Diffusion Derivation for Arbitrary Order DFEM with Spatially Varying Cross Section

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1 Diffusion Equations

We begin with the analytic transport equation (with isotropic scattering):

$$\mu \frac{d\psi}{dx} + \sigma_t \psi = \frac{\sigma_s}{2}\phi + q(x,\mu)\,.$$

Integrating over angle we have:

$$\frac{dJ}{dx} + \sigma_t \phi = \sigma_s \phi + Q(x)\,, \tag{1}$$

and we use the diffusion approximation for the current:

$$J(x) = -D(x)\frac{d\phi}{dx} \tag{2a}$$

$$D = \frac{1}{3\sigma_t}\,. \tag{2b}$$

We fill follow a path similar to the first derivation of Adams and Martin [1]. Spatially discretizing the analytic diffusion equation, rather than generating a diffusion equation from the spatially discretized transport equation.

2 Spatial Discretization

We spatially discretize our equations, expanding in a P degree polynomial, discontinuous finite element trial space. First, transforming to a generic reference element:

$$\begin{aligned} x &= x_i + \frac{\Delta x_i}{2} s \\ s &\in [-1,1] \\ \Delta x_i &= x_{i+1/2} - x_{i-1/2} \\ x_i &= \frac{x_{i+1/2} + x_{i-1/2}}{2} \end{aligned}$$

For generality, let $\widetilde{y}$ be approximate the analytic variables y:

$$y \approx \widetilde{y}(s) = \sum_{j=1}^{N_P} y_j B_j(s)\,,$$

where

$$B_j = \prod_{\substack{k=1 \\ k\neq j}}^{N_P} \frac{s_k - s}{s_k - s_j} \, ,$$

$N_P = P + 1$, and s_j is the interpolation point corresponding to basis function B_j. Multiplying Eq. (1) by basis function B_i and integrating within a reference cell, we have:

$$\int_{-1}^{1} B_i(s) \left[\frac{d\widetilde{J}(s)}{ds} + \sigma_a(s) \frac{\Delta x_k}{2} \widetilde{\phi}(s) \right] ds = \frac{\Delta x_k}{2} \int_{-1}^{1} B_i(s) Q(s) \; ds \tag{3}$$

We handle the derivative terms of Eqs. (3) by integrating by parts, to yield:

$$B_i(1)\widehat{J}_{k+1/2} - B_i(-1)\widehat{J}_{k-1/2} - \int_{-1}^{1} \frac{dB_i(s)}{ds} \widetilde{J}(s) \; ds \\ + \frac{\Delta x_k}{2} \int_{-1}^{1} B_i(s)\sigma_a(s)\widetilde{\phi}(s) ds = \frac{\Delta x_k}{2} \int_{-1}^{1} B_i(s) Q(s) \; ds \tag{4}$$

where $\widehat{J}_{k\pm1/2}$ is the net current in the $+x$ direction at $x_{k\pm1/2}$. With DFEM, we need to uniquely define the vertex current, and do so using the P_1 approximation. By definition of the upwinding scheme used in the transport scheme, the P_1 approximation to the angular flux at $x_{k-1/2}$ is:

$$\widetilde{\psi}(x_{k-1/2}, \mu) = \begin{cases} \frac{\widetilde{\phi}_{k-1,R}}{2} + \frac{3\mu}{2} \widetilde{J}_{k-1,R} & \mu > 0 \\ \frac{\widetilde{\phi}_{k,L}}{2} + \frac{3\mu}{2} \widetilde{J}_{k,L} & \mu < 0 \end{cases} . \tag{5}$$

