independent variables. The outermost iteration is over energy. Angle and space constitute the inner iterations.

3.1 Multigroup Iterations

In Eq. (2.63) the full multigroup discrete ordinates equations are presented in matrix form. This presentation assumes a full scattering matrix that includes downscattering, within-group scattering, and upscattering. For many problems, upscattering either does not exist or is not important, and $\mathbf{S}$ assumes a lower-triangular form,

$$\mathbf{S} = \begin{pmatrix} [\mathbf{S}]_{00} & 0 & 0 & 0 & 0 \\ [\mathbf{S}]_{10} & [\mathbf{S}]_{11} & 0 & 0 & 0 \\ [\mathbf{S}]_{20} & [\mathbf{S}]_{21} & [\mathbf{S}]_{22} & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ [\mathbf{S}]_{G0} & [\mathbf{S}]_{G1} & [\mathbf{S}]_{G2} & \cdots & [\mathbf{S}]_{GG} \end{pmatrix} . \tag{3.1}$$

The transport series in Eq. (2.69) can now be written,

$$\begin{aligned} \mathbf{L}[\psi]_0 &= [\mathbf{M}][\mathbf{S}]_{00}[\phi]_0 + [\mathbf{M}][q_e]_0 \,, \\ \mathbf{L}[\psi]_1 &= [\mathbf{M}]\big([\mathbf{S}]_{10}[\phi]_0 + [\mathbf{S}]_{11}[\phi]_1\big) + [\mathbf{M}][q_e]_1 \,, \\ &\vdots \\ \mathbf{L}[\psi]_g &= [\mathbf{M}]\big([\mathbf{S}]_{g0}[\phi]_0 + [\mathbf{S}]_{g1}[\phi]_1 + \ldots + [\mathbf{S}]_{gg}[\phi]_g\big) + [\mathbf{M}][q_e]_g \,, \\ &\vdots \\ \mathbf{L}[\psi]_G &= [\mathbf{M}]\big([\mathbf{S}]_{G0}[\phi]_0 + [\mathbf{S}]_{G1}[\phi]_1 + \ldots + [\mathbf{S}]_{GG}[\phi]_G\big) + [\mathbf{M}][q_e]_G \,. \end{aligned} \tag{3.2}$$

This series can be solved without iteration using forward-substitution:

$$\begin{aligned}\mathbf{L}[\psi]_g &= [\mathbf{M}][\mathbf{S}]_{gg}[\phi]_g + [\mathbf{M}]\Big(\sum_{g'=0}^{g-1}[\mathbf{S}]_{gg'}[\phi]_{g'} + [q_e]_g\Big) \\ &= [\mathbf{M}][\mathbf{S}]_{gg}[\phi]_g + \bar{Q}_g \,.\end{aligned} \tag{3.3}$$

What remains to be determined is the method by which the $[\psi]$ and $[\phi]$ are related. The solution of $[\phi]_g$ is determined in the inner-iterations that we shall discuss next.

3.2 Solution of Flux Moments

Equation (3.3) is equivalent to a one-group transport problem with the following form,

$$\mathbf{L}\psi = \mathbf{MS}\phi + \bar{Q} \,, \tag{3.4}$$

where the group indices have been suppressed, and

$$\psi \equiv [\psi]_g \,, \quad \mathbf{M} \equiv [\mathbf{M}] \,, \quad \mathbf{S} \equiv [\mathbf{S}]_{gg} \,, \quad \phi \equiv [\phi]_g \,, \quad \bar{Q} \equiv \bar{Q}_g \,.$$

The discrete angular fluxes are related to the flux moments through the operator $\mathbf{D}$,

$$\phi = \mathbf{D}\psi \,. \tag{3.5}$$

Clearly, the discrete form of $\mathbf{D}$ is defined by the quadrature integration rules in Eqs. (2.51) and (2.52),

$$\begin{aligned}\mathbf{D} &= \mathbf{M}^T\mathbf{W} \\ &= \sum_{a=1}^{n} Y_{lm}^{(e/o)} w_a \,,\end{aligned} \tag{3.6}$$

where $\mathbf{W}$ is an $(a \times a)$ diagonal matrix of the quadrature weights. Using the definition of $\mathbf{M}$ from Eq. (2.62), the size of $\mathbf{D}$ can be determined from

$$\mathbf{D} \equiv (f \times a)(a \times a) = (f \times a) \,. \tag{3.7}$$

Also, even though $\mathbf{M}$ maps angular flux moments onto discrete angular fluxes, in general $\psi \neq \mathbf{M}\phi$.

