Lecture 26

Self-Adjoint Forms of the Transport Equation

1 Introduction

The transport equation can be put in several second-order diffusion-like forms that make it possible to use certain discretization and solution techniques originally developed for the diffusion equation. A significant problem with this approach is that conservative second-order forms invariably have a diffusion-like coefficient proportional to σ_t^{-1}. This obviously causes problems in voids, but it also causes accuracy problems as well as conditioning problems when high optical depth material is adjacent to low optical depth material. These approaches have been standard for neutronics methods at Argonne National Laboratory for some time, and form the basis of the UNIC code. However, the recent goal eliminating homogenization techniques in reactor physics will render these techniques essentially obsolete in the long term unless the void problem can be dealt with. If one is willing to give up conservation, many possibilities present themselves, but very little work has been done in this regard.

2 Even and Odd-Parity Equations

Let us begin with the steady-state transport equation:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi(\overrightarrow{\Omega}) + (\sigma_t - \mathbf{S})\, \psi(\overrightarrow{\Omega}) = q(\overrightarrow{\Omega})\,, \tag{1}$$

where S denotes the scattering operator. We next evaluate this equation at $-\overrightarrow{\Omega}$:

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi(\overrightarrow{-\Omega}) + (\sigma_t - \mathbf{S})\, \psi(-\overrightarrow{\Omega}) = q(\overrightarrow{-\Omega})\,. \tag{2}$$

Note that in the above equation, we have used the fact that the scattering source evaluated at $-\overrightarrow{\Omega}$ is equal to the the scattering source applied to $\psi(-\overrightarrow{\Omega})$. One can prove this using an infinite spherical-harmonic expansion for the scattering source. Adding Eqs. (1) and (2), we get the first-order even-parity transport equation:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi^{-}(\overrightarrow{\Omega}) + (\sigma_t - \mathbf{S})\, \psi^{+}(\overrightarrow{\Omega}) = q^{+}(\overrightarrow{\Omega})\,, \tag{3}$$

where the even-parity angular flux is given by

$$\psi^{+}(\overrightarrow{\Omega}) = \frac{1}{2}\left(\psi(\overrightarrow{\Omega}) + \psi(-\overrightarrow{\Omega})\right)\,, \tag{4}$$

the odd-parity flux is given by

$$\psi^{-}(\overrightarrow{\Omega}) = \frac{1}{2}\left(\psi(\overrightarrow{\Omega}) - \psi(-\overrightarrow{\Omega})\right)\,, \tag{5}$$

and even-parity and odd-parity inhomogeneous sources are analogously defined. Subtracting Eq. (2) from Eq. (1), we obtain the first-order odd-parity transport equation:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi^{+}(\overrightarrow{\Omega}) + (\sigma_t - \mathbf{S})\, \psi^{-}(\overrightarrow{\Omega}) = q^{-}(\overrightarrow{\Omega})\,. \tag{6}$$

Solving Eq. (6) for ψ^-, we obtain

$$\psi^- = -\left(\sigma_t - \mathbf{S}\right)^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi^+(\overrightarrow{\Omega}) + \left(\sigma_t - \mathbf{S}\right)^{-1} q^- \,. \tag{7}$$

Substituting from Eq. (7) into Eq. (3), we obtain the second-order even-parity transport equation:

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \left(\sigma_t - \mathbf{S}\right)^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi^+(\overrightarrow{\Omega}) + \left(\sigma_t - \mathbf{S}\right) \psi^+(\overrightarrow{\Omega}) = q^+(\overrightarrow{\Omega}) + \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \left(\sigma_t - \mathbf{S}\right)^{-1} q^- \,. \tag{8}$$

Solving Eq. (3) for ψ^+ and substituting into Eq. (6), we obtain the second-order odd-parity transport equation:

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \left(\sigma_t - \mathbf{S}\right)^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi^-(\overrightarrow{\Omega}) + \left(\sigma_t - \mathbf{S}\right)^{-1} \psi^-(\overrightarrow{\Omega}) = q^-(\overrightarrow{\Omega}) + \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \left(\sigma_t - \mathbf{S}\right)^{-1} q^+ \,. \tag{9}$$

