Lecture 18

S_n Discretization of the 1-D Spherical-Geometry Equations

1 Introduction

The purpose of the lecture is to describe the S_n discretization for the 1-D spherical-geometry equations. These equations are significantly more complicated than the 1-D slab geometry equations because of the angular derivative. Thus, in a limited sense, the spherical geometry equation is more like a 2-D equation than a 1-D equation.

2 Angular Discretization

The monoenergetic transport equation in 1-D spherical-geometry is

$$\frac{\mu}{r^2}\frac{\partial}{\partial r}r^2\psi + \frac{1}{r}\frac{\partial}{\partial \mu}\left[(1-\mu^2)\psi\right] + \sigma_t\psi = 2\pi\int_{-1}^{+1}\sigma_s(\mu'\to\mu)\psi(\mu')\,d\mu' + Q\,. \tag{1}$$

We first discretize all of the terms in Eq. (1) except the angular derivative term in analogy with the discretization of the slab-geometry equation. We start with a standard S_N quadrature set, $\{\mu_m, w_m\}_{m=1}^N$, then use a Legendre polynomial expansion of degree L to represent

the scattering and inhomogeneous sources, and collocate at the quadrature directions to obtain

$$\frac{\mu_m}{r^2}\frac{\partial}{\partial r}r^2\psi_m + \frac{1}{r}\left\{\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\right\}_m + \sigma_t\psi_m = \sum_{k=0}^{L}\frac{2k+1}{4\pi}\left(\sigma_k\phi_k + q_k\right)P_k(\mu_m)\,, \tag{2}$$

where $P_k(\mu)$ is the Legendre polynomial of degree k , the Legendre moments of the differential scattering cross-section are given by

$$\sigma_k = 2\pi\int_{-1}^{+1}\sigma_s(\mu_0)P_k(\mu_0)\,d\mu_0\,, \tag{3a}$$

the Legendre moments of the flux are given by

$$\phi_k = \sum_{m=1}^{N}\psi_m P_k(\mu)w_m\,, \tag{3b}$$

and the Legendre moments of the inhomogeneous source are given by

$$q_k = 2\pi\int_{-1}^{+1}Q(\mu)P_k(\mu)\,d\mu\,. \tag{3c}$$

We next discretize the angular derivative term. Assuming that the cosines are ordered in ascending order, we define angular cell-edge cosines using renormalized quadrature weights as follows:

$$\mu_{m+\frac{1}{2}} = \mu_{m-\frac{1}{2}} + \hat{w}_m\,, \quad m = 1, N, \quad \mu_{\frac{1}{2}} = -1\,, \tag{4}$$

where the renormalized weights sum to 2 rather than 4π:

$$\hat{w}_m = \frac{w_m}{2\pi}\,. \tag{5}$$

For future reference, it is important to note that the m'th angular interval, $(\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}})$, will contain μ_m, i.e., $\mu_{m-\frac{1}{2}} < \mu_m < \mu_{m+\frac{1}{2}}$, but μ_m will not be at the center of the interval, i.e.,

$$\mu_m \neq (\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}})/2\,. \tag{6}$$

A naive discretization if the angular derivative term would take the following form:

$$\frac{1}{r}\left\{\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\right\}_m = \frac{1}{r}\left[\frac{(1-\mu^2_{m+\frac{1}{2}})\psi_{m+\frac{1}{2}} - (1-\mu^2_{m-\frac{1}{2}})\psi_{m-\frac{1}{2}}}{\mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}}\right]\,, \tag{7}$$

where the cell-edge fluxes, $\psi_{m\pm\frac{1}{2}}$ are as yet undefined. This discretization is undesirable because it does not preserve the constant solution. To see this, we assume that the angular flux, ψ_c, is constant in space and isotropic in angle. It is clear that $\overrightarrow{\Omega}\cdot\overrightarrow{\nabla}\psi_c = 0$, but evaluating our discretization for this quantity, we get

