Lecture 25

Discretization and Solution of the Spherical-Geometry S_n Equations

1 Introduction

The 1-D spherical-geometry transport equation can really be thought of as being a 2-D equation in that you have advection in both space and angle. Thus the sweep process is quite different in this geometry as opposed to slab-geometry. As we shall see, the S_n discretization in angle of this equation is complicated by the fact that the quadrature cosines generally do not lie at the center of their associated angular cells. The equation we discretize is

$$\frac{\mu}{r^2}\frac{\partial[r^2\psi]}{\partial r} + \frac{1}{r}\frac{\partial[(1-\mu^2)\psi]}{\partial \mu} + \sigma_t\psi = \sum_{k=0}^{\infty}\frac{2k+1}{2}(\sigma_k\phi_k + q_k)P_k(\mu)\,. \tag{1}$$

2 Angular Discretization

It is easier to discretize this transport equation if we temporarily assume that the quadrature weights sum to 2. Doing so enables us to define cell-edge cosines. We index the quadrature directions in order of increasing cosine. Thus μ_1 is the smallest cosine (nearest

$\mu = -1$). With this ordering we can define a simple recursion formula for the angular cell-edge cosines assuming an N-point quadrature set:

$$\mu_{m+1/2} = \mu_{m-1/2} + w_m \,, \quad \mu_{1/2} = -1, \quad m = 1, N. \tag{2}$$

Next we integrate Eq. (1) over angular cell m using the quadrature formula for all terms except the derivative term, which we integrate exactly.

$$\frac{\mu_m}{r^2}\frac{\partial\,[r^2\psi]}{\partial r}w_m + \frac{1}{r}[(1-\mu_{m+1/2}^2)\psi_{m+1/2} - (1-\mu_{m-1/2}^2)\psi_{m-1/2}] + \sigma_t\psi_m w_m = \sum_{k=0}^{K}\frac{2k+1}{2}(\sigma_k\phi_k + q_k)P_k(\mu_m)w_m \,, \tag{3}$$

where K is chosen to be the minimum of $N-1$ and the degree of the "exact" cross section expansion. By "exact" we mean the mimimum expansion degree that yields adequate accuracy. Note that we use the standard S_n quadrature treatment here rather than a Galerkin quadrature treatment. This is fine as long as the scattering is weakly anisotropic or Gauss quadrature is used. The first property we test is the ability of this discretization to preserve the constant isotropic solution. Under the assumption that the inhomogeneous source is isotropic and constant in space, this solution is given by

$$\psi_c = \frac{1}{2}(q_0/\sigma_a) \,, \tag{4}$$

Substituting from Eq. (4), into Eq. (3), we first note that

$$\begin{aligned} \frac{1}{2}\sigma_t(q_0/\sigma_a)w_m - \frac{1}{2}[\sigma_s(q_0/\sigma_a) - q_0]w_m &= ((\sigma_a+\sigma_s)/\sigma_a)q_0 - (\sigma_s/\sigma_a)q_0 - q_0 \\ &= 0 \,. \end{aligned} \tag{5}$$

Thus we need only further consider the space-angle advection term, which should be equal to zero:

$$\begin{aligned}
&\frac{\mu_m}{r^2}\frac{\partial\left[r^2\psi_c\right]}{\partial r}w_m + \frac{1}{r}[(1-\mu_{m+1/2}^2)\psi_c - (1-\mu_{m-1/2}^2)\psi_c]\,, \\
&= 2\frac{\mu_m}{r}\psi_c w_m + \frac{1}{r}[\mu_{m-1/2}^2 - \mu_{m+1/2}^2]\psi_c\,, \\
&= \left\{2\mu_m w_m + (\mu_{m+1/2}+\mu_{m-1/2})\left(\mu_{m-1/2}-\mu_{m+1/2}\right)\right\}\frac{\psi_c}{r}\,, \\
&= \left\{2\mu_m w_m - (\mu_{m+1/2}+\mu_{m-1/2})w_m\right\}\frac{\psi_c}{r}\,, \\
&= \left\{\mu_m - (\mu_{m+1/2}+\mu_{m-1/2})/2\right\}\frac{2\psi_c w_m}{r}\,.
\end{aligned} \tag{6}$$

However, it is clear from Eq. (6) that this will only be the case if each quadrature point lies at the center of the angular cell. While the m'th quadrature point can always be expected to lie within the m'th angular cell, it will almost never lie at the center of that cell. Thus our discretization fails to preserve the constant solution in it's present form. We can remedy this. First we replace $1-\mu_{m+1/2}^2$ by the (as yet undefined) coefficient $\alpha_{m+1/2}$. Equation (3) becomes

$$\begin{aligned}
&\frac{\mu_m}{r^2}\frac{\partial\left[r^2\psi\right]}{\partial r}w_m + \frac{1}{r}[(\alpha_{m+1/2}\psi_{m+1/2} - \alpha_{m-1/2}\psi_{m-1/2}] + \sigma_t\psi_m w_m = \\
&\qquad\qquad \sum_{k=0}^{K}\frac{2k+1}{2}(\sigma_k\phi_k + q_k)P_k(\mu_m)w_m\,.
\end{aligned} \tag{7}$$