Note that the second-order equations are self-adjoint because $\sigma_t - \mathbf{S}$ is self-adjoint. In particular, it has the following form in 1D when defined with respect to the Legendre moments of the angular flux:

$$\sigma_t - \mathbf{S} = diag(\sigma_t - \sigma_0, \sigma_t - \sigma_1, \sigma_t - \sigma_2, \ldots) \,. \tag{10}$$

Note that in the even-parity transport equation, the inverse of this operator only operates on odd-parity functions, while in the odd-parity transport equation, the inverse of this operator only operates on even-parity functions. When c=1, the P_0 eigenvalue of this operator, $\sigma_t - \sigma_0$, is zero, and the even-party part of the operator is not invertible. Hence the odd-parity equation cannot be solved when $c = 1$. The even-parity equation can be discretized using continuous finite-element methods, which results in symmetric positive-definite coefficient matrices and results in far better behavior than when such methods are applied to the first-order form of the transport equation. Furthermore, conjugate-gradient methods can be used to solve these equations. However, it should be noted that while these equations are self-adjoint and second-order, they are not elliptic, so multigrid preconditioners for diffusion are not applicable. In the 1-D case, these second-order transport equations really are diffusion equations, and all standard techniques can be applied.

It is important to note that the even-parity and odd-parity fluxes are completely defined by their dependence on half the unit sphere. Thus one need only define half the unit sphere as the angular domain.

There are versions of these second-order equations that are specific to S_n methods. In particular, one groups the scattering source with the inhomogeneous source and does source iteration. For instance, the S_n form of the even-parity equation is:

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \sigma_t^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi^{+,\ell+1} + \sigma_t \psi^{+,\ell+1} = \mathbf{S}^{+,\ell} \psi^{+\ell} + q^{+} + \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \sigma_t^{-1} \left(\mathbf{S} \psi^{-,\ell} + q^{-} \right) . \quad (11)$$

Each operator on the left side if Eq. (11) corresponds to tensor diffusion with a singular (rank 1) tensor. It is not difficult to show that the spectral radius for source iteration as defined above is identical to that for the first-order transport equation. Thus one can apply DSA here as well. One no longer has trouble with $c = 1$ problems, but voids are still a problem.

2.1 Boundary Conditions

At inflow boundaries, the boundary conditions take the usual form when written in terms of the angular flux. For instance, at a source boundary with incoming angular flux, $f(\overrightarrow{\Omega})$, and outward normal, $\overrightarrow{n}$,

$$\psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) = f(\overrightarrow{\Omega}), \quad \overrightarrow{\Omega} \cdot \overrightarrow{n} < 0. \tag{12}$$

One need simply express the angular flux in terms of the even-parity and odd-parity fluxes:

$$\psi(\overrightarrow{\Omega}) = (\psi^{+}(\overrightarrow{\Omega}) + \psi^{-}(\overrightarrow{\Omega}))/2\,, \tag{13}$$

Thus Eq. (12) becomes

$$\psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) = f(\overrightarrow{\Omega}), \quad \overrightarrow{\Omega} \cdot \overrightarrow{n} < 0. \tag{14}$$

At an outflow boundary, the solution simply satisfies the first-order transport equation:

$$\psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) = -\,(\sigma_t - \mathbf{S})^{-1}\,\overrightarrow{\Omega} \cdot \overrightarrow{\nabla}\psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) + (\sigma_t - \mathbf{S})^{-1}\,q(\overrightarrow{r}_b, \overrightarrow{\Omega})\,. \tag{15}$$

Unlike the case for the even-parity and odd-parity equation, reflective conditions are straightforward for the self-adjoint equation.

3 The Self-Adjoint Angular Flux Equation

One need not decompose the angular flux into even and odd components to obtain a self-adjoint transport equation. For instance, we can use Eq. (1) to solve for ψ as follows:

$$\psi^{-} = -\left(\sigma_t - \mathbf{S}\right)^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi + \left(\sigma_t - \mathbf{S}\right)^{-1} q \,. \tag{16}$$

Substituting from Eq. (16) into Eq. (1), we get obtain the self-adjoint angular flux equation:

$$-\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \left(\sigma_t - \mathbf{S}\right)^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi + \left(\sigma_t - \mathbf{S}\right)^{-1} \psi^{-} = q + \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \left(\sigma_t - \mathbf{S}\right)^{-1} q \,. \tag{17}$$

Solving this equation is basically equivalent to solving both the second-order even-parity and odd-parity equations simultaneously. The main advantage to this is that all components of the angular flux (even-parity and odd-parity) are similarly treated. The angular domain associated with this equation is the unit sphere.