$$\begin{aligned}
\left[\Omega\cdot\overrightarrow{\nabla}\psi_c\right]_m &= \frac{\mu_m}{r^2}\frac{\partial}{\partial r}r^2\psi_c + \frac{1}{r}\left[\frac{(1-\mu^2_{m+\frac{1}{2}})\psi_c - (1-\mu^2_{m-\frac{1}{2}})\psi_c}{\mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}}\right]\,,\\
&= \mu_m\frac{2}{r}\psi_c - \frac{1}{r}\left[\frac{\mu^2_{m+\frac{1}{2}} - \mu^2_{m-\frac{1}{2}}}{\mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}}\right]\psi_c\,,\\
&= \mu_m\frac{2}{r}\psi_c - \left[(\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}})/2\right]\frac{2}{r}\psi_c\,.
\end{aligned} \tag{8}$$

The right side of Eq. (8) will only be zero if Eq. (6) is satisfied. Since Eq. (6) is never satisfied with a standard S_n quadrature set, it follows that the naive discretization does not preserve the constant solution.

To remedy this situation, we re-express the S_n discretization for the angular derivative

term as follows:

$$\frac{1}{r}\left\{\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\right\}_m = \frac{1}{r}\left[\frac{\beta_{m+\frac{1}{2}}\psi_{m+\frac{1}{2}} - \beta_{m-\frac{1}{2}}\psi_{m-\frac{1}{2}}}{w_m}\right], \tag{9}$$

where the β-coefficients are as yet undefined. Evaluating $\overrightarrow{\Omega}\cdot\overrightarrow{\nabla}\psi_c$ using the discretization defined by Eq. (9), we obtain

$$\begin{aligned}\left[\Omega\cdot\overrightarrow{\nabla}\psi_c\right]_m &= \frac{\mu_m}{r^2}\frac{\partial}{\partial r}r^2\psi_c + \frac{1}{r}\left[\frac{\beta_{m+\frac{1}{2}}\psi_c - \beta_{m-\frac{1}{2}}\psi_c}{w_m}\right], \\ &= \mu_m\frac{2}{r}\psi_c - \frac{1}{r}\left[\frac{\beta_{m+\frac{1}{2}} - \beta_{m-\frac{1}{2}}}{w_m}\right]\psi_c\,. \end{aligned} \tag{10}$$

We obtain a recursion relationship for the β-coefficients by *requiring* that the right side of Eq. (10) be zero, or equivalently, that the constant solution be preserved. The resulting recursion relationship is

$$\beta_{m+\frac{1}{2}} = \beta_{m-\frac{1}{2}} - 2\mu_m w_m\,. \tag{11}$$

To begin the recursion, we set $\beta_{\frac{1}{2}} = 0$ on purely physical grounds, namely, the first and last β-coefficients must be zero to ensure particle conservation. This follows from the fact that

$$2\pi\int_{-1}^{+1}\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\,d\mu = 2\pi\left|_{-1}^{+1}(1-\mu^2)\psi\right. = 0\,. \tag{12}$$

Integrating Eq. (9) over all directions using the quadrature formula, and assuming that $\beta_{N+\frac{1}{2}} = \beta_{\frac{1}{2}} = 0$, we get the discrete equivalent of Eq. (12):

$$\sum_{m=1}^{N}\left\{\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\right\}_m w_m = \beta_{N+\frac{1}{2}}\psi_{N+\frac{1}{2}} - \beta_{\frac{1}{2}}\psi_{\frac{1}{2}} = 0\,. \tag{13}$$

