Lecture 22
More on Anisotropic Scattering

1 Introduction

The standard $\mathrm{S_N}$ treatment for the scattering source, which is based on a Legendre polynomial expansion for the scattering cross section in conjunction with quadrature-generated spherical-harmonic moments of the angular flux, is still the workhorse for modern discrete-ordinates calculations, even though it is not always satisfactory. There are several reasons why it remains in widespread use: (i) fundamentally different approaches usually require significant processing of raw cross section data; (ii) such techniques often have memory requirements that are significantly larger than those of the standard treatment; and (iii) the standard technique is often much more accurate than one would expect, even when highly-truncated cross-section expansions are used in a calculation. Next, we describe the standard method, together with an improvement that has had a notable impact on charged-particle calculations.

We previously used the spherical-harmonics addition theorem to show that the scattering source corresponding to an angular flux that is representable as a linear combination of spherical harmonics of degree L is itself a representable as a linear combination of spherical harmonics of degree no higher than L. This result follows from the fact that the spherical-harmonic functions (which include the Legendre polynomials) are eigenfunctions of the Boltzmann scattering operator. Furthermore, the only cross section information appearing in the scattering source is the first $L + 1$ moments of the scattering cross section. *This same result is obtained if a cross section expansion of degree L is used, rather than an exact expansion of infinite degree.* In this case, the convergence of the cross-section expansion is irrelevant. This powerful result is not widely appreciated.

We now discuss how this property impacts S_N calculations. For simplicity, we consider the 1-D slab-geometry scattering source. Assuming that an N-point angular quadrature set is used in conjunction with a cross-section expansion of degree $N - 1$, the S_N scattering source takes the form:

$$(S\psi)_n(x) = \sum_{m=0}^{N-1} \frac{2m+1}{4\pi} P_m(\mu_n)\sigma_m\phi_m(x) \quad , \tag{1}$$

where

$$\phi_m(x) = \sum_{n=1}^{N} P_m(\mu_n)\psi_n(x)w_n \quad . \tag{2}$$

We assume Gauss quadrature. With N quadrature points, one can uniquely interpolate those points with a polynomial of degree $N - 1$. Furthermore, since an N-point Gauss set exactly integrates polynomials of degree $2N - 1$, the Legendre moments in Eq. (2) are exactly the moments of the interpolatory polynomial. Considering our previous results regarding the scattering source for a polynomial angular flux representation, we see that the discrete scattering source values given in Eq. (1) are exactly those of the scattering source generated with the polynomial interpolation for the angular flux. Thus, if the true angular flux is well-represented by the polynomial interpolation of the discrete angular flux values, the true scattering source will similarly be well-represented by the polynomial interpolation of the discrete scattering source values.

We again stress that this is true regardless of the convergence of the cross-section expansion. This property does not guarantee positive discrete scattering source values, given positive discrete angular flux values, because the polynomial interpolation of the discrete angular fluxes can be negative at some points, even though the discrete values themselves are positive. However, since polynomial interpolation at the Gauss points is known to be stable, any negativities in the angular flux interpolation will be small relative to the maximum discrete angular flux value. Therefore, any negativities in the discrete scattering source values will also be small relative to the maximum discrete scattering source value. Hence, accurate S_N solutions for angle-integrated quantities can be obtained in a wide variety of problems in 1-D slab geometry with highly-anisotropic scattering using Gauss quadrature, even if the scattering cross section expansion is highly truncated.