3.1 Boundary Conditions

At inflow boundaries, the boundary conditions take the usual form. For instance, at a source boundary with incoming angular flux, $f(\overrightarrow{\Omega})$, and outward normal, $\overrightarrow{n}$,

$$\psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) = f(\overrightarrow{\Omega}), \quad \overrightarrow{\Omega} \cdot \overrightarrow{n} < 0. \tag{18}$$

At an outflow boundary, the solution simply satisfies the first-order transport equation:

$$\psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) = -\left(\sigma_t - \mathbf{S}\right)^{-1} \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \psi(\overrightarrow{r}_b, \overrightarrow{\Omega}) + \left(\sigma_t - \mathbf{S}\right)^{-1} q(\overrightarrow{r}_b, \overrightarrow{\Omega}) \,. \tag{19}$$

Unlike the case for the even-parity and odd-parity equation, reflective conditions are straightforward for the self-adjoint equation.

4 The SP$_n$ Equations

There is an even-parity approximation to the P$_n$ equations that is worth discussing. It is called the simplified P$_n$ or SP$_n$ method. The usual derivation of the SP$_n$ method starts with the 1-D slab-geometry P$_n$ equations. However, for reasons that will eventually become clear, we will start with the S$_N$ equations with Gauss quadrature, which are equivalent to the P$_N$ equations:

$$\mu_m \frac{\partial \psi_m}{\partial x} + \sigma_t \psi_m = Q_m \,, \quad m = 1, N, \tag{20}$$

where we have grouped the scattering and inhomogeneous sources together. We next perform the even-party/odd-parity decomposition of Eq. (20) and derive the following second-order even-parity equation:

$$-\mu_m^2 \frac{\partial}{\partial x} \frac{1}{\sigma_t} \frac{\partial \psi_m^+}{\partial x} + \sigma_t \psi_m^+ = Q_m^+ + \mu_m \psi \frac{\partial}{\partial x} \frac{1}{\sigma_t} Q_m^- \,, \quad \mu_m > 0, \quad , m = 1, N/2, \tag{21}$$

and the corresponding first-order odd-parity equation:

$$\psi_m^- = -\frac{\mu_m}{\sigma_t} \frac{\partial \psi_m^+}{\partial x} + \frac{1}{\sigma_t} Q_m^- \,, \quad \mu_m > 0, \quad , m = 1, N/2, \tag{22}$$

We next "convert" these equations to 3-D rotationally-symmetric form by

1. Declaring the even-parity flux to be a scalar and declaring the odd-parity flux to be a vector.

2. Replacing any derivative operator acting upon the even-parity flux with a gradient operator.

3. Replacing any derivative operator acting upon the odd-parity flux or a derivative of the even-parity

The resulting equations are called the canonical SP$_n$ equations, and they are completely equivalent to the standard SP$_n$ equations:

$$-\mu_m^2 \overrightarrow{\nabla} \cdot \frac{1}{\sigma_t} \overrightarrow{\nabla} \psi_m^+ + \sigma_t \psi_m^+ = Q_m^+ + \mu_m \psi \overrightarrow{\nabla} \cdot \frac{1}{\sigma_t} \overrightarrow{Q}_m^-, \quad \mu_m > 0, \quad , m = 1, N/2, \tag{23}$$

$$\overrightarrow{\psi}_m^- = -\frac{\mu_m}{\sigma_t} \overrightarrow{\nabla} \psi_m^+ + \frac{1}{\sigma_t} \overrightarrow{Q}_m^-, \quad \mu_m > 0, \quad , m = 1, N/2, \tag{24}$$

The essential nature of these equations is that they will exactly preserve a P$_{N-1}$ solution along any direction. Thus they tend to work well for problems that are locally 1-D. That is, problems that have a 1-D angular dependence with respect to some direction $\overrightarrow{k}$, i.e., $\psi(\overrightarrow{\Omega}) = \psi(\overrightarrow{\Omega} \cdot \overrightarrow{k})$ where $\overrightarrow{k}$ at any material interface or boundary coincides with the normal to that material interface or boundary.