Having defined a relationship between ϕ and ψ, schemes for solving Eq. (3.4) can be postulated. The classic method is so-called *source-iteration*,

$$\mathbf{L}\psi^{k+1} = \mathbf{MS}\phi^k + \bar{Q} \,, \tag{3.8}$$

$$\phi^{k+1} = \mathbf{D}\psi^{k+1} \,. \tag{3.9}$$

Source-iteration is simply a form of fixed-point, or Richardson, iteration,

$$\mathbf{A}x = b \Rightarrow x^{k+1} = (\mathbf{I} - \mathbf{A})x^k + b \,, \tag{3.10}$$

which will converge as long as the spectral radius, $\rho((\mathbf{I} - \mathbf{A})$, is less than 1.

The spectral radius of Eq. (3.9) is

$$\rho = c = \frac{\sigma_\mathrm{s}}{\sigma} \,. \tag{3.11}$$

Thus, as the problem becomes more scattering-dominated, source-iteration will be increasingly inefficient. There are many schemes that accelerate the convergence of source-iteration including Diffusion Synthetic Acceleration (DSA), Transport Synthetic Acceleration (TSA), partial-current rebalance, and others. Unfortunately, most of these schemes can suffer from severe stability problems in multi-D, particularly in physical domains with large material discontinuities. Therefore, instead of source-iteration, we will apply more advanced iteration schemes that do not have stability problems.

First, let us pose Eq. (3.4) in a more conventional form that mimics a standard linear system, $\mathbf{A}x = b$. Operating by $\mathbf{L}^{-1}$ and $\mathbf{D}$ and moving ϕ-terms to the left-hand side gives

$$(\mathbf{I} - \mathbf{D}\mathbf{L}^{-1}\mathbf{M}\mathbf{S})\phi = \mathbf{D}\mathbf{L}^{-1}\bar{Q} \,. \tag{3.12}$$

Defining

$$\tilde{\mathbf{A}} = (\mathbf{I} - \mathbf{D}\mathbf{L}^{-1}\mathbf{M}\mathbf{S}) \,, \quad \tilde{b} = \mathbf{D}\mathbf{L}^{-1}\bar{Q} \,,$$

gives the desired form,

$$\tilde{A}\phi = \tilde{b} \,.$$

Writing the transport equation in the form of Eq. (3.12) allows the application of non-stationary linear solvers. In particular, Krylov iteration schemes are particular ammenable because Krylov methods only require the action of the operator on an iteration vector, $\tilde{A}v$. Thus, applying a Krylov method to Eq. (3.12) requires the following steps:

$$\begin{aligned} \text{matrix-vector multiply}: &\quad y = \mathbf{M}\mathbf{S}v \,, \\ \text{sweep}: &\quad z = \mathbf{D}\mathbf{L}^{-1}y \,, \\ \text{return}: &\quad \Leftarrow v - z \,, \end{aligned}$$

where v is the iteration vector generated by the Krylov method. Before the Krylov method can be used, a single sweep through the mesh is required to calculate the source,

$$\tilde{b} = \mathbf{D}\mathbf{L}^{-1}\bar{Q} \,.$$

In the above steps, the operation $\mathbf{L}^{-1}$ represents a sweep through the mesh in the direction of particle travel. This operation is performed for each angle in the S_N quadrature set. Therefore, every Krylov iteration requires n sweeps of the mesh, and the solution of the transport equation is defined by the efficiency of the sweep algorithm. The details of the sweep algorithm are discussed in the following section.

Chapter 4

The Adjoint Transport Solution

The solution to the adjoint form of the transport equation is useful in hybrid Monte Carlo/-deterministic transport methods and sensitivity analysis. The adjoint form of Eq. (2.1) is

$$\begin{aligned} -\hat{\mathbf{\Omega}}\cdot\nabla\psi^{\dagger}(\mathbf{r},\mathbf{\Omega},E)+\sigma(\mathbf{r},E)\psi^{\dagger}(\mathbf{r},\mathbf{\Omega},E) \\ =\int_0^{\infty}\int_{4\pi}\sigma_{\mathrm{s}}(\mathbf{r},\hat{\mathbf{\Omega}}\cdot\hat{\mathbf{\Omega}}',E\rightarrow E')\psi^{\dagger}(\mathbf{r},\mathbf{\Omega}',E')\,d\mathbf{\Omega}'dE'+q^{\dagger}(\mathbf{r},\mathbf{\Omega},E)\,. \end{aligned} \tag{4.1}$$