It follows from Eq. (7) that the space-angle advection term will yield zero for the constant isotropic solution if

$$2\mu_m w_m + \alpha_{m+1/2} - \alpha_{m-1/2} = 0\,. \tag{8}$$

We can use Eq. (8) as a recursion relationship to generate all of the α-coefficients once we initialize the recursion with $\alpha_{1/2} = 1 - \mu_{1/2}^2 = 0$:

$$\alpha_{m+1/2} = \alpha_{m-1/2} - 2\mu_m w_m\,, \quad m = 1, N, \quad \alpha_{1/2} = 0\,. \tag{9}$$

Note that since we require a symmetric quadrature both $\alpha_{1/2} = \alpha_{N+1/2} = 0$. First and final values of zero are needed to obtain particle conservation in angular advection approximation. At that point we have three angular unknowns per angular cell in Eq. (7). We can view $\psi_{m-1/2}$ as known since particles advect from small μ to large μ. That leaves two unknowns and only one equation. We need an auxilliary equation. We could use the diamond relationship (which was the standard for many years,) but it is not consistent with the fact that the quadrature points do not lie at the angular cell centers. Instead we use a weighted-diamond relationship that is consistent with a local linear dependence of ψ within each angular cell:

$$\psi_m = \beta_m \psi_{m+1/2} + (1 - \beta_m)\psi_{m-1/2}\,, \quad m = 1, N, \tag{10}$$

where β_m is defined by the following relationship:

$$\mu_m = \beta_m \mu_{m+1/2} + (1 - \beta_m)\mu_{m-1/2}\,, \qquad m = 1, N, \tag{11}$$

or equivalently

$$\beta_m = \frac{\mu_m - \mu_{m-1/2}}{\mu_{m+1/2} - \mu_{m-1/2}}\,, \qquad m = 1, N. \tag{12}$$

At this point, we lack an equation for $\psi_{1/2}$, which is the flux value on the "angular inflow boundary." This flux corresponds to $\mu = -1$ regardless of the quadrature set used. For obvious reasons, we call it the starting-direction flux. We could obtain this value in some implicit manner, e.g., by interpolation of the angular fluxes at the quadrature points. However, this would give us implicit coupling which would prevent us from solving our equations via a sweep. The transport equation in non-conservative form is given by:

$$\mu\frac{\partial\psi}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial\psi}{\partial\mu} + \sigma_t\psi = Q_m\,. \tag{13}$$

Evaluating Eq. (13) at $\mu = -1$ assuming that the derivative of ψ with respect to μ is bounded at $\mu = -1$ we find that the starting direction flux satisfies the slab geometry equation:

$$-\frac{\partial\psi_s}{\partial r} + \sigma_t\psi_s = Q_s\,. \tag{14}$$

We have already discussed the spatial discretization of this equation. We should use the same method for both the starting direction equation and the main transport equation, e.g., diamond difference or linear discontinuous Galerkin. With anisotropic scattering, one must decide how to evaulate the source at $\mu = -1$. The most stable way to obtain it is by linear interpolation of the two source values with cosines nearest the starting cosine. In

this case, one obtains

$$Q_s = Q_1 \frac{\mu_2 + 1}{\mu_2 - \mu_1} - Q_2 \frac{1 + \mu_1}{\mu_2 - \mu_1} \,. \tag{15}$$

If this value is negative, it can simply be set to zero. An easier but less stable alternative is to evaluate the Legendre expansion for the source at $\mu = -1$. With a reflective condition at the outer boundary, a value of the flux is needed at $\mu = 1$ to "reflect" into the starting direction. This value can similarly be obtained by linear interpolation of the angular fluxes with cosines nearest $\mu = 1$. In particular, we obtain

$$\psi\big|_{\mu=1} = \psi_N \frac{1 - \mu_{N-1}}{\mu_N - \mu_{N-1}} - \psi_{N-1} \frac{1 - \mu_N}{\mu_N - \mu_{N-1}} \,. \tag{16}$$

If this value is negative, it can simply be set to zero. A final point regarding use of the starting-direction flux is that the fluxes in all directions are equal to the starting-direction flux at the origin.

