Lecture 13
Discretization of the Diffusion Equation

The purpose of this lecture is to discuss the finite-difference and finite-element methods for discretizing the diffusion equation. The equation to be solved is:

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

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

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

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

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

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

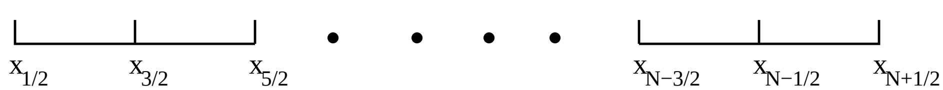

Figure 1: Grid indexing.

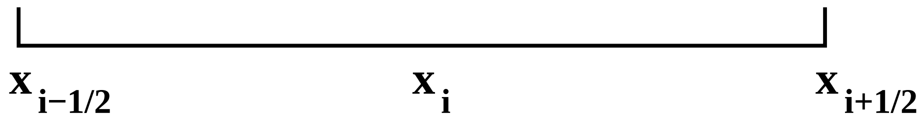

Figure 2: A single cell.

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.

1 The Cell-Centered Finite-Difference Method

We first consider the classic cell-centered finite-difference method, which is conservative over each spatial cell. To derive the cell-centered difference equations, we first consider a single cell, which is illustated in Fig. 2, and 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

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

where

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

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:

$$-\frac{D_{3/2}}{h_{3/2}}(\phi_2 - \phi_1) + \left(\frac{2D_1}{h_1 + 4D_1}\right)\phi_1 + \sigma_{a,1}h_1\phi_1 = q_1h_1 + \left(\frac{2D_1}{h_1 + 4D_1}\right)\phi_L^b . \tag{23}$$

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

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

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

2 The Linear-Continuous Finite-Element Method

We next consider the linear-continuous finite-element method. Using the same grid notation and cross-section assumptions used in the previous section, we define piecewise-linear vertex-centered basis functions as follows:

$$\begin{aligned}
B_{\frac{1}{2}}(x) &= \frac{x_{\frac{3}{2}} - x}{x_{\frac{3}{2}} - x_{\frac{1}{2}}}\,, \quad x \in [x_{\frac{1}{2}}, x_{\frac{3}{2}}], \\
&= 0\,, \text{otherwise}, && \text{(25a)} \\
B_{i+\frac{1}{2}}(x) &= \frac{x - x_{i-\frac{1}{2}}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}}\,, \quad x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \\
&= \frac{x_{i+\frac{3}{2}} - x}{x_{i+\frac{3}{2}} - x_{i+\frac{1}{2}}}\,, \quad x \in [x_{i+\frac{1}{2}}, x_{i+\frac{3}{2}}], \\
&= 0\,, \text{otherwise}, \quad i = 1, N-1, && \text{(25b)} \\
B_{N+\frac{1}{2}}(x) &= \frac{x - x_{N-\frac{1}{2}}}{x_{N+\frac{1}{2}} - x_{N-\frac{1}{2}}}\,, \quad x \in [x_{N-\frac{1}{2}}, x_{N+\frac{1}{2}}], \\
&= 0\,, \text{otherwise}. && \text{(25c)}
\end{aligned}$$

These basis functions are interpolatory, i.e., $B_{i+\frac{1}{2}}(x) = 1$ at $x = x_{i+\frac{1}{2}}$ and is zero at all other vertices. Thus the trial-space solution takes the following form:

$$\tilde{\phi}(x) = \sum_{i=0}^{N} \phi_{i+\frac{1}{2}} B_{i+\frac{1}{2}}(x)\,, \tag{26}$$

where

$$\phi_{i+\frac{1}{2}} = \tilde{\phi}(x_{i+\frac{1}{2}})\,. \tag{27}$$

The linear-continuous method is a Galerkin method. Thus the equation for $\phi_{i+\frac{1}{2}}$ is obtained by substituting from Eq. (26) into Eq. (1), multiplying that equation by $B_{i+\frac{1}{2}}(x)$, and integrating that equation over the entire spatial domain. An integration by parts is performed to deal with the delta-function second derivatives of the basis functions:

$$-\Big|_{x_{\frac{1}{2}}}^{x_{N+\frac{1}{2}}} B_{i+\frac{1}{2}} D\frac{d\tilde{\phi}}{dx} + \int_{x_{\frac{1}{2}}}^{x_{N+\frac{1}{2}}} D\frac{d\tilde{\phi}}{dx}\frac{dB_{i+\frac{1}{2}}}{dx}\,dx + \int_{x_{\frac{1}{2}}}^{x_{N+\frac{1}{2}}} B_{i+\frac{1}{2}}\sigma\tilde{\phi}\,dx = \int_{x_{\frac{1}{2}}}^{x_{N+\frac{1}{2}}} B_{i+\frac{1}{2}} q\,dx\,. \tag{28}$$

