Arbitrary Order DFEM Diffusion Discretization with Spatially Varying Cross Section Derived via the M4S Method

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1 Diffusion Equations

We begin with the analytic diffusion equation:

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

We will generate a set of DFEM diffusion equations following the first route proposed by Adams and Martin [1].

2 Spatial Discretization

We approximate the true scalar flux ϕ in each cell as a P degree polynomial, $\widetilde{\phi}$,

$$\phi(x) \approx \widetilde{\phi}(x) = \sum_{j=1}^{N_P} \phi_j B_j(x), \quad x \in \left[x_{k-1/2}, x_{k+1/2}\right], \tag{2}$$

where $N_P = P+1$, and

$$B_j(x) = \prod_{\substack{i=1 \\ i \neq j}}^{N_P} \frac{s_i - s}{s_i - s_j}\,.$$

To determine the N_P unknowns of $\widetilde{\phi}(x)$, ϕ_j, within each cell, we follow a Galarkin procedure, succesively multiplying Eq. (1) by basis functions $B_i(x)$, and integrating, generating N_P moment equations:

$$\int_{x_{k-1/2}}^{x_{k+1/2}} B_i(x) \left[\frac{dJ}{dx} + \sigma_a(x)\phi(x) = Q(x)\right] dx\,. \tag{3}$$

First, we transform to transforming to a generic reference element,

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

With this transformation, Eq. (3) becomes:

$$\int_{-1}^{1} B_i(s)\left[\frac{2}{\Delta x_k}\frac{dJ}{ds} + \sigma_a(s)\phi(s) = Q(s)\right]\frac{\Delta x_k}{2} ds\,. \tag{4}$$

Integrating the first term by parts, we have:

$$B_i(1)\widehat{J}_{k+1/2} - B_i(-1)\widehat{J}_{k-1/2} + \frac{2}{\Delta x_k}\int_{-1}^{1}\frac{dB_i}{ds}D(s)\frac{d\phi}{ds}\;ds + \frac{\Delta x_k}{2}\int_{-1}^{1}\sigma_a(s)B_i(s)\phi(s)\,, \tag{5}$$

where we have made the standard diffusion approximation:

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

within the cell, and $\widehat{J}_{k\pm1/2}$ denotes the vertex currents. However, with the DFEM spatial discretization, there is no unique value for the current at each cell edges. One possible solution is to use a P_1 approximation of the angular flux at each cell edge:

$$\psi(x_{k\pm1/2},\mu) \approx \frac{\phi(x_{k\pm1/2})}{2} + \frac{3\mu}{2}J(x_{k\pm1/2})\,,$$

for which the upwinding scheme used to define the angular flux at cell edges in the transport solution process is well defined. Looking specifically at $k-1/2$ vertex we have:

$$\widetilde{\psi}(x_{k-1/2},\mu) = \begin{cases} \frac{\widetilde{\phi}_{k-1,R}}{2} + \frac{3\mu}{2}\widetilde{J}_{k-1,R} & \mu > 0 \\ \frac{\widetilde{\phi}_{k,L}}{2} + \frac{3\mu}{2}\widetilde{J}_{k,L} & \mu < 0 \end{cases}\,. \tag{6}$$

With the definition of $\widetilde{\phi}(s)$given in Eq. (2) and the diffusion approximation, $\widetilde{\phi}_{k-1,R}$ and $\widetilde{J}_{k-1,R}$ become

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

$$\widetilde{J}_{k-1,R} = -D_{k-1}(x_{k-1/2})\frac{d\phi}{dx} = -\frac{2D_{k-1}(1)}{\Delta x_{k-1}}\frac{d\phi}{ds} = -\frac{2D_{k-1}(1)}{\Delta x_{k-1}}\sum_{j=1}^{N_P}\left.\frac{dB_j}{ds}\right|_{s=1}\phi_{k-1,j}\,, \tag{7b}$$

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

$$\widetilde{\phi}_{k,L} = \sum_{j=1}^{N_P} B_j(-1)\phi_{k,j} \tag{8a}$$

$$\widetilde{J}_{k,L} = -\frac{2D(-1)}{\Delta x_k}\sum_{j=1}^{N_P}\left.\frac{dB_j}{ds}\right|_{s=-1}\phi_{k,j}\,. \tag{8b}$$

The $\frac{2}{\Delta x}$ terms appear in the $\widetilde{J}$ definitions of Eq. (7) and Eq. (8) as a result of the change of variables from physical to reference coordinates. Using the definitions of Eq. (6), we can now define $\widehat{J}_{k-1/2}$. We will integrate with the same angular quadrature used in our S_N scheme.

$$\widehat{J}_{k-1/2} = \int_{-1}^{1}\mu\psi(x_{k-1/2},\mu)\;d\mu \approx \sum_{\substack{d=1\\ \mu_d>0}}^{N_{dir}} w_d\mu_d\left[\frac{\widetilde{\phi}_{k-1,R}}{2} + \frac{3\mu_d}{2}\widetilde{J}_{k-1,R}\right] + \sum_{\substack{d=1\\ \mu_d<0}}^{N_{dir}} w_d\mu_d\left[\frac{\widetilde{\phi}_{k,L}}{2} + \frac{3\mu_d}{2}\widetilde{J}_{k,L}\right] \tag{9}$$