Since standard S_n quadrature sets are required to be symmetric about $\mu = 0$, the last β-coefficient generated with Eq. (11) will be zero whenever the first coefficient is zero. Thus we see that the β-coefficients are uniquely determined by requiring that the constant solution be preserved and that the discretization be conservative. This is very elegant, but it does not help us to see how the original derivative is being approximated. To achieve a better understanding, we first note that one can define a differential equation for the quantity, $\gamma = 1 - \mu^2$, over the interval, $[-1, +1]$, as follows:

$$\frac{\partial}{\partial \gamma} = -2\mu\,, \quad \gamma(-1) = 0. \tag{14}$$

We next note that the S_n discretization for the angular derivative term can be re-expressed in the following alternate form:

$$\frac{1}{r}\left\{\frac{\partial}{\partial \mu}\left[(1-\mu^2)\psi\right]\right\}_m = \frac{1}{r}\left[\frac{\gamma_{m+\frac{1}{2}}\psi_{m+\frac{1}{2}} - \gamma_{m-\frac{1}{2}}\psi_{m-\frac{1}{2}}}{\hat{w}_m}\right], \tag{15}$$

where

$$\gamma_{m+\frac{1}{2}} = \gamma_{m-\frac{1}{2}} - 2\mu_m \hat{w}_m\,, \quad m = 1, N, \quad \gamma_{\frac{1}{2}} = 0. \tag{16}$$

Thus we see that the S_n discretization for the angular derivative term is equivalent to using discrete values of γ obtained by solving a differential equation for *gamma* via a quadrature integration. Substituting from Eq. (9) into Eq. (2) we get the final form of the S_n equations:

$$\frac{\mu_m}{r^2}\frac{\partial}{\partial r}r^2\psi_m + \frac{1}{r}\left(\frac{\beta_{m+\frac{1}{2}}\psi_{m+\frac{1}{2}} - \beta_{m+\frac{1}{2}}\psi_{m-\frac{1}{2}}}{w_m}\right) + \sigma_t\psi_m = \sum_{k=0}^{L}\frac{2k+1}{4\pi}\left(\sigma_k\phi_k + q_k\right)P_k(\mu_m)\,, \tag{17}$$

We next consider the definition of the cell-edge angular fluxes, $\psi_{m\pm\frac{1}{2}}$. We will present three possible definitions. The first is just the step method, which states that the outflow value is equal to the average value. However, we must establish whether $\psi_{m-\frac{1}{2}}$ or $\psi_{m+\frac{1}{2}}$ is the outflow value. Recalling a previous lecture on the $\overrightarrow{\Omega} \cdot \overrightarrow{\nabla}$ operator in 1-D spherical-geometry, we recall that a particle entering a voided sphere with direction $\mu = -1$ is directed toward the origin, and remains in direction $\mu = -1$ until it passes through the origin. As it passes through the origin, it transitions to the direction $\mu = +1$ and stays in direction $\mu = +1$ until it passes out of the sphere. A particle that enters a voided sphere in any direction other than $\mu = -1$, continuously changes its μ-coordinate as it streams. More specifically, this coordinate continuously increases, asymptotically approaching $\mu = +1$ as the total distance traveled in the sphere increases without bound. Thus the angular derivative term represents a type of advection operator that "advects" particles in the direction of increasing μ. This means that $\psi_{m-\frac{1}{2}}$ is the inflow flux and $\psi_{m+\frac{1}{2}}$ is the outflow flux in angular cell m. Applying the step discretization, we get

$$\psi_m = \psi_{m+\frac{1}{2}}\,, \quad m = 1, M. \tag{18}$$

Substituting from Eq. (18) into Eq. (9), we get the following discretization for the angular deivative:

$$\frac{1}{r}\left\{\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\right\}_m = \frac{1}{r}\left[\frac{\beta_{m+\frac{1}{2}}\psi_m - \beta_{m-\frac{1}{2}}\psi_{m-\frac{1}{2}}}{w_m}\right], \tag{19}$$

The step or upwind assumption closes the semi-discrete S$-n$ system of equations.