The adjoint equation obeys the boundary condition

$$\psi^{\dagger}(\mathbf{r},\mathbf{\Omega},E)=0\,,\quad \mathbf{r}\in\partial\Gamma\,,\quad \hat{\mathbf{\Omega}}\cdot\hat{n}>0\,, \tag{4.2}$$

which defines the *outgoing* flux on all problem boundaries. The adjoint source is defined

$$q^{\dagger}(\mathbf{r},\mathbf{\Omega},E)=\frac{1}{4\pi}\Sigma(\mathbf{r},E)\delta(\mathbf{r}-\mathbf{r}')\delta(E-E')\,, \tag{4.3}$$

where Σ is a normalized response function in a detector region defined in the phase-space of $\mathbf{r}'$ and E'.

4.1 Discrete Adjoint Equation

Following the same multigroup discretizations applied in § 2.1, the multigroup, adjoint S_N equations are defined

$$-\hat{\mathbf{\Omega}}\cdot\nabla\psi^{\dagger\,g}(\mathbf{r},\mathbf{\Omega})+\sigma^{g}(\mathbf{r})\psi^{\dagger\,g}(\mathbf{r},\mathbf{\Omega})=Q^{\dagger\,g}(\mathbf{r},\mathbf{\Omega})\,. \tag{4.4}$$

The adjoint source is defined

$$\begin{aligned} Q^{\dagger\,g}(\mathbf{r},\mathbf{\Omega}) &= q_s^{\dagger\,g}(\mathbf{r},\mathbf{\Omega})+\frac{1}{4\pi}\Sigma^{g}(\mathbf{r}) \\ &=\sum_{g'=0}^{G}\int_{4\pi}\sigma_{\mathrm{s}}^{g\rightarrow g'}(\mathbf{r},\hat{\mathbf{\Omega}}'\cdot\hat{\mathbf{\Omega}})\psi^{\dagger\,g'}(\mathbf{r},\mathbf{\Omega}')\,d\mathbf{\Omega}'+\frac{1}{4\pi}\Sigma^{g}(\mathbf{r})\,. \end{aligned} \tag{4.5}$$

The boundary conditions are

$$\psi^{\dagger\, g}(\mathbf{r}, \mathbf{\Omega}) = 0\,, \quad \mathbf{r} \in \partial\Gamma\,, \quad \hat{\mathbf{\Omega}} \cdot \hat{\mathbf{n}} > 0\,. \tag{4.6}$$

Applying the standard angular expansions of the scattering and the discrete ordinates approximation as described in §§ 2.2 and 2.4 gives

$$\begin{aligned} -\,\hat{\mathbf{\Omega}}_a \cdot \nabla \psi_a^{\dagger\, g}(\mathbf{r}) + \sigma^g(\mathbf{r})\psi_a^{\dagger\, g}(\mathbf{r}) = \sum_{g'=0}^{G}\sum_{l=0}^{N} \sigma_{\mathrm{s}\,l}^{g'g}(\mathbf{r}) \Big[Y_{l0}^e(\mathbf{\Omega}_a)\phi_{l0}^{\dagger\, g'}(\mathbf{r}) + \\ \sum_{m=1}^{l} \big(Y_{lm}^e(\mathbf{\Omega}_a)\phi_{lm}^{\dagger\, g'}(\mathbf{r}) + Y_{lm}^o(\mathbf{\Omega}_a)\vartheta_{lm}^{\dagger\, g'}(\mathbf{r}) \big) \Big] + \frac{1}{4\pi}\Sigma^g(\mathbf{r})\,. \end{aligned} \tag{4.7}$$

This equation is the adjoint version of Eq. (2.56) defined in § 2.5.

