Lecture 10

Numerical Solution of the Diffusion Equation

The purpose of this lecture is to discuss the methods required to write a 1-D slab diffusion code. The equation to be solved is:

$$-\frac{d}{dx} D \, \frac{d\phi}{dx} + \sigma_a \, \phi = q \, . \tag{1}$$

The spatial grid on which we solve Eq. (1) has edge coordinates $\{x_{i-1/2}\}_{i=0}^{N}$, where

$$x_{1/2} = 0 \, , \quad x_{i+1/2} = x_{i-1/2} + h_i \quad , i = 1, N, \tag{2}$$

and center coordinates, $\{x_i\}_{i=1}^{N}$, where

$$x_i = \frac{1}{2}(x_{i-1/2} + x_{i+1/2}) \, . \tag{3}$$

A grid is illustrated in Fig. 1. There is a unique absorption and scattering cross section associated with each cell, $\{\sigma_{a,i}\}_{i=1}^{N}$ and $\{\sigma_{t,i}\}_{i=1}^{N}$, respectively. These may vary between cells, but are constant within each cell. Finally, there is an isotropic inhomogeneous source associated with each cell, $\{Q_i\}_{i=1}^{N}$. These may vary between cells, but are constant within

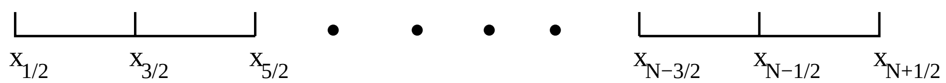

Figure 1: Grid indexing.

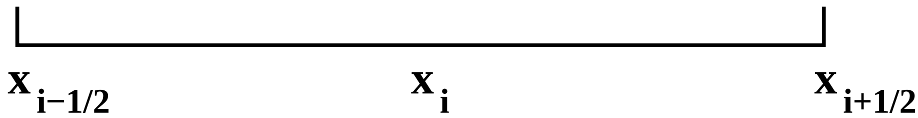

Figure 2: A single cell.

each cell. The scalar fluxes are located at both cell center and cell edge, but the cell edge fluxes will eventually be eliminated. The currents are located at cell faces.

To derive our difference equations, we first consider a single cell, which is illustated in Fig. 2. We first rewrite Eq. (1) in first-order form:

$$\frac{\partial J}{\partial x} + \sigma_a \phi = Q \,, \tag{4a}$$

$$J = -\frac{1}{3\sigma_t}\,\frac{\partial \phi}{\partial x} \,. \tag{4b}$$

Equation (4a) is rigorously integrated over the cell:

$$J_{i+1/2} - J_{i-1/2} + \sigma_{a,i} h_i \phi_i = q_i h_i \,. \tag{5}$$

Care must be taken in differencing Eq. (4b). We first consider cell interfaces on the mesh interior. It seems natural to take a difference between the scalar fluxes in cells x_i and x_{i+1} to compute a current at $x_{i+1/2}$. This is perfectly reasonable if cells i and $i+1$ have the same diffusion coefficient. However, we allow the diffusion coefficient to differ between cells. In this case, the derivative of the flux is discontinuous at the cell interface, so one cannot take a difference across that interface. This is the reason for the cell edge scalar fluxes. Instead, we use the cell-edge scalar flux and the adjacent cell center scalar fluxes to compute separate fluxes on each side of the interface, i.e.,

$$J_{i+\frac{1}{2},i} = -\frac{2D_i}{h_i}\left(\phi_{i+\frac{1}{2}} - \phi_i\right) , \tag{6a}$$

$$J_{i+\frac{1}{2},i+1} = -\frac{2D_{i+1}}{h_{i+1}}\left(\phi_{i+1} - \phi_{i+\frac{1}{2}}\right) , \tag{6b}$$

where $J_{i+\frac{1}{2},k}$ denotes the current associated with interface $i+\frac{1}{2}$ and cell k. The interface conditions for the 1-D diffusion equation state that the scalar flux and current must be continuous. The former condition is automatically met by having one scalar flux at each interface, but we must enforce the latter condition since there are two currents at each interface. The continuity-of-current condition provides the equation for the cell-edge fluxes, i.e., the equation for $\phi_{i+\frac{1}{2}}$ is

$$-\frac{2D_i}{h_i}\left(\phi_{i+\frac{1}{2}} - \phi_i\right) = -\frac{2D_{i+1}}{h_{i+1}}\left(\phi_{i+1} - \phi_{i+\frac{1}{2}}\right) . \tag{7}$$

Solving for the cell-edge scalar flux in Eq. (7), we get

$$\phi_{i+1/2} = \frac{\sigma_{i+1}h_{i+1}\phi_i + \sigma_i h_i \phi_{i+1}}{\sigma_{i+1}h_{i+1} + \sigma_i h_i} . \tag{8}$$

