Lecture 18

Spatial Discretization and Solution of the S_n Equations

1 Source Iteration

The S_n equations can be expressed as follows,

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

where

$$Q_m = \sum_{k=0}^{L} \frac{2k+1}{4\pi} (\sigma_k \phi_k + q_k) P_k(\mu_m) \,, \tag{2a}$$

$$\sigma_k = 2\pi \int_{-1}^{+1} \sigma_s(\mu_0) P_k(\mu_0) \, d\mu_0 \,, \tag{2b}$$

$$\phi_k = \sum_{m=1}^{N} \psi_m P_k(\mu_m) w_m \,, \tag{2c}$$

$$q_k = 2\pi \int_{-1}^{+1} q(\mu) P_k(\mu) \, d\mu. \tag{2d}$$

It is important to recognize that all coupling between directions occurs on the right side of Eq. (1), and that the left side of that equation represents a set of angularly-independent

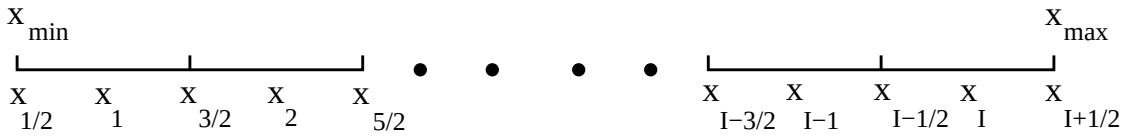

Figure 1: Spatial indexing.

first-order differential equations. Since such equations are easily solved once they have been spatially discretized, the following iterative solution technique naturally comes to mind:

$$\mu_m \frac{\partial \psi_m^{\ell+1}}{\partial x} + \sigma_t \psi_m^{\ell+1} = Q_m^{\ell}\,, \tag{3}$$

where ℓ is the iteration index. This is called source iteration simply because the scattering source lagged. The source iteration process has a physical interpretation. If one initially starts with a zero guess for the scalar flux, each source iteration adds the contribution from another generation of scatter to the flux solution. For instance, the first iteration yields the uncollided flux, the second iteration yields the uncollided plus first-collided flux, the third iteration yields the uncollided plus first-collided plus second-collided flux, etc. To understand the numerical solution process for solving the source iteration equations, we must first consider spatial discretization of the S_n equations.

2 Spatial Discretization

The indexing for spatial discretization is shown in Fig. 1. Note from that figure that cell-edge quantities carry half-integral indices and cell-average quantities carry integral indices, and that the total number of mesh cells is denoted by I. For reasons that will eventually

become clear, we need only consider the spatial discretization for a single cell and the solution of the source iteration equations for that cell. The first step in the discretization process is to spatially integrate Eq. (3) over the cell to obtain a balance equation:

$$\mu_m \left(\psi_{1+\frac{1}{2},m} - \psi_{i-\frac{1}{2},m} \right) + \sigma_{t,i} \Delta x_i \psi_{i,m} = Q_{i,m} \Delta x_i \,, \tag{4}$$

where

$$\psi_{i,m} = \frac{1}{\Delta x_i} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \psi_m(x) dx \,, \tag{5a}$$

$$Q_{i,m} = \frac{1}{\Delta x_i} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} Q_m(x)\, dx \,. \tag{5b}$$

It is important to note that Eq. (4) is exact. All we have done is integrate the equation over the cell. Since we seek to solve our equations over a single cell, we must assume that the *incoming* cell-edge fluxes are known, i.e., $\psi_{i-\frac{1}{2},m}$ for $\mu_m > 0$ and $\psi_{i+\frac{1}{2},m}$ for $\mu_m < 0$. This would be the case on a mesh consisting of a single cell since these fluxes would be defined by boundary conditions. We will see later that the assumption of known incoming fluxes is fully justified. This means that we must solve for the average and *outgoing* fluxes in each direction. Thus we need two equations for each direction. However at present we have only one equation per direction - the balance equation. To close the system, we must define an additional equation for each direction. This additional equation per direction is known as the auxiliary equation. One of the most common auxiliary equations is the

diamond difference relationship:

$$\psi_{i,m} = \frac{1}{2}\left(\psi_{i+\frac{1}{2},m} + \psi_{i-\frac{1}{2},m}\right) . \tag{6}$$

Perhaps the simplest auxiliary equation is the step relationship:

$$\begin{aligned} \psi_{i+\frac{1}{2},m} &= \psi_{i,m} \quad \mu_m > 0, \\ \psi_{i-\frac{1}{2},m} &= \psi_{i,m} \quad \mu_m < 0, \end{aligned} \tag{7}$$

The diamond relationship gives second-order accuracy, but is not necessarily positive. The step relationship is positive, but only gives first-order accuracy. Equation (4) and either Eq. (6) or Eq. (7)) enable us to solve for the average and outgoing fluxes in a cell given the incoming fluxes. We stress that the equations for each direction are completely independent of one another. All angular coupling appears on the right side of the equation and is iterated upon.