4.2 Operator From of the Adjoint Equation

In operator notation Eq. (4.7) is written,

$$\mathbf{L}^\dagger \psi^\dagger = \mathbf{M}\mathbf{S}^\dagger \phi^\dagger + q^\dagger\,. \tag{4.8}$$

The adjoint scattering operator is simply the transpose of the forward operator defined in Eq. (2.63),

$$\mathbf{S}^\dagger = \mathbf{S}^T\,. \tag{4.9}$$

Then, we have (for no upscattering)

$$\mathbf{L}^\dagger \begin{pmatrix} [\psi^\dagger]_0 \\ [\psi^\dagger]_1 \\ [\psi^\dagger]_2 \\ \vdots \\ [\psi^\dagger]_G \end{pmatrix} = [\mathbf{M}] \begin{pmatrix} [\mathbf{S}]_{00} & [\mathbf{S}]_{10} & [\mathbf{S}]_{20} & \cdots & [\mathbf{S}]_{G0} \\ 0 & [\mathbf{S}]_{11} & [\mathbf{S}]_{21} & \cdots & [\mathbf{S}]_{G1} \\ 0 & 0 & [\mathbf{S}]_{22} & \cdots & [\mathbf{S}]_{G2} \\ 0 & 0 & 0 & \ddots & \vdots \\ 0 & 0 & 0 & 0 & [\mathbf{S}]_{GG} \end{pmatrix} \begin{pmatrix} [\phi^\dagger]_0 \\ [\phi^\dagger]_1 \\ [\phi^\dagger]_2 \\ \vdots \\ [\phi^\dagger]_G \end{pmatrix} + \begin{pmatrix} [q^\dagger]_0 \\ [q^\dagger]_1 \\ [q^\dagger]_2 \\ \vdots \\ [q^\dagger]_G \end{pmatrix}\,. \tag{4.10}$$

The resulting series of equations can be solved over energy groups using back-substitution:

$$\begin{aligned} \mathbf{L}^\dagger [\psi^\dagger]_g &= [\mathbf{M}][\mathbf{S}]_{gg}[\phi^\dagger]_g + [\mathbf{M}]\Big(\sum_{g'=g+1}^{G} [\mathbf{S}]_{g'g}[\phi^\dagger]_{g'} \Big) + [q^\dagger]_g \\ &= [\mathbf{M}][\mathbf{S}]_{gg}[\phi^\dagger]_g + \bar{Q}_g^\dagger\,, \quad g = G, G-1, G-2, \ldots, 0\,. \end{aligned} \tag{4.11}$$

Spherical Harmonics Expansions

Any function of $\mathbf{\Omega}$ can be expanded in Spherical Harmonics using

$$f(\mathbf{\Omega}) = \sum_{l=0}^{N} \sum_{m=-l}^{l} Y_{lm}(\mathbf{\Omega}) f_{lm} \, . \tag{12}$$

The $Y_l m$ are the Spherical Harmonics, and they constitute a complete, orthonormal set. They are defined

$$Y_{lm}(\theta, \varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \, P_{lm}(\cos\theta) \mathrm{e}^{im\varphi} \, , \tag{13}$$

where the P_{lm} are the associated Legendre Polynomials. We note that some treatments prefer to include the Condon-Shortley phase factor, $(-1)^m$, in the definition of P_{lm}, whereas here it is applied to the definition of Y_{lm}. The orthogonality of Spherical Harmonics is

$$\int_{4\pi} Y^*_{l'm'} Y_{lm} \, d\mathbf{\Omega} = \delta_{ll'} \delta_{mm'} \, . \tag{14}$$

Using this property the moments of f are calculated

$$f_{lm} = \int_{4\pi} Y^*_{lm}(\mathbf{\Omega}) f(\mathbf{\Omega}) \, d\mathbf{\Omega} \, . \tag{15}$$

If $f \in \mathscr{R}$ then the expansion given in Eq. (12) will be inappropriate because it is complex. We seek a real expansion of f. First, we rewrite Eq.(12) by explicitly breaking it into $\pm$ components of m,

$$f = \sum_{l=0}^{N} \sum_{m=0}^{l} \left[C_{lm} P_{lm} f_{lm} \mathrm{e}^{im\varphi} + C_{l-m} P_{l-m} \mathrm{e}^{-im\varphi} \right] \, , \tag{16}$$

where

$$C_{lm} = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \tag{17}$$

Noting that the imaginary terms vanish when $m = 0$, we define the complex form of f_{lm} as follows,

$$f_{lm} = \begin{cases} \alpha_{lm} & m = 0\,, \\ \alpha_{lm} + i\beta_{lm} & m > 0\,. \end{cases} \tag{18}$$