In Eq. (5), $\widetilde{\phi}_{k-1,R}$ and $\widetilde{J}_{k-1,R}$ are:

$$\widetilde{\phi}_{k-1,R} = \sum_{j=1}^{N_P} B_j(1)\phi_{k-1,j} \tag{6a}$$

$$\widetilde{J}_{k-1,R} = -D_{k-1}(x_{k-1/2})\frac{d\phi}{dx} = -\frac{2D_{k-1}(1)}{\Delta x_{k-1}} \frac{d\phi}{ds} = -\frac{2D_{k-1}(1)}{\Delta x_{k-1}} \sum_{j=1}^{N_P} \left. \frac{dB_j}{ds} \right|_{s=1} \phi_{k-1,j} \, , \tag{6b}$$

with $\widetilde{\phi}_{k,L}$ and $\widetilde{J}_{k,L}$ being defined as:

$$\widetilde{\phi}_{k,L} = \sum_{j=1}^{N_P} B_j(-1)\phi_{k,j} \tag{7a}$$

$$\widetilde{J}_{k,L} = -\frac{2D(-1)}{\Delta x_k} \sum_{j=1}^{N_P} \left. \frac{dB_j}{ds} \right|_{s=-1} \phi_{k,j} \, . \tag{7b}$$

The $\frac{2}{\Delta x}$ terms appear in the $\widetilde{J}$ definitions of Eq. (6) and Eq. (7) as a result of the change of variables from physical to reference coordinates. Using the definitions of Eq. (5), we can now define $\widehat{J}_{k-1/2}$. We will integrate with the same angular quadrature used in our S_N scheme.

$$\widehat{J}_{k-1/2} = \int_{-1}^{1} \mu\psi(x_{k-1/2}, \mu) \; d\mu \approx \\ \sum_{\substack{d=1 \\ \mu_d>0}}^{N_{dir}} w_d\mu_d \left[\frac{\widetilde{\phi}_{k-1,R}}{2} + \frac{3\mu_d}{2} \widetilde{J}_{k-1,R} \right] + \sum_{\substack{d=1 \\ \mu_d<0}}^{N_{dir}} w_d\mu_d \left[\frac{\widetilde{\phi}_{k,L}}{2} + \frac{3\mu_d}{2} \widetilde{J}_{k,L} \right] \tag{8}$$

Since we are integrating half range quantities, symmetric quadrature sets defined for $\mu \in [-1,1]$ will not exactly integrate functions over the intervals $\mu \in [-1,0]$ and $\mu \in [0,1]$. Thus, we introduce α:

$$\alpha = \sum_{\substack{d=1 \\ \mu_d > 0}}^{N_{dir}} w_d \mu_d \approx \frac{1}{2} \,. \tag{9}$$

In general, symmetric quadrature sets will integrate even functions of μ exactly over the half range, so we do not need to introduce a quadrature approximation for this. We further assume that $\sum_{d=1}^{N_{dir}} w_d = 2$. Performing the quadrature integration of Eq. (8) we have

$$\widehat{J}_{k-1/2} = \alpha \frac{\widetilde{\phi}_{k-1,R}}{2} + \frac{\widetilde{J}_{k-1,R}}{2} - \alpha \frac{\widetilde{\phi}_{k,L}}{2} + \frac{\widetilde{J}_{k,L}}{2} \tag{10}$$

and using Eq. (6) and Eq. (7), we have:

$$\begin{aligned} \widehat{J}_{k-1/2} = \frac{\alpha}{2} \left[\sum_{j=1}^{N_P} B_j(1) \phi_{k-1,j} \right] + \frac{1}{2} \left[-\frac{2 D_{k-1}(1)}{\Delta x_{k-1}} \sum_{j=1}^{N_P} \left. \frac{dB_j}{ds} \right|_{s=1} \phi_{k-1,j} \right] \\ - \frac{\alpha}{2} \left[\sum_{j=1}^{N_P} B_j(-1) \phi_{k,j} \right] + \frac{1}{2} \left[-\frac{2 D_k(-1)}{\Delta x_k} \sum_{j=1}^{N_P} \left. \frac{dB_j}{ds} \right|_{s=-1} \phi_{k,j} \right] . \end{aligned} \tag{11}$$