Assuming that q is expanded in the vertex basis functions, we obtain the following equation for interior-mesh vertices:

$$\begin{gathered} -\frac{D_{i+1}}{h_{i+1}}\left(\phi_{i+\frac{3}{2}} - \phi_{i+\frac{1}{2}}\right) + \frac{D_i}{h_i}\left(\phi_{i+\frac{1}{2}} - \phi_{i-\frac{1}{2}}\right) + \\ \sigma_{a,i+1}\left(\frac{1}{3}\phi_{i+\frac{3}{2}} + \frac{2}{3}\phi_{i+\frac{1}{2}}\right)\frac{h_{i+1}}{2} + \sigma_{a,i}\left(\frac{2}{3}\phi_{i+\frac{1}{2}} + \frac{1}{3}\phi_{i-\frac{1}{2}}\right)\frac{h_i}{2} = \\ \left(\frac{1}{3}q_{i+\frac{3}{2}} + \frac{2}{3}q_{i+\frac{1}{2}}\right)\frac{h_{i+1}}{2}\left(\frac{2}{3}q_{i+\frac{1}{2}} + \frac{1}{3}q_{i-\frac{1}{2}}\right)\frac{h_i}{2} \qquad i = 1, N-1. \end{gathered} \tag{29}$$

Note that this equation represents a pseudo-balance equation for the median mesh cell centered about $x_{i+\frac{1}{2}}$ with faces at x_i and x_{i+1} respectively. Since the currents are evaluated at cell centers, differences are never taken across material discontinuities and there is no averaging of diffusion coefficients. This makes the linear-continuous finite-element method much simpler than the cell-centered finite-difference method. The equations for the first and last vertex fluxes are respectively,

$$-\frac{D_1}{h_1}\left(\phi_{\frac{3}{2}} - \phi_{\frac{1}{2}}\right) - J_{\frac{1}{2}} + \sigma_{a,1}\left(\frac{1}{3}\phi_{\frac{3}{2}} + \frac{2}{3}\phi_{\frac{1}{2}}\right)\frac{h_1}{2} = \left(\frac{1}{3}q_{\frac{3}{2}} + \frac{2}{3}q_{\frac{1}{2}}\right)\frac{h_1}{2}\,, \tag{30}$$

and

$$J_{n+\frac{1}{2}} - \frac{D_N}{h_N}\left(\phi_{N+\frac{1}{2}} - \phi_{N-\frac{1}{2}}\right) + \sigma_{a,N}\left(\frac{2}{3}\phi_{N+\frac{1}{2}} + \frac{1}{3}\phi_{N-\frac{1}{2}}\right)\frac{h_N}{2} = \left(\frac{2}{3}q_{N+\frac{1}{2}} + \frac{1}{3}q_{N-\frac{1}{2}}\right)\frac{h_i}{2}\,, \tag{31}$$

where we have made the following respective interpretations:

$$-B_1 D\left.\frac{d\tilde{\phi}}{dx}\right|_{x_{\frac{1}{2}}} \rightarrow J_{\frac{1}{2}}\,, \tag{32}$$

$$-B_{N+\frac{1}{2}} D\left.\frac{d\tilde{\phi}}{dx}\right|_{x_{N+\frac{1}{2}}} \rightarrow J_{N+\frac{1}{2}}\,, \tag{33}$$

where $J_{\frac{1}{2}}$ and $J_{N+\frac{1}{2}}$ are determined by boundary conditions. This process is much easier than it is for the cell-centered finite-difference method. In particular, assuming source boundary conditions at the left and right faces, one directly obtains the following respective expressions from the Marshak boundary condition:

$$J_{\frac{1}{2}} = \frac{1}{2}\left(\phi_L^b - \phi_{\frac{1}{2}}\right)\,, \tag{34}$$

and

$$J_{N+\frac{1}{2}} = \frac{1}{2}\left(\phi_R^b - \phi_{N+\frac{1}{2}}\right) . \tag{35}$$