Expanding $\exp(im\varphi) = \cos m\varphi + i \sin m\varphi$, we write

$$\begin{aligned} f = \sum_{l=0}^{N} \sum_{m=0}^{l} \big[& C_{lm} P_{lm} (\alpha_{lm} + i\beta_{lm})(\cos m\varphi + i \sin m\varphi) \\ & + C_{l-m} P_{l-m} (\alpha_{l-m} + i\beta_{l-m})(\cos m\varphi - i \sin m\varphi) \big]\,. \end{aligned} \tag{19}$$

Grouping terms into real and imaginary parts gives

$$\begin{aligned} f = \sum_{l=0}^{N} \sum_{m=0}^{l} \Big[& (C_{lm} P_{lm} \alpha_{lm} + C_{l-m} P_{l-m} \alpha_{l-m}) \cos m\varphi \\ & + (C_{l-m} P_{l-m} \beta_{l-m} - C_{lm} P_{lm} \beta_{lm}) \sin m\varphi \\ & + i \big[(C_{lm} P_{lm} \beta_{lm} + C_{l-m} P_{l-m} \beta_{l-m}) \cos m\varphi \\ & + (C_{lm} P_{lm} \alpha_{lm} - C_{l-m} P_{l-m} \alpha_{l-m}) \sin m\varphi \big] \Big]\,. \end{aligned} \tag{20}$$

Because $f \in \mathscr{R}$, the imaginary parts must vanish, which gives the following condition:

$$C_{l-m} P_{l-m} \beta_{l-m} = -C_{lm} P_{lm} \beta_{lm}\,, \tag{21}$$

$$C_{l-m} P_{l-m} \alpha_{l-m} = C_{lm} P_{lm} \alpha_{lm}\,. \tag{22}$$

Substituting these expressions into Eq. (20), yields

$$f(\mathbf{\Omega}) = \sum_{l=0}^{N} \sum_{m=0}^{l} C_{lm} P_{lm} (2\alpha_{lm} \cos m\varphi - 2\beta_{lm} \sin m\varphi)\,. \tag{23}$$

The new basis for the real expansion of f consists of the following functions

$$\hat{Y}^{e}_{lm} = C_{lm} P_{lm} \cos m\varphi\,, \tag{24}$$

$$\hat{Y}^{o}_{lm} = C_{lm} P_{lm} \sin m\varphi\,, \tag{25}$$

and

$$\begin{aligned} Y_{lm} &= C_{lm} P_{lm} \cos m\varphi + i C_{lm} P_{lm} \sin m\varphi \\ &= \hat{Y}^{e}_{lm} + i \hat{Y}^{o}_{lm}\,. \end{aligned} \tag{26}$$

This basis needs to constitute an orthonormal set, applying orthogonality to the even harmonic gives

$$\begin{aligned} \int_{4\pi} \hat{Y}^{e}_{lm} \hat{Y}^{e}_{l'm'}\, d\mathbf{\Omega} &= C^2_{lm} \frac{2\pi}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'} (1 + \delta_{m0}) \delta_{mm'} \\ &= \frac{(1 + \delta_{m0})}{2} \delta_{mm'} \delta_{ll'}\,, \end{aligned} \tag{27}$$

where we have used orthogonality relations for cos and P_{lm} listed in § 4.2. In order for $\hat{Y}^e_{lm}$ to be orthonormal, we must have

$$\mathcal{C}^2 \frac{(1+\delta_{m0})}{2} \delta_{mm'} \delta_{ll'} = 1 \,, \tag{28}$$

which yields the following conditions on $\mathcal{C}$,

$$\mathcal{C} = \begin{cases} 1 & m = 0 \,, \\ \sqrt{2} & m > 0 \,. \end{cases} \tag{29}$$

Defining $\mathcal{C} = \sqrt{2 - \delta_{m0}}$ satisfies both constraints. The odd harmonics are developed similarly with the exception that they vanish when $m = 0$, ie.

$$\int_{4\pi} \hat{Y}^o_{lm} \hat{Y}^o_{l'm'} \, d\mathbf{\Omega} = \frac{(1-\delta_{m0})}{2} \delta_{ll'} \delta_{mm'} \,. \tag{30}$$

Applying $\mathcal{C}$ to $\hat{Y}^e$ and $\hat{Y}^o$, the real basis for f is

$$Y^e_{lm} = D_{lm} P_{lm} \cos m\varphi \,, \tag{31}$$

$$Y^o_{lm} = D_{lm} P_{lm} \sin m\varphi \,, \tag{32}$$

where

$$D_{lm} = (-1)^m \sqrt{(2-\delta_{m0}) \frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \,. \tag{33}$$