When simplified (slightly), this becomes:

$$\widehat{J}_{k-1/2} = \frac{1}{2} \sum_{j=1}^{N_P} \left[\alpha B_j(1) - \frac{2}{\Delta x_{k-1}} D_{k-1} \left. \frac{dB_j}{ds} \right|_{s=1} \right] \phi_{k-1,j} - \frac{1}{2} \sum_{j=1}^{N_P} \left[\alpha B_j(-1) + \frac{2}{\Delta x_k} D_k(-1) \left. \frac{dB_j}{ds} \right|_{s=-1} \right] \phi_{k,j} \,. \tag{12}$$

Analogously, the equation for $\widehat{J}_{k+1/2}$ is:

$$\widehat{J}_{k+1/2} = \frac{1}{2} \sum_{j=1}^{N_P} \left[\alpha B_j(1) - \frac{2}{\Delta x_k} D_k \left. \frac{dB_j}{ds} \right|_{s=1} \right] \phi_{k,j} - \frac{1}{2} \sum_{j=1}^{N_P} \left[\alpha B_j(-1) + \frac{2}{\Delta x_{k+1}} D_{k+1}(-1) \left. \frac{dB_j}{ds} \right|_{s=-1} \right] \phi_{k+1,j} \,. \tag{13}$$

If we consider the N_P moments of Eq. (4) at once, we have the following $N_P \times N_P$ system of equations:

$$\left[\mathbf{S}_+ \left(\mathbf{J}_{L,k+1} \vec{\phi}_{k+1} + \mathbf{J}_{R,k} \vec{\phi}_k \right) - \mathbf{S}_- \left(\mathbf{J}_{L,k} \vec{\phi}_k + \mathbf{J}_{R,k-1} \vec{\phi}_{k-1} \right) \right] + \mathbf{L} \vec{\phi}_k + \widehat{\mathbf{M}}_{\sigma_a} \vec{\phi}_k = \mathbf{M} \vec{Q} \,, \tag{14}$$

where we make the following definitions:

$$\mathbf{J}_{L,k,1 \ldots N_P,j} = -\frac{1}{2} \left[\frac{2}{\Delta x_k} D_k(-1) \left. \frac{dB_j}{ds} \right|_{s=-1} + \alpha B_j(-1) \right] \tag{15}$$

$$\mathbf{J}_{R,k,1 \ldots N_P,j} = \frac{1}{2} \left[\alpha B_j(1) - \frac{2}{\Delta x_k} D_k(1) \left. \frac{dB_j}{ds} \right|_{s=1} \right] \tag{16}$$

$$\mathbf{S}_{\pm,ij} = \begin{cases} B_i(\pm 1) & i = j \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

$$\mathbf{L}_{ij} = \frac{2}{\Delta x_k} \int_{-1}^{1} D_k(s) \frac{dB_i}{ds} \frac{dBj}{ds} \; ds \tag{18}$$

$$\vec{\phi}_k = \begin{bmatrix} \phi_{1,k} \\ \vdots \\ \phi_{N_P,k} \end{bmatrix}, \tag{19}$$

$$\widehat{\mathbf{M}}_{\sigma_a,ij} = \frac{\Delta x}{2} \int_{-1}^{1} \sigma_a(s) B_i(s) B_j(s) \; ds \,, \tag{20}$$

$$\mathbf{M}_{ij} = \frac{\Delta x}{2} \int_{-1}^{1} B_i(s) B_j(s) \; ds \,, \tag{21}$$

$$\vec{Q} = \begin{bmatrix} Q_{1,k} \\ \vdots \\ Q_{N_P,k} \end{bmatrix}. \tag{22}$$

In practice, we will approximate the $\mathbf{L}$, $\widehat{\mathbf{M}}$, and $\mathbf{M}$ matrices using numerical quadrature:

$$\begin{aligned}
\mathbf{M}_{ij} &\approx \frac{\Delta x_k}{2} \sum_{q=1}^{N_q} w_q B_i(s_q) B_j(s_q) \\
\widehat{\mathbf{M}}_{\sigma_a,ij} &\approx \frac{\Delta x_k}{2} \sum_{q=1}^{N_q} w_q \sigma_a(s_q) B_i(s_q) B_j(s_q) \\
\mathbf{L}_{ij} &\approx \frac{1}{\Delta x_k} \sum_{q=1}^{N_q} w_q D_k(s_q) \left.\frac{dB_i}{ds}\right|_{s_q} \left.\frac{dB_j}{ds}\right|_{s_q}
\end{aligned}$$