3 The Mixed-Hybrid Finite-Element Method

There is a class of finite-element methods that produces cell-centered-type discretizations rather than vertex-centered discretizations. These methods a actually applied to the diffusion equation in P_1 or first-order form:

$$\frac{dJ}{dx} + \sigma_a \phi = q \,, \tag{36a}$$

$$\frac{1}{3}\frac{d\phi}{dx} + \sigma_t J = 0 \,. \tag{36b}$$

These methods correspond to Galerkin methods. Furthermore, one applies the method on a single cell and then applies interface conditions to obtain the equations for the full mesh. The lowest-order trial space is defined as follows on the cell illustrated in Fig. 2:

$$\begin{aligned}
\tilde{\phi}(x) &= \phi_{i-\frac{1}{2}} \,, \quad x = x_{i-\frac{1}{2}}, \\
&= \phi_{i+\frac{1}{2}} \,, \quad x = x_{i+\frac{1}{2}}, \\
&= \phi_i \,, \quad x \in \left(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right), \qquad (37a) \\
\tilde{J}(x) &= J_{i-\frac{1}{2}}\, B_{i-\frac{1}{2}}(x) + J_{i+\frac{1}{2}}\, B_{i+\frac{1}{2}}(x) \,, \quad x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \qquad (37b)
\end{aligned}$$

where

$$
\begin{aligned}
B_{i-\frac{1}{2}}(x) &= \frac{x_{i+\frac{1}{2}} - x}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}}, \quad x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \\
B_{i+\frac{1}{2}}(x) &= \frac{x - x_{i-\frac{1}{2}}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}}, \quad x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}].
\end{aligned} \tag{38a}
$$

Thus the scalar flux is piecewise-constant with jumps at the left and right cell boundaries, while the current is simply piecewise-linear. The equation for ϕ_i is obtained by substituting from Eqs. (37a) through (37b) into Eq. (36a), multiplying Eq. (36a) by the basis function for $\tilde{\phi}$, and integrating that equation over the cell. The basis function for $\tilde{\phi}$ is just constant and equal to unity except for the jumps at the cell edges, which are of no consequence in Eq. (36a) because there are no derivatives of ϕ in that equation. Thus the equation we obtain for ϕ_i is just the balance equation:

$$
J_{i+\frac{1}{2}} - J_{i-\frac{1}{2}} + \sigma_{a,i}\phi_i h_i = q_i h_i \,, \tag{39}
$$

where q_i denotes the cell-averaged value of q. The equation for $J_{i-\frac{1}{2}}$ is obtained by substituting from Eqs. (37a) through (37b) into Eq. (36b), multiplying Eq. (36b) by $B_{i-\frac{1}{2}}$, and integrating over the cell. To accomodate the jumps in $\tilde{\phi}$ the gradient term is integrated by parts. The following equation is obtained:

$$
\frac{1}{3}\left(\phi_i - \phi_{i-\frac{1}{2}}\right) + \sigma_{t,i}\left(\frac{2}{3}J_{i-\frac{1}{2}} + \frac{1}{3}J_{i+\frac{1}{2}}\right)\frac{h_i}{2} = 0\,. \tag{40}
$$

Following an analogous procedure to obtain the equation for $J_{i+\frac{1}{2}}$, we obtain:

$$\frac{1}{3}\left(\phi_{i+\frac{1}{2}} - \phi_i\right) + \sigma_{t,i}\left(\frac{1}{3}J_{i-\frac{1}{2}} + \frac{2}{3}J_{i+\frac{1}{2}}\right)\frac{h_i}{2} = 0\,. \tag{41}$$

Equations (40) and (41) are more accurate but more complicated than those corresponding to the cell-centered finite-difference method. However, if we lump the current equations, i.e., use a two-point trapezoidal quadrature rule to perform the integrations, we obtain the current equations of the cell-centered finite-difference method, Eqs. (6a) and (6b). The full equations actually result in a dense diffusion matrix if the cell-edge scalar fluxes are algebraically eliminated from the system. Alternatively, one can eliminate only the currents, leaving a symmetric positive-definite system containing both cell-center and cell-edge scalar fluxes.