Given the equations for a single cell, it is very easy to solve for all of the fluxes on a multicell mesh. For instance, let assume that the quadrature points are indexed in order of increasing cosine. Then μ_1 through $\mu_{\frac{N}{2}}$ are negative and $\mu_{\frac{N}{2}+1}$ through μ_N are positive. One can begin the solution process by solving for $\psi_{I,1}$ and $\psi_{I-\frac{1}{2},1}$, where I is the total number of cells in the mesh. One will know $\psi_{I+\frac{1}{2},1}$ from the boundary condition at the right face. With a vacuum or source condition, these values are explicitly known, but with a reflective condition, one must set the incoming values to the appropriate outgoing flux

values using the latest iterate for the outgoing values. Such a boundary condition is called implicit because the incoming fluxes are implicitly known rather than explicitly known. After solving for $\psi_{I-\frac{1}{2},1}$, one has the necessary values to solve for $\psi_{I-1,1}$ and $\psi_{I-\frac{3}{2},1}$. The solution process or "sweep" proceeds across each cell until the left boundary is reached. The process is then repeated for all remaining fluxes with $\mu < 0$. Next one uses the boundary condition at the left face to determine $\psi_{\frac{1}{2},\frac{N}{2}+1}$, and then similarly proceeds through the mesh successively solving for the average and outgoing fluxes in each cell until the right boundary is reached. The process is then repeated for all remaining fluxes having $\mu > 0$. At this point, one full sweep (and one full source iteration) has been completed. If there is no scattering and both of the boundary conditions are explicit, the S_N equations will be completely solved after one sweep. This completes our description of the source iteration or sweep process.

3 Advanced Spatial Discretizations

Advanced spatial discretizations are generally characterized by either having more than two spatial unknowns per cell or having an auxilliary equation that captures some form of transport physics. Note that the diamond and step relationships are not specific to the transport equation. On the other hand, the linear-discontinuous (LD) finite element scheme has an

auxilliary equation that is obtained by a Galerkin process. Such an auxilliary equation clearly captures some transport physics since it is obtained from the transport equation itself. We note that the LD scheme can be derived in many ways. We choose to derive it in a way that results in an auxilliary equation with an obvious physical interpretation. The trial space is defined as follows for $\mu_m > 0$,

$$\begin{aligned} \tilde{\psi} &= \psi_{i-\frac{1}{2},m}\,, && \text{for } x = x_{i-\frac{1}{2}}, \\ &= \psi_{i,m} + \left(\psi_{i+\frac{1}{2},m} - \psi_{i,m}\right)\frac{2(x-x_i)}{\Delta x_i}\,, && \text{for } x \in (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \end{aligned} \tag{8a}$$

and as follows for $\mu_m < 0$,

$$\begin{aligned} \tilde{\psi} &= \psi_{i,m} + \left(\psi_{i,m} - \psi_{i-\frac{1}{2},m}\right)\frac{2(x-x_i)}{\Delta x_i}\,, && \text{for } x \in [x_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}), \\ &= \psi_{i+\frac{1}{2},m}\,, && \text{for } x = x_{i+\frac{1}{2}}, \end{aligned} \tag{8b}$$

An analogous representation is assumed for the inhomogeneous source. The auxilliary equation for $\mu_m > 0$ is obtained by substituting from Eq. (8a) (and its analogue for the source representation) into Eq. (1), multiplying by $(x - x_{i-\frac{1}{2}})/\Delta x_i$, and integrating over the cell:

$$\mu(\psi_{i+\frac{1}{2},m} - \psi_{i,m}) + \sigma_{t,i}\left(\frac{2}{3}\psi_{i,m} + \frac{1}{3}\psi_{i+\frac{1}{2},m}\right)\frac{\Delta x_i}{2} = \left(\frac{2}{3}Q_{i,m} + \frac{1}{3}\hat{Q}_{i+\frac{1}{2},m}\right)\frac{\Delta x_i}{2}\,, \tag{9}$$