Another obvious possiblity for defining the cell-edge angular fluxes is the diamond scheme:

$$\psi_m = (\psi_{m+\frac{1}{2}} - \psi_{m-\frac{1}{2}})/2\,, \quad m = 1, M. \tag{20}$$

Substituting from Eq. (20) into Eq. (9), we get the following discretization for the angular derivative:

$$\frac{1}{r}\left\{\frac{\partial}{\partial\mu}\left[(1-\mu^2)\psi\right]\right\}_m = \frac{1}{r}\left[\frac{\beta_{m+\frac{1}{2}}(2\psi_m - \psi_{m-\frac{1}{2}}) - \beta_{m-\frac{1}{2}}\psi_{m-1}}{w_m}\right], \tag{21}$$

The diamond assumption does not close the semi-discrete S_n system of equations because $\psi_{\frac{1}{2}}$ appears in the equation for ψ_1. To close the system, we must define $\psi_{\frac{1}{2}}$, which is called the starting direction flux. The simplest way to do this is to use the so-called "step-start" definition:

$$\psi_{\frac{1}{2}} - \psi_1\,. \tag{22}$$

This is equivalent to simply using step differencing in the first angular cell. A much more accurate treatment is to include an equation for the $\psi_{\frac{1}{2}}$, which corresponds to $mu = -1$. It is important to remember that to obtain such an equation, we first express the transport equation in the non-conservative form:

$$\mu\frac{\partial\psi}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial\psi}{\partial\mu} + \sigma_t\psi = 2\pi\int_{-1}^{+1}\sigma_s(\mu'\to\mu)\psi(\mu')\,d\mu' + Q\,. \tag{23}$$

Evaluating Eq. (24) at $\mu = 1$ and assuming that $\frac{\partial\psi}{\partial\mu}$ is bounded, we obtain the starting

direction flux equation:

$$-\frac{\partial \psi}{\partial r} + \sigma_t \psi = 2\pi \int_{-1}^{+1} \sigma_s(\mu' \to \mu)\psi(\mu')\, d\mu' + Q\,. \tag{24}$$

Note that this is actually the *slab* geometry equation. It is important to note that the starting direction flux is not part of the quadrature set, i.e., it has no weight. This flux satisfies the slab geometry equation because it is assumed to have a bounded angular derivative. This precludes a delta-function angular dependence. Problems with angular delta-function sources or incident fluxes along $\mu- = 1$ cannot be directly solved using the S_n method. The uncollided singular components of such solutions should be specially treated, and the S_n method used only to compute the collided flux component.

A more accurate definition for the cell-edge angular fluxes arises from the observation that standard S_n quadrature points do not lie at the center of the angular cells. Thus we use the relationship between the quadrature cosines and the edge cosines to relate the cell-center and cell-edge angular fluxes:

$$\psi_m = \frac{1+\alpha_m}{2}\psi_{m-\frac{1}{2}} + \frac{1+\alpha_m}{2}\psi_{m+\frac{1}{2}}\,, \quad m = 1, M, \tag{25}$$

where

$$\mu_m = \frac{1+\alpha_m}{2}\mu_{m-\frac{1}{2}} + \frac{1+\alpha_m}{2} m u_{m+\frac{1}{2}}\,, \quad m = 1, M, \tag{26}$$

or equivalently,

$$\alpha_m = \frac{2\mu_m - (\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}})}{\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}}}\,, \quad m = 1, M. \tag{27}$$

This "weighted-diamond" scheme also requires the starting direction flux to close the equations. It is the preferred scheme because it has a significant advantage over the step and diamond schemes in the diffusion limit. This will be discussed in a later lecture.

3 Spatial Discretization

In this section, we spatially discretize the S_n equations using the diamond-difference approximation. We begin by exactly integrating Eq. (17) over the spherical volume associated with the interval $[r_{i-\frac{1}{2}}, r_{i+\frac{1}{2}}]$:

$$\mu_m \left(A_{i+\frac{1}{2}} \psi_{i+\frac{1}{2},m} - A_{i-\frac{1}{2}} \psi_{i-\frac{1}{2},m} \right) + \frac{\Delta A_i}{2} \left(\frac{\beta_{m+\frac{1}{2}} \psi_{i,m+\frac{1}{2}} - \beta_{m+\frac{1}{2}} \psi_{i,m-\frac{1}{2}}}{w_m} \right) + \sigma_t \psi_{i,m} V_i =$$