If a Gauss quadrature set is not used, some of the scattering source moments of the interpolatory polynomial will be properly computed, but others will not, depending upon the accuracy of the quadrature set. It can be seen from Eq. (1) that the m'th moment of the scattering source is just the product of the m'th moment of the scattering cross section and the m'th moment of the angular flux. Thus, any flux moment that is erroneous yields a corresponding scattering source moment that is erroneous. This deficiency can be treated by generating a separate set of quadrature weights for each moment. In particular, for each $0 \leq m \leq N-1$, one can generate N weights, $\{w_{m,n}\}_{n=1}^{N}$ that are defined by the N linear equations:

$$\sum_{n=1}^{N} P_m(\mu_n) P_j(\mu_n) w_{m,n} = \frac{4\pi}{2m+1}\delta_{mj} \quad , \quad 1 \leq j \leq N \quad . \tag{3}$$

Then Eq. (2) is replaced by

$$\phi_m(x) = \sum_{n=1}^{N} P_m(\mu)\psi_n(x) w_{m,n} \quad . \tag{4}$$

This method gives the desirable properties of Gauss quadrature to non-Gauss quadrature for the purpose of calculating the scattering source. (However, there is no guarantee that the weights generated in this way will be positive.)

This is one variant of a more general technique known as *Galerkin quadrature.* To present the more general method, we re-express the standard S_N technique for calculating the scattering source in terms of matrix algebra. In particular, we write Eqs. (1) and (2) as:

$$\overrightarrow{S} = \mathbf{M\Sigma D}\overrightarrow{\psi} \quad , \tag{5}$$

where $\overrightarrow{\psi}$ is the vector of discrete angular flux values:

$$(\psi_1, \psi_2, \ldots, \psi_N)^T \quad , \tag{6}$$

D is the $N \times N$ matrix:

$$D_{m,n} = P_m(\mu_n) w_n \quad , \tag{7}$$

Σ is the $N \times N$ diagonal matrix:

$$\mathbf{\Sigma} = diag\,(\sigma_0, \sigma_1, \sigma_2, \ldots) \quad , \tag{8}$$

and **M** is the $N \times N$ matrix:

$$M_{n,m} = \frac{2m+1}{4\pi} P_m(\mu_n) \quad . \tag{9}$$

The *discrete-to-moment* matrix **D** maps a vector of discrete angular flux values to a corresponding vector of Legendre flux moments. We note from Eq. (7) that the first row of this matrix consists of the standard quadrature weights, because $P_0(\mu) = 1$. The matrix **Σ** is the *scattering matrix* in the Legendre basis, or equivalently, the scattering matrix for the $\mathrm{P_{N-1}}$ approximation. It maps a vector of Legendre flux moments to a corresponding vector of Legendre scattering source moments. The *moment-to-discrete* matrix **M** maps a vector of Legendre scattering source moments to a corresponding vector of discrete scattering source values. Using the orthogonal property of the Legendre polynomials, one can show that with Gauss quadrature, $\mathbf{M} = \mathbf{D}^{-1}$:

$$\mathbf{DM} = \sum_{k=1}^{N} D_{i,k} M_{k,j} = \sum_{k=1}^{N} P_i(\mu_k) \frac{2j+1}{4\pi} P_j(\mu_k) w_k = \delta_{i,j} \quad . \tag{10}$$

Thus, using Eq. (10), we can re-express Eq. (5) as:

$$\overrightarrow{S} = \mathbf{D}^{-1} \mathbf{\Sigma} \mathbf{D} \overrightarrow{\psi} \quad . \tag{11}$$

Eq. (11) shows that the S_N scattering matrix represents a similarity transformation of the Legendre scattering matrix, $\mathbf{\Sigma}$. This means that the standard S_N scattering source with Gauss quadrature (and a Legendre cross-section expansion of degree $N-1$) is equivalent to the scattering source of the P_{N-1} approximation. This is to be expected, considering the well-known equivalence between the S_N and P_N approximations in 1-D slab geometry. If Gauss quadrature is not used, then $\mathbf{M} \neq \mathbf{D}^{-1}$, a result which is undesirable. The matrix $\mathbf{D}$ maps a vector of N discrete function values to N Legendre moments, and the matrix $\mathbf{M}$ maps a vector of N Legendre moments to N discrete function values. One can uniquely define a polynomial of degree $N-1$ either in terms of N Legendre moments or in terms of N discrete function values at N distinct points. Therefore, $\mathbf{D}$ and $\mathbf{M}$ should be inverses of one another. The moment-dependent weights defined in Eq. (3) ensure that this will be the case. We note that it is not necessary to actually generate the moment-dependent weights; one can directly obtain the correct matrix $\mathbf{D}$ simply by calculating the inverse of $\mathbf{M}$.