where $\hat{Q}_{i+\frac{1}{2}}$ denotes the "cell-interior" angular flux at $x_{i+\frac{1}{2}}$,

$$\begin{aligned} \hat{Q}_{i+\frac{1}{2}} &= Q_{i+\frac{1}{2},m}\,, & \text{for } \mu_m > 0, \\ &= 2Q_{i,m} - Q_{i-\frac{1}{2},m}\,, & \text{for } \mu_m < 0, \end{aligned} \tag{10a}$$

generated with the cell-interior angular fluxes at $x = x_{i+\frac{1}{2}}$:

$$\begin{aligned} \hat{\psi}_{i+\frac{1}{2},m} &= \psi_{i+\frac{1}{2},m}\,, & \text{for } \mu_m > 0, \\ &= 2\psi_{i,m} - \psi_{i-\frac{1}{2},m}\,, & \text{for } \mu_m < 0, \end{aligned} \tag{10b}$$

Equation (9) clearly represents an approximate statement of balance over the right half of the cell. Many advanced schemes can be represented in terms of a rigorous balance equation for the whole cell together with auxilliary equations that represent approximate balance equations for portions of the cell. This is often referred to as the multiple-balance representation for a discretization scheme. The auxilliary equation for $\mu_m < 0$ is completely analogous to that for $\mu > 0$, and is obtained by substituting from Eq. (8b) into Eq. (1), multiplying by $(x_{i+\frac{1}{2}} - x)/\Delta x_i$, and integrating over the cell:

$$\mu(\psi_{i,m} - \psi_{i-\frac{1}{2},m}) + \sigma_{t,i}\left(\frac{2}{3}\psi_{i,m} + \frac{1}{3}\psi_{i-\frac{1}{2},m}\right)\frac{\Delta x_i}{2} = \left(\frac{2}{3}Q_{i,m} + \frac{1}{3}\hat{Q}_{i-\frac{1}{2},m}\right)\frac{\Delta x_i}{2}\,. \tag{11}$$

Many advanced discretization schemes can also be represented in terms of approximate balance equations over subregions of the cell, where the subregions are disjoint and the union of the subregions is the whole cell. For instance, let us assume an LD trial space

representation as follows for $\mu > 0$,

$$\begin{aligned}
\tilde{\psi}_m &= \psi_{i-\frac{1}{2},m}\,, && \text{for } x = x_{i-\frac{1}{2}}, \\
&= \psi_{L,i,m}\frac{(x_{i+\frac{1}{2}} - x)}{\Delta x_i} + \psi_{R,i,m}\frac{(x - x_{i-\frac{1}{2}})}{\Delta x_i}\,, && \text{for } x \in (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}],
\end{aligned} \tag{12a}$$

and as follows for $\mu_m < 0$,

$$\begin{aligned}
\tilde{\psi}_m &= \psi_{L,i,m}\frac{(x_{i+\frac{1}{2}} - x)}{\Delta x_i} + \psi_{R,i,m}\frac{(x - x_{i-\frac{1}{2}})}{\Delta x_i}\,, && \text{for } x \in [x_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}), \\
&= \psi_{i+\frac{1}{2},m}\,, && \text{for } x = x_{i+\frac{1}{2}},
\end{aligned} \tag{12b}$$

An analogous representation is assumed for the distributed source. Substituting from Eq. (12a) into the Eq. (1) multiplying by $\frac{(x_{i+\frac{1}{2}} - x)}{\Delta x_i}$ and integrating over the the cell, we obtain an equation for $\psi_{L,i,m}$:

$$\mu_m \left[\frac{1}{2}\left(\psi_{L,i,m} + \psi_{R,i,m}\right) - \psi_{R,i-1,m}\right] + \sigma_{t,i}\left(\frac{2}{3}\psi_{L,i,m} + \frac{1}{3}\psi_{R,i,m}\right)\frac{\Delta x_i}{2} = \left(\frac{2}{3}Q_{L,i,m} + \frac{1}{3}Q_{R,i,m}\right)\frac{\Delta x_i}{2}\,. \tag{13}$$

Note that Eq. (13) represents an approximate balance equation for the left half of the cell. Proceeding similarly, but weighting with $\frac{(x - x_{i-\frac{1}{2}})}{\Delta x_i}$, we obtain an equation for $\psi_{R,i,m}$:

$$\mu_m \left[\psi_{R,i,m} - \frac{1}{2}\left(\psi_{L,i,m} + \psi_{R,i,m}\right)\right] + \sigma_{t,i}\left(\frac{2}{3}\psi_{R,i,m} + \frac{1}{3}\psi_{L,i,m}\right)\frac{\Delta x_i}{2} = \left(\frac{2}{3}Q_{R,i,m} + \frac{1}{3}Q_{L,i,m}\right)\frac{\Delta x_i}{2}\,. \tag{14}$$