Note that $\phi_{i+\frac{1}{2}}$ is a weighted-average of ϕ_i and ϕ_{i+1} that favors the flux in the most optically-thin cell, i.e., the cell whose thickness is smallest in total mean-free-paths. Substituting from Eq. (8) into either Eq. (6a) or Eq. (6b), we get

$$J_{i+1/2} = -\frac{D_{i+1/2}}{h_{i+1/2}}\ \left(\phi_{i+1} - \phi_i\right) , \tag{9}$$

where

$$D_{i+1/2} = \left[\frac{\frac{h_i}{D_i} + \frac{h_{i+1}}{D_{i+1}}}{h_i + h_{i+1}}\right]^{-1}, \tag{10a}$$
$$= \frac{h_i + h_{i+1}}{3(\sigma_{t,i}h_i + \sigma_{t,i+1}h_{i+1})},$$

and

$$h_{i+1/2} = \frac{h_i + h_{i+1}}{2}. \tag{10b}$$

Note that Eq. (9) indicates that a difference *can* be taken across a material discontinutity if the diffusion coefficient is *properly averaged.* It can be seen from Eq. (10a) that the correct average is a weighted harmonic average. If this average is not used, the solution will not converge as the mesh is refined. A discontinuity in diffusion coefficient is not to be confused with a continuous variation in the diffusion coefficient. In the latter case one may average coefficients as desired and still retain convergence as the mesh is refined. Substituting from Eq. (9) into Eq. (5), we obtain the standard 3-point cell-centered diffusion operator:

$$-\frac{D_{i+1/2}}{h_{i+1/2}}\,(\phi_{i+1} - \phi_i) + \frac{D_{i-1/2}}{h_{i-1/2}}\,(\phi_i - \phi_{i-1}) + \sigma_{a,i}h_i\phi_i = q_i h_i\,. \tag{10c}$$

Equation (10c) applies for all interior cells. We next consider the boundary currents. To obtain initial equations for $J_{\frac{1}{2}}$ and $J_{N+\frac{1}{2}}$, we first apply the Marshak conditions. In particular, assuming an incident flux at the left boundary, $f_L(\mu)$, and using the extrapolation form of the Marshak boundary condition, we get

$$\phi_{\frac{1}{2}} + 2J_{\frac{1}{2}} = \phi_L^b\,, \tag{11}$$

where ϕ_L^b is the effective scalar flux on the left boundary arising from the incident flux, i.e.,

$$\phi_L^b = 4j^+ = 8\pi \int_0^1 \mu f_L(\mu)\, d\mu \,. \tag{12}$$

Proceeding similarly for the right face, we get

$$\phi_{N+\frac{1}{2}} - 2J_{N+\frac{1}{2}} = \phi_R^b \,, \tag{13}$$

where ϕ_R^b is the effective scalar flux on the right boundary arising from the incident flux, $f_R(\mu)$, i.e.,

$$\phi_R^b = 4j^- = -8\pi \int_{-1}^0 \mu f_R(\mu)\, d\mu \,. \tag{14}$$

Solving Eqs. (11) and (13) for $J_{\frac{1}{2}}$ and $J_{N+\frac{1}{2}}$, respectively, we get

$$J_{\frac{1}{2}} = \frac{1}{2}\left(\phi_L^b - \phi_{\frac{1}{2}}\right) \,, \tag{15}$$

and

$$J_{N+\frac{1}{2}} = \frac{1}{2}\left(\phi_{N+\frac{1}{2}} - \phi_R^b\right) \,. \tag{16}$$

To get equations for $\phi_{\frac{1}{2}}$ and $\phi_{N+\frac{1}{2}}$, we again impose a form of current continuity by requiring that the expressions for the boundary currents from the Marshak condition equal the expressions for the boundary currents from Fick's law:

$$\frac{1}{2}\left(\phi_L^b - \phi_{\frac{1}{2}}\right) = -\frac{2D_1}{h_1}\left(\phi_1 - \phi_{\frac{1}{2}}\right) \,, \tag{17}$$

$$\frac{1}{2}\left(\phi_{N+\frac{1}{2}} - \phi_R^b\right) = -\frac{2D_N}{h_N}\left(\phi_{N+\frac{1}{2}} - \phi_N\right) \,, \tag{18}$$

Solving for $\phi_{\frac{1}{2}}$ and $\phi_{N+\frac{1}{2}}$, respectively, we get

$$\phi_{1/2} = \frac{\left(\phi_L^b + 4\frac{D_1}{h_1}\phi_1\right)}{\left(1 + \frac{4D_1}{h_1}\right)} \,, \tag{19}$$

and

$$\phi_{N+1/2} = \frac{\left(\phi_R^b + 4\frac{D_N}{h_N}\phi_N\right)}{\left(1 + \frac{4D_N}{h_N}\right)} \,. \tag{20}$$

Note from Eqs. (19) and (20) that the scalar flux on the boundary is a weighted average of the effective incident scalar flux and the center flux in the boundary cell. Substituting from Eqs. (19) and (20) into Eqs. (15) and (16), respectively, we get the final expressions for the boundary currents:

$$J_{1/2} = \frac{-2D_1}{h_1 + 4D_1}\left(\phi_1 - \phi_L^b\right) \,, \tag{21}$$

and

$$J_{N+1/2} = \frac{2D_N}{h_N + 4D_N}\left(\phi_N - \phi_R^b\right) \,. \tag{22}$$

Using Eqs. (21), (9), and (5), we obtain the equation for the first cell:

$$-\frac{D_{3/2}}{h_{3/2}}(\phi_2 - \phi_1) + \left(\frac{2D_1}{h_1 + 4D_1}\right)\phi_1 + \sigma_{a,1}h_1\phi_1 = q_1 h_1 + \left(\frac{2D_1}{h_1 + 4D_1}\right)\phi_L^b \,. \tag{23}$$

Using Eqs. (22), (9), and (5), we obtain the equation for the last cell:

$$\left(\frac{2D_N}{h_N + 4D_N}\right)\phi_N + \frac{D_{N-1/2}}{h_{N-1/2}}(\phi_N - \phi_{N-1}) + \sigma_{a,N}h_N\phi_N = q_N h_N + \left(\frac{2D_N}{h_N + 4D_N}\right)\phi_R^b \,. \tag{24}$$

This completes the derivation of the difference equations. Note that the diffusion matrix is tridiagonal and symmetric positive definite.