This Galerkin quadrature method is useful for 1-D calculations when quadrature with special directions are desired. For example, Lobatto and double Radau quadrature sets, which have quadrature points at $\mu = \pm 1$, are particularly useful for simulating a normally incident plane-wave of radiation.

In 2-D and 3-D, the Galerkin quadrature method is based upon spherical-harmonic interpolation of the discrete angular fluxes rather than polynomial interpolation. Choosing the correct spherical harmonics for interpolation is more complicated in multidimensions because the number of spherical-harmonic functions of order $N-1$ does not equal the number of discrete directions in a multidimensional $\mathrm{S_N}$ quadrature set. Nonetheless, suitable interpolation functions can be defined for triangular quadrature sets. They can also been defined for product quadrature sets, but this has not yet been published. The Galerkin quadrature method in 2-D and 3-D can be much more accurate than the standard quadrature method with highly anisotropic scattering because there is no analog of Gauss quadrature in 2-D and 3-D, i.e., there is no 2-D or 3-D quadrature set that will exactly calculate all of the spherical-harmonic moments of the interpolated angular flux. In fact, fewer than half of the moments are exactly calculated with typical sets, e.g., even-moment symmetric sets, etc.

The Galerkin quadrature method can also accommodate non-polynomial or non-spherical-harmonic interpolation functions. To demonstrate this in 1-D, we consider a general interpolatory basis set for a given set of N discrete directions:

$$\psi(x,\mu) = \sum_{n=1}^{N} \psi_n(x) B_n(\mu) \quad , \tag{12}$$

where

$$B_i(\mu_j) = \delta_{ij} \quad . \tag{13}$$

Multiplying Eq. (12) by $P_m(\mu)$ and integrating over all directions, we obtain

$$\phi_m(x) = \sum_{n=1}^{N} \psi_n(x) \left[2\pi \int_{-1}^{+1} P_m(\mu) B_n(\mu)\, d\mu \right] \quad . \tag{14}$$

It follows from the definition of the discrete-to-moment matrix $\mathbf{M}$ and Eq. (13) that the components of $\mathbf{D}$ are:

$$D_{m,n} = 2\pi \int_{-1}^{+1} P_m(\mu) B_n(\mu)\, d\mu \quad . \tag{15}$$

Eq. (15) is valid for all types of interpolation functions, including polynomials. We note that the first row of the discrete-to-moment matrix consists of standard quadrature weights that are exact for integrating the interpolated angular flux:

$$\phi(x) = 2\pi \int_{-1}^{+1} \psi(x,\mu)\, d\mu = \sum_{n=1}^{N} \psi_n w_n \quad , \tag{16}$$

where

$$w_n = 2\pi \int_{-1}^{+1} B_n(\mu)\, d\mu \quad . \tag{17}$$

These are called the *companion quadrature weights*. Non-polynomial interpolation requires much more computational effort to generate the discrete-to-moment matrix, because the interpolatory basis functions must be explicitly formed and their products with the Legendre polynomials must be integrated. Also, one must invert the discrete-to-moment matrix to obtain the moment-to-discrete matrix, because the standard S_N expression for the moment-to-discrete matrix, Eq. (9), is only correct for polynomial interpolation.

We refer to the scattering source obtained by operating on the interpolated angular flux with the exact scattering kernel as the *exact interpolation-generated scattering source*. When the interpolation functions are non-polynomial, the exact interpolation-generated scattering source is generally not expressible in terms of the interpolation functions. Thus, if the discrete scattering source values obtained from the Galerkin quadrature method are interpolated, one generally does not obtain the exact interpolation-generated scattering source. Rather, one obtains a scattering source that has the same Legendre moments of degree 0 through $N-1$ as the exact interpolation-generated scattering source.