Note that Eq. (14) represents an approximate balance equation for the right half of the cell. The equations for $\mu < 0$ are analogous:

$$\mu_m \left[\frac{1}{2} \left(\psi_{L,i,m} + \psi_{R,i,m} \right) - \psi_{L,i-1,m} \right] + \sigma_{t,i} \left(\frac{2}{3} \psi_{L,i,m} + \frac{1}{3} \psi_{R,i,m} \right) \frac{\Delta x_i}{2} = \left(\frac{2}{3} Q_{L,i,m} + \frac{1}{3} Q_{R,i,m} \right) \frac{\Delta x_i}{2} . \tag{15}$$

and

$$\mu_m \left[\psi_{L,i+1,m} - \frac{1}{2} \left(\psi_{L,i,m} + \psi_{R,i,m} \right) \right] + \sigma_{t,i} \left(\frac{2}{3} \psi_{R,i,m} + \frac{1}{3} \psi_{L,i,m} \right) \frac{\Delta x_i}{2} = \left(\frac{2}{3} Q_{R,i,m} + \frac{1}{3} Q_{L,i,m} \right) \frac{\Delta x_i}{2} . \tag{16}$$

Equations (13) through (16) represent the LD equation in corner balance form. Summing the approximate balance equations for the left and right halves of the cell yields the balance equation for the whole cell.

3.1 Finite Element Lumping

It is often useful to give up a certain degree of accuracy in return for more robustness in a discretization scheme. By robustness, we generally mean the ability to yield well behaved (though not necessarily accurate) solutions on poorly resolved meshes. In general, this is achieved in finite-element methods by using a quadrature formula with quadrature points at the mesh-cell vertices to perform the finite-element integrations rather than performing them analytically or with Gauss quadrature. The effect of using such quadrature sets

is to reduce the span of the discrete stencil or make the matrix representation for the discretization "more diagonal." For instance, let us consider the LD method and perform the integrals using a trapezoidal-rule quadrature. This quadrature has two points that are located at $x_{i-\frac{1}{2}}$ and $x_{i+\frac{1}{2}}$, and each point carries a weight of $\Delta x_i/2$. The integration of the perfect derivative resulting from the integration by parts is always carried out before applying the quadrature formula because quadratures can never be expected to properly integrate delta-function derivatives. For instance, let us assume an arbitrary LD trial space representation, $\tilde{\psi}$, and an arbitary weighting function, $W(x)$. A lumped approximation for the equation associated with the weighting function, would be obtained by applying the trapezoidal quadrature to the following equation:

$$\mu_m \left(W_{i+\frac{1}{2}} \tilde{\psi}_{i+\frac{1}{2},m} - W_{i-\frac{1}{2}} \tilde{\psi}_{i-\frac{1}{2},m} \right) - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tilde{\psi} \, \frac{\partial W}{\partial x} \, dx +$$

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \sigma_t W \tilde{\psi}_m \, dx = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} W Q_m \, dx \, . \tag{17}$$

Note from that the perfect derivative arising from the integration by parts of the gradient term has been performed analytically. In general, maintaining acceptable accuracy in the lumping process requires that the integration be exact if the weight function is unity, i.e. for the balance equation. The trapezoidal quadrature is indeed exact for the integrals in Eq. (17) when $W(x) = 1$. To give a specific example, we substitute from Eq. (8a) (and its analogue for the source representation) into Eq. (1), multiply that equation by

$(x - x_{i-\frac{1}{2}})/\Delta x_i$, and integrating over the cell using the trapezoidal quadrature formula:

$$\mu(\psi_{i+\frac{1}{2},m} - \psi_{i,m}) + \sigma_{t,i}\psi_{i+\frac{1}{2},m}\frac{\Delta x_i}{2} = \hat{Q}_{i+\frac{1}{2},m}\frac{\Delta x_i}{2}\,, \tag{18}$$

where $\hat{Q}_{i+\frac{1}{2}}$ is defined by Eqs. (10a) and (10b). Comparing Eq. (18) with its unlumped analogue given by Eq. (9), we find that the the removal and source terms in Eq. (18) do have reduced spatial coupling.