If we use numerical quadrature restricted to the DFEM interpolation points, $\mathbf{M}$ and $\widehat{\mathbf{M}}_{\sigma_a}$ become diagonal matrices since,

$$B_i(s_q) = \begin{cases} 1 & s_i = s_q \\ 0 & \text{otherwise} \end{cases}. \tag{23}$$

Using self-lumping quadrature, $\mathbf{M}$ and $\widehat{\mathbf{M}}_{\sigma_a}$ are:

$$\mathbf{M}_{ij} = \begin{cases} w_i & i = j \\ 0 & \text{otherwise} \end{cases} \tag{24}$$

$$\widehat{\mathbf{M}}_{ij,\sigma_a} = \begin{cases} w_i \sigma_a(s_i) & i = j \\ 0 & \text{otherwise} \end{cases}. \tag{25}$$

3 Boundary Conditions

We'll now consider the boundary conditions for our DSA equations.

3.1 Vacuum (Incident Flux Transport BC)

For a fixed incident flux transport boundary condition, we do not wish to have any correction to the inward directed flux. Thus, on the left boundary, $\widehat{J}_{1/2}$ is:

$$\widehat{J}_{1/2} = \int_{-1}^{1} \mu\psi(x_{1/2},\mu)\, d\mu \approx 0 + \sum_{\substack{d=1 \\ \mu_d<0}}^{N_{dir}} w_d\mu_d \left[\frac{\widetilde{\phi}_1}{2} + \frac{3\mu_d\widetilde{J}_1}{2}\right] \tag{26}$$

$$\widehat{J}_{1/2} = -\frac{1}{2}\left[\sum_{j=1}^{N_P} \alpha B_j(-1)\phi_{1,j} + \frac{2D_1(-1)}{\Delta x}\sum_{j=1}^{N_P} \left.\frac{dB_j}{ds}\right|_{s=-1} \phi_{1,j}\,.\right] \tag{27}$$

This make the N_P moment equation in the leftmost cell:

$$\left[\mathbf{S}_+\left(\mathbf{J}_{L,2}\vec{\phi}_2 + \mathbf{J}_{R,1}\vec{\phi}_1\right) - \mathbf{S}_-\mathbf{J}_{L,1}\vec{\phi}_1\right] + \mathbf{L}\vec{\phi}_k + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_k = \mathbf{M}\vec{Q}\,. \tag{28}$$

Similarly on the rightmost cell, the moment equations become:

$$\left[\mathbf{S}_+\mathbf{J}_{R,N_{cell}}\vec{\phi}_{N_{cell}} - \mathbf{S}_-\left(\mathbf{J}_{L,N_{cell}}\vec{\phi}_{N_{cell}} + \mathbf{J}_{R,N_{cell}-1}\vec{\phi}_{N_{cell}-1}\right)\right] + \mathbf{L}\vec{\phi}_{N_{cell}} + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_{N_{cell}} = \mathbf{M}\vec{Q}\,. \tag{29}$$

3.2 Reflecting (Reflecting Transport BC)

For reflective transport boundary conditions, we need a reflective DSA boundary condition. This is implemented most clearly by setting $\widehat{J}_{1/2} = 0$, since everything that goes out of the slab is reflected back in, result in a net current of 0. The moment equation at the left most and right most cell are then:

$$\mathbf{S}_+\left(\mathbf{J}_{L,2}\vec{\phi}_2 + \mathbf{J}_{R,1}\vec{\phi}_1\right) + \mathbf{L}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_1 = \mathbf{M}\vec{Q}\,, \tag{30}$$

$$\mathbf{S}_-\left(\mathbf{J}_{L,N_{cell}}\vec{\phi}_{N_{cell}} + \mathbf{J}_{R,N_{cell}-1}\vec{\phi}_{N_{cell}-1}\right) + \mathbf{L}\vec{\phi}_{N_{cell}} + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_{N_{cell}} = \mathbf{M}\vec{Q}\,, \tag{31}$$