3 Spatial Discretization

We next spatially discretize Eq. (3). Integrating over all space, we get the following balance equation:

$$\mu_m \left(A_{i+1/2} \psi_{i+1/2,m} - A_{i-1/2} \psi_{i-1/2,m} \right) +$$
$$\frac{1}{2} \left(A_{i+1/2} - A_{i-1/2} \right) \frac{\left(\alpha_{m+1/2} \hat{\psi}_{i,m+1/2} - \alpha_{m-1/2} \hat{\psi}_{i,m-1/2} \right)}{w_m} +$$

$$\sigma_{t,i} V_i \psi_{i,m} = Q_{i,m} V_i \,, \quad m = 1, N, \quad i = 1, I, \tag{17}$$

where

$$A_{i+1/2} = 4\pi r_{i+1/2}^2 \,, \tag{18}$$

$$V_i = \frac{4\pi}{3} \left(r_{i+1/2}^3 - r_{i-1/2}^3 \right) \,, \tag{19}$$

$\hat{\psi}_i$ denotes an r-averaged flux and ψ_i denotes an r^2-weighted average. Thus two spatial averages appear in this equation. The spatial discretization results in a total of four unknowns, the angular outflow, $\psi_{i,m+1/2}$, the spatial outflow: $\psi_{i-1/2,m}$, for $\mu_m < 0$ and $\psi_{i+1/2,m}$ for $\mu_m > 0$, the r-weighted cell average, $\hat{\psi}_{i,m}$, and the r^2 weighted $\psi_{i,m}$. We currently have two equations: the balance equation and the weighted-diamond angular relationship. Thus, we need to two more. The spatial diamond approximation provides both equations:

$$\hat{\psi}_{i,m} = \frac{1}{2} \left(\psi_{i-1/2,m} + \psi_{i+1/2,m} \right) \,, \tag{20}$$

and

$$\psi_{i,m} = \frac{1}{2} \left(\psi_{i-1/2,m} + \psi_{i+1/2,m} \right) \,. \tag{21}$$

Note that when the spatial diamond approximation is used, there is no difference between the r-averaged and r^2-averaged fluxes. Our discretized equations enable us to solve in a space-angle cell i, m given spatial and angular inflow fluxes. In particular, the angular inflow flux is $\hat{\psi}_{i,m-1/2}$, the spatial inflow flux for $\mu_m < 0$ is $\psi_{i+1/2,m}$, and the spatial inflow flux for $\mu_m > 0$ is $\psi_{i-1/2,m}$.

4 The Source Iteration Algorithm

We use source iteration to solve these equations. This process has been previously described for slab geometry. The flux iterate consists of the cell-centered flux moments, the starting direction flux at the origin, and the outflow angular flux values at the right boundary, which may be required to iterate on implicit outer boundary conditions. These outer boundary fluxes are needed in any case to compute the outflow current, which is required for a particle conservation check. We now need only explain how to perform a sweep.

1. Given an angular flux iterate, The angular flux at the outer boundary is set from boundary conditions and a slab-geometry sweep to the origin is performed for that direction. All of the fluxes at the origin take on the starting-direction flux value since the origin can only be reached by particles traveling in the starting direction. The number of particles born at the origin through scattering or the inhomogeneous source is negligible (differentially small).

2. The starting direction flux provides the angular inflow for the first angular cell (quadrature direction) in each spatial cell. Thus one next sweeps to the origin to obtain the flux in the first quadrature direction. The flux in this direction must be set to the starting-direction flux value at the origin. This requires replacement of the diamond-difference relationship in the cell containing the origin with the starting-

direction flux specification. The balance equation is maintained.

3. The solution in the first angular cell provides the angular inflows for the second angular cell, and so on. Thus one sequentially performs an analogous sweep to the origin for each negative direction, updating the angular inflows for the next angular cell in each spatial cell.

4. Once the fluxes in the negative directions have been swept, the angular inflow values are known for the first postive angular cell. The flux in the first positive direction is set to the starting-direction flux value at the origin and that direction is swept to the outer boundary. No modification of the equations is required in the cell containing the origin because it is the spatial inflow value rather than the spatial outflow value that is defined.

5. Once the first positive direction has been swept, the angular inflows for the next positive direction can be computed, and so on. Thus the remaining positive directions are sequentially swept to the outer boundary. This completes the overall sweep. Unlike the slab-geometry case, the spherical-geometry angular sweeps must be performed sequentially because of the angular coupling resulting from the angular derivative term.

5 Alternate Weights

One may use quadrature weights that sum to 4π or 1 if desired. The edge cosines must be computed using renormalized weights that sum to 2, and the denominator of the first factor in the Legendre expansion for the scattering source must equal the sum of the weights:

$$\frac{2k+1}{2} \rightarrow \frac{2k+1}{\sum_{m=1}^{N} w_m} \,. \tag{22}$$

Interestingly, the recursion relationship for the α-coefficients uses the actual weights rather than the renormalized weights. No other changes have to be made to accomodate weights with an arbitrary normalization.