$$\sum_{k=0}^{L} \frac{2k+1}{4\pi} \left(\sigma_k \phi_{i,k} + q_{i,k} \right) V_i \, P_k(\mu_m) \, , \tag{28}$$

where

$$A_{i\pm\frac{1}{2}} = 4\pi r_{i\pm\frac{1}{2}}^2 \, , \tag{29a}$$

$$\Delta A_i = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} \, , \tag{29b}$$

$$V_i = \frac{4\pi}{3} \left(r_{i+\frac{1}{2}}^3 - r_{i-\frac{1}{2}}^3 \right) \, , \tag{29c}$$

$$\psi_{i,m+\frac{1}{2}} = \frac{4\pi}{\Delta A_i} \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} r \psi_{m+\frac{1}{2}} \, dr \, , \tag{29d}$$

$$\psi_{i,m} = \frac{4\pi}{V_i} \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} r^2 \psi_{m+\frac{1}{2}} \, dr \, , \tag{29e}$$

$$\phi_{i,k} = \frac{4\pi}{V_i} \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} r^2 \phi_k \, dr \,, \tag{29f}$$

$$q_{i,k} = \frac{4\pi}{V_i} \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} r^2 q_k \, dr \,. \tag{29g}$$

Next we exactly integrate the starting direction flux equation over the interval, $[r_{i-\frac{1}{2}}, r_{i+\frac{1}{2}}]$:

$$-\psi_{i+\frac{1}{2},\frac{1}{2}} - \psi_{i-\frac{1}{2},\frac{1}{2}} + \sigma_t \psi^*_{i,\frac{1}{2}} \Delta r_i =$$

$$\sum_{k=0}^{L} \frac{2k+1}{4\pi} \left(\sigma_k \phi^*_{i,k} + q^*_{i,k} \right) \Delta r_i \, P_k(\mu_m) \,, \tag{30}$$

where

$$\Delta r_i = r_{i+\frac{1}{2}} - r_{i-\frac{1}{2}} \,, \tag{31a}$$

$$\psi^*_{i,m} = \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} \psi_{\frac{1}{2}} \, dr \,, \tag{31b}$$

$$\phi^*_{i,k} = \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} \phi_{i,k} \, dr \,, \tag{31c}$$

$$q^*_{i,k} = \int_{r_{i-\frac{1}{2}}}^{r_{i+\frac{1}{2}}} \phi_{i,k} \, dr \,. \tag{31d}$$

Note that no spatial approximations have been made at this point, but our equations are not closed. To do this, we must relate the spatial cell-edge fluxes to the various types of cell-centered fluxes. To do this, we use the diamond difference relationship:

$$\psi_{i,m\pm\frac{1}{2}} = (\psi_{i+\frac{1}{2},m\pm\frac{1}{2}} + \psi_{i-\frac{1}{2},m\pm\frac{1}{2}})/2 \,, \tag{32a}$$

$$\psi_{i,m} = (\psi_{i+\frac{1}{2},m} + \psi_{i-\frac{1}{2},m})/2 \,. \tag{32b}$$

$$\phi_{i,k} = (\phi_{i+\frac{1}{2},k} + \phi_{i-\frac{1}{2},k})/2\,. \tag{32c}$$

$$\psi^*_{i,\frac{1}{2}} = (\psi_{i+\frac{1}{2},\frac{1}{2}} + \psi_{i-\frac{1}{2},\frac{1}{2}})/2\,, \tag{32d}$$

$$\phi^*_{i,k} = (\phi_{i+\frac{1}{2},k} + \phi_{i-\frac{1}{2},k})/2\,. \tag{32e}$$

Equations (32a) through (32e) close the system of S_n equations. Other discretizations such as step and the discontinuous finite-element method can be used, but do not discuss these in detail here.