As an example of a useful non-polynomial interpolation scheme, we consider a linear-discontinuous angular trial space in 1-D spherical geometry. Such a trial space is fully compatible with a linear-discontinuous treatment for the angular derivative term. An "S_N" trial space of this type is defined to consist of $N/2$ equal-width piecewise-linear segments in μ, where N is even and $N > 2$. There are two discrete angular flux unknowns per segment located at the local Gauss S_2 quadrature points, i.e., the points corresponding to $\pm 1/\sqrt{3}$ obtained by mapping $[-1, +1]$ onto each segment. A Galerkin quadrature set is generated for this trial space by exactly evaluating the Legendre angular flux moments of degree 0 through $N-1$ associated with the linear-discontinuous interpolation of the N discrete flux values. The companion quadrature set corresponding to the Galerkin set, i.e., the standard quadrature set having the same quadrature points as the Galerkin set with quadrature weights that exactly integrate the interpolated angular flux representation, corresponds to a local Gauss S_2 set on each linear segment. Since each local Gauss set exactly integrates cubic polynomials, it follows that the companion set will exactly evaluate the zero'th, first, and second Legendre moments of the interpolated angular flux. However, all higher flux moments will be inexactly evaluated, regardless of the quadrature order N. This is in contrast to the Galerkin quadrature set of order N, which always exactly evaluates the Legendre angular flux moments of degree 0 through $N-1$. Furthermore, because the companion quadrature set never exactly integrates polynomials of degree greater than 3, one cannot use a Legendre cross-section expansion of degree greater than 3 with the companion quadrature set (otherwise particle conservation will be lost). Thus, the accuracy of the scattering source with highly anisotropic scattering can be greatly improved for linear-discontinuous angular trial spaces in 1-D by using Galerkin quadrature. This enables one to use a linear-discontinuous approximation for the angular derivative term in 1-D spherical geometry in conjunction with an accurate treatment for highly anisotropic scattering.

Perhaps the most important property of the Galerkin quadrature method, independent of the type of functions used to interpolate the discrete angular flux values, is that straight-ahead delta-function scattering is exactly treated. This has a very important impact in charged-particle calculations, because it enables the total scattering cross section to be dramatically reduced (with an attendant decrease in the scattering ratio) while leaving the $\mathrm{S_N}$ solution invariant. To demonstrate why straight-ahead scattering is exactly treated, let us consider the following differential scattering cross section:

$$\sigma_s(\mu_0) = \frac{\alpha}{2\pi}\delta(\mu_0 - 1) \ , \tag{18}$$

where α is an arbitrary constant. The Boltzmann scattering operator associated with this cross section is α times the identity operator:

$$\begin{aligned} S\psi &= 2\pi \int_{-1}^{+1} \frac{\alpha}{2\pi}\delta(\mu_0 - 1)\psi(\mu')\, d\mu' \\ &= \alpha\psi(\mu) \ . \end{aligned} \tag{19}$$

Furthermore, the Legendre moments of this cross section are all equal to alpha:

$$\sigma_m = \frac{\alpha}{2\pi}2\pi \int_{-1}^{+1} \delta(\mu_0 - 1)P_m(\mu')\, d\mu' = \alpha P_m(1) = \alpha \ , \ \ 0 \leq m \leq \infty \ . \tag{20}$$

Thus, the diagonal matrix of cross-section moments used to construct the vector of discrete scattering source values is α times the identity matrix:

$$\mathbf{\Sigma} = \alpha \mathbf{I} \ . \tag{21}$$

Substituting from Eq. (21) into Eq. (11), and recognizing that $\mathbf{M} = \mathbf{D}^{-1}$, we obtain

$$\begin{aligned} \overrightarrow{S} &= \mathbf{M}\alpha\mathbf{I}\mathbf{D}\overrightarrow{\psi} \ , \\ &= \alpha\mathbf{M}\mathbf{D}\overrightarrow{\psi} \ , \\ &= \alpha\overrightarrow{\psi} \ , \end{aligned} \tag{22}$$

which agrees with Eq. (19). We have explicitly considered only the 1-D case, but this result also applies in multiple dimensions.