The orthogonality conditions of Y^e and Y^o are now correctly defined

$$\int_{4\pi} Y^e_{lm} Y^e_{l'm'} \, d\mathbf{\Omega} = \frac{(2-\delta_{m0})(1+\delta_{m0})}{2} \delta_{mm'} \delta_{ll'} = \delta_{mm'} \delta_{ll'} \,, \tag{34}$$

$$\int_{4\pi} Y^o_{lm} Y^o_{l'm'} \, d\mathbf{\Omega} = \frac{(2-\delta_{m0})(1-\delta_{m0})}{2} \delta_{mm'} \delta_{ll'} = (1-\delta_{m0}) \delta_{mm'} \delta_{ll'} \,. \tag{35}$$

Defining

$$a_{lm} = \sqrt{2 - \delta_{m0}} \, \alpha_{lm} \,, \tag{36}$$

$$b_{lm} = \sqrt{2} (\delta_{m0} - 1) \beta_{lm} \,, \tag{37}$$

and applying the set in Eqs. (31) and (32) to Eq. (23) yields

$$\boxed{f(\mathbf{\Omega}) = \sum_{l=0}^{N} \Big[Y^e_{l0} a_{l0} + \sum_{m=1}^{l} (Y^e_{lm} a_{lm} + Y^o_{lm} b_{lm}) \Big] \,.} \tag{38}$$

Applying the orthogonality conditions, Eqs. (34) and (35), to Eq. (38) defines the moments, a_{lm} and b_{lm},

$$a_{lm} = \int_{4\pi} Y^e_{lm}(\mathbf{\Omega}) f(\mathbf{\Omega})\, d\mathbf{\Omega}\,, \quad m \geq 0\,, \tag{39}$$

$$b_{lm} = \int_{4\pi} Y^o_{lm}(\mathbf{\Omega}) f(\mathbf{\Omega})\, d\mathbf{\Omega}\,, \quad m > 0\,. \tag{40}$$

Equation (38) defines the Spherical Harmonics expansion of a real-valued function $f(\mathbf{\Omega})$. The orthonormal Spherical Harmonics used in Eq. (38) are defined in Eqs. (31) and (32). The moments of f are defined in Eqs. (39) and (40).

Mathematical Properties and Identities

Useful orthogonality properties that are used in the text are:

$$\int_0^{2\pi} \cos m'x \cos mx \, dx = \pi(1+\delta_{m0})\delta_{mm'} \,, \qquad \text{cosine} \tag{41}$$

$$\int_0^{2\pi} \sin m'x \sin mx \, dx = \pi(1-\delta_{m0})\delta_{mm'} \,, \qquad \text{sine} \tag{42}$$

$$\int_{-1}^{1} P_n(x)P_m(x) \, dx = \frac{2}{2n+1}\delta_{nm} \,, \qquad \text{Legendre polynomials} \tag{43}$$

$$\int_{-1}^{1} P_{lm}(x)P_{l'm}(x) \, dx = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'} \,. \qquad \text{associated Legendre polynomials} \tag{44}$$

The relationship between m and $-m$ associated Legendre polynomials is

$$P_{l-m} = (-1)^m \frac{(l-m)!}{(l+m)!} P_{lm} \,. \tag{45}$$

In Eqs. (24) and (25) the complex components of the Spherical Harmonics are given that satisfy

$$Y_{lm} = \hat{Y}^e_{lm} + i\hat{Y}^o_{lm} \,. \tag{46}$$

Using Eq. (45) the relationship between the positive and negative m-components of Y_{lm} can be found:

$$\begin{aligned} \hat{Y}^e_{l-m} &= (-1)^m C_{l-m} \frac{(l-m)!}{(l+m)!} P_{lm} \cos m\varphi \\ &= \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}}\,\frac{(l-m)!}{(l+m)!} P_{lm} \cos m\varphi \\ &= (-1)^{-m}\hat{Y}^e_{lm} \equiv (-1)^m \hat{Y}^e_{lm} \,. \end{aligned} \tag{47}$$

Similarly,

$$\hat{Y}^o_{l-m} = -(-1)^m \hat{Y}^o_{lm} \,. \tag{48}$$