4 Alternative Use of Integration By Parts

$$B_i\left[\widehat{J}_{out} - \widehat{J}_{in}\right] \tag{32}$$

$$\left(B_i(1)J_{+,k,k+1/2} + B_i(-1)J_{-,k,k-1/2}\right) - \left(B_i(-1)J_{+,k-1,k-1/2} + B_i(1)J_{-,k+1,k-1/2}\right) \tag{33}$$

$$
\left(B_i(1) \sum_{\substack{d=1 \\ \mu_d>0}}^{N_{dir}} w_d\mu_d \sum_{j=1}^{N_P} \phi_{k,j} \left[\frac{B_j(1)}{2} - \frac{3\mu_d}{2} D_k(1) \frac{2}{\Delta x_k} \frac{dB_j}{ds}\bigg|_{s=1} \right] \right.
$$

$$
\left. + B_i(-1) \sum_{\substack{d=1 \\ \mu_d<0}}^{N_{dir}} w_d\mu_d \sum_{j=1}^{N_P} \phi_{k,j} \left[\frac{B_j(-1)}{2} - \frac{3\mu_d}{2} D_k(-1) \frac{2}{\Delta x_k} \frac{dB_i}{ds}\bigg|_{s=-1} \right] \right)
$$

$$
- \left(B_i(-1) \sum_{\substack{d=1 \\ \mu_d>0}}^{N_{dir}} w_d\mu_d \sum_{j=1}^{N_P} \phi_{k-1,j} \left[\frac{B_j(1)}{2} - \frac{3\mu_d}{2} \frac{\Delta x_{k-1}}{2} D_{k-1} \frac{dB_j}{ds}\bigg|_{s=1} \right] \right.
$$

$$
\left. + B_i(1) \sum_{\substack{d=1 \\ \mu_d<0}}^{N_{dir}} w_d\mu_d \sum_{j=1}^{N_P} \phi_{k+1,j} \left[\frac{B_j(-1)}{2} - \frac{2}{\Delta x_{k+1}} D_{k+1}(-1) \frac{dB_j}{ds}\bigg|_{s=-1} \right] \right) \tag{34}
$$

$$
\left(\mathbf{S}_+ \mathbf{J}_{R,k} \vec{\phi}_k + \mathbf{S}_- \mathbf{J}_{L,k} \vec{\phi}_k \right) - \left(\mathbf{S}_+ \mathbf{J}_{L,k+1} \vec{\phi}_{k+1} + \mathbf{S}_- \mathbf{J}_{R,k-1} \right) \vec{\phi}_{k-1} \tag{35}
$$

5 Stencil Size

The stencil of this DSA scheme will be dependent on the DFEM interpolation points selected. If there is not a DFEM interpolation point located at each cell vertex, the stencil increases significantly. This is caused by $\mathbf{S}_{\pm}$. If there is a DFEM interpolation point on each cell edge, then $\mathbf{S}_+ \mathbf{J}_{L,k+1} \vec{\phi}_{k+1}$ will result in a non-zero coefficient of only one $\phi_{k+1,j}$, $\phi_{k+1,1}$ in the N_P moment equation of $\vec{\phi}_k$. Assuming there is a DFEM interpolation point at each vertex, in matrix form, the N_P moment equations for $\vec{\phi}_k$ have $N_P \times N_P + 2$ non-zero entries. However, if there is no DFEM interpolation point at the cell edges, rather than coupling to 1 unknown of each neighboring cell, the moment equations of $\vec{\phi}$ are fully coupled to the neighboring cells, creating a $3(N_P \times N_P)$ diffusion equation stencil.

References

[1] M. L. Adams and W. R. Martin , "Diffusion Synthetic Acceleration of Discontinuous Finite Element Transport Iterations," *Nuclear Science and Engineering*, **111**, pp. 145-167 (1992).