For charged particles, the scattering ratio for each group is generally very close to unity, and the mean free path is very small; nonetheless, the transport process is not diffusive. This is because the "transport-corrected" scattering ratio, $(\sigma_0 - \sigma_1)/\sigma_t$, is not close to unity. Within-group straight-ahead scattering is equivalent to no scattering at all, since the particle scatters into the same group and direction it had before the scattering. Thus, one can add or subtract a straight-ahead differential scattering cross section from any physically correct within-group cross section without changing the analytic transport solution. Since all Galerkin quadratures treat straight-ahead scattering exactly, one can subtract the truncated expansion for a within-group straight-ahead scattering cross section from the physically correct cross section expansion without changing the S_N solution.

For instance, let us consider the total Boltzmann scattering operator (outscatter minus inscatter) associated with a 1-D S_N Galerkin quadrature:

$$\begin{aligned}\Sigma_0 \overrightarrow{\psi} - \overrightarrow{S} &= [\mathbf{M\Sigma_0 D} - \mathbf{M\Sigma D}]\,\overrightarrow{\psi} \quad , \\ &= \mathbf{M}\left[\mathbf{\Sigma_s} - \mathbf{\Sigma}\right]\mathbf{D}\,\overrightarrow{\psi} \quad , \\ &= \mathbf{M}\left[diag\left(\sigma_0 - \sigma_0, \sigma_0 - \sigma_1, \ldots, \sigma_0 - \sigma_{N-1}\right)\right]\mathbf{D}\,\overrightarrow{\psi} \quad . \end{aligned} \tag{23}$$

Subtracting the delta-function cross section given in Eq. (18) from the physically correct cross section, we obtain the following modified outscatter matrix:

$$\mathbf{\Sigma_0^*} = (\mathbf{\Sigma_0} - \alpha\mathbf{I}) \quad , \tag{24}$$

and the following modified inscatter matrix:

$$[\mathbf{M\Sigma D}]^* = \mathbf{M\Sigma^* D} \quad , \tag{25}$$

where

$$\mathbf{\Sigma}^* = diag\left(\sigma_0 - \alpha, \sigma_1 - \alpha, \ldots, \sigma_{N-1} - \alpha\right) \quad . \tag{26}$$

We note that while the outscatter and inscatter matrices are modified by subtraction of the straight-ahead scattering cross section, the total Boltzmann matrix, Eq. (23), does not change, i.e.,

$$\mathbf{\Sigma_0^*} - \mathbf{M\Sigma^* D} = \mathbf{\Sigma_0} - \mathbf{M\Sigma D} \quad . \tag{27}$$

Thus, the S_N solution does not change. However, the convergence properties of the source iteration process can be dramatically changed. A discussion of the optimal choice of α is beyond the scope of this paper, but the traditional choice (which is nearly optimal) is to set $\alpha = \Sigma_N$. This *extended transport correction* can greatly reduce both the total scattering cross section and the scattering ratio in relativistic charged-particle transport calculations. We note that the significance of this cross-section modification depends upon the convergence of the cross-section expansion. If the expansion is essentially converged, Σ_{N-1} will be very small relative to Σ_0 , resulting in a negligible reduction in Σ_0; and if the cross-section expansion is highly truncated, Σ_{N-1} will be comparable to Σ_0, resulting in a significant reduction in Σ_0. Acceptable computational efficiency often cannot be achieved without the use of the extended transport correction in charged-particle calculations.

Thus, with Galerkin quadrature, the extended transport correction (correctly) leaves the S_N solution invariant. This is a powerful motivation for using the Galerkin method in charged-particle calculations.