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:

$$\alpha = \sum_{\substack{d=1 \\ \mu_d > 0}}^{N_{dir}} w_d \mu_d \approx \frac{1}{2}\,. \tag{10}$$

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. (9) we have

$$\widehat{J}_{k-1/2} = \alpha\frac{\widetilde{\phi}_{k-1,R}}{2} + \frac{\widetilde{J}_{k-1,R}}{2} - \alpha\frac{\widetilde{\phi}_{k,L}}{2} + \frac{\widetilde{J}_{k,L}}{2} \tag{11}$$

and using Eq. (7) and Eq. (8), we have:

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

When simplified (slightly), this becomes:

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

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

$$\widehat{J}_{k+1/2} = \frac{1}{2}\sum_{j=1}^{N_P}\left[\alpha B_j(1) - \frac{2}{\Delta x_k} D_k\left.\frac{dB_j}{ds}\right|_{s=1}\right]\phi_{k,j} - \frac{1}{2}\sum_{j=1}^{N_P}\left[\alpha B_j(-1) + \frac{2}{\Delta x_{k+1}} D_{k+1}(-1)\left.\frac{dB_j}{ds}\right|_{s=-1}\right]\phi_{k+1,j}\,. \tag{14}$$

If we consider the N_P moments equations in a given mesh cell at once, we have the following $N_P \times N_P$ system of equations:

$$\left[\mathbf{S}_+\left(\mathbf{J}_{L,k+1}\vec{\phi}_{k+1} + \mathbf{J}_{R,k}\vec{\phi}_k\right) - \mathbf{S}_-\left(\mathbf{J}_{L,k}\vec{\phi}_k + \mathbf{J}_{R,k-1}\vec{\phi}_{k-1}\right)\right] + \mathbf{L}\vec{\phi}_k + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_k = \mathbf{M}\vec{Q}\,, \tag{15}$$

where we make the following definitions:

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

$$\mathbf{J}_{R,k,1\ldots N_P,j} = \frac{1}{2}\left[\alpha B_j(1) - \frac{2}{\Delta x_k} D_k(1)\left.\frac{dB_j}{ds}\right|_{s=1}\right] \tag{17}$$

$$\mathbf{S}_{\pm,ij} = \begin{cases} B_i(\pm 1) & i = j \\ 0 & \text{otherwise} \end{cases} \tag{18}$$

$$\mathbf{L}_{ij} = \frac{2}{\Delta x_k}\int_{-1}^{1} D_k(s)\frac{dB_i}{ds}\frac{dBj}{ds}\; ds \tag{19}$$

$$\vec{\phi}_k = \begin{bmatrix} \phi_{1,k} \\ \vdots \\ \phi_{N_P,k} \end{bmatrix}, \tag{20}$$

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

$$\mathbf{M}_{ij} = \frac{\Delta x}{2} \int_{-1}^{1} B_i(s) B_j(s) \; ds \,, \tag{22}$$

$$\vec{Q} = \begin{bmatrix} Q_{1,k} \\ \vdots \\ Q_{N_P,k} \end{bmatrix}. \tag{23}$$

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,

$$B_i(s_q) = \begin{cases} 1 & s_i = s_q \\ 0 & \text{otherwise} \end{cases}. \tag{24}$$

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

$$\mathbf{M}_{ij} = \begin{cases} w_i & i = j \\ 0 & \text{otherwise} \end{cases} \tag{25}$$

$$\widehat{\mathbf{M}}_{ij,\sigma_a} = \begin{cases} w_i \sigma_a(s_i) & i = j \\ 0 & \text{otherwise} \end{cases}. \tag{26}$$

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:

$$\widehat{J}_{1/2} = \int_{-1}^{1} \mu\psi(x_{1/2},\mu)\, d\mu \approx 0 + \sum_{\substack{d=1 \\ \mu_d<0}}^{N_{dir}} w_d\mu_d \left[\frac{\widetilde{\phi}_1}{2} + \frac{3\mu_d\widetilde{J}_1}{2}\right] \tag{27}$$

$$\widehat{J}_{1/2} = -\frac{1}{2}\left[\sum_{j=1}^{N_P} \alpha B_j(-1)\phi_{1,j} + \frac{2D_1(-1)}{\Delta x}\sum_{j=1}^{N_P} \frac{dB_j}{ds}\bigg|_{s=-1}\phi_{1,j}\,.\right] \tag{28}$$

This make the N_P moment equation in the leftmost cell:

$$\left[\mathbf{S}_+\left(\mathbf{J}_{L,2}\vec{\phi}_2 + \mathbf{J}_{R,1}\vec{\phi}_1\right) - \mathbf{S}_-\mathbf{J}_{L,1}\vec{\phi}_1\right] + \mathbf{L}\vec{\phi}_k + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_k = \mathbf{M}\vec{Q}\,. \tag{29}$$

Similarly on the rightmost cell, the moment equations become:

$$\left[\mathbf{S}_+\mathbf{J}_{R,N_{cell}}\vec{\phi}_{N_{cell}} - \mathbf{S}_-\left(\mathbf{J}_{L,N_{cell}}\vec{\phi}_{N_{cell}} + \mathbf{J}_{R,N_{cell}-1}\vec{\phi}_{N_{cell}-1}\right)\right] + \mathbf{L}\vec{\phi}_{N_{cell}} + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_{N_{cell}} = \mathbf{M}\vec{Q}\,. \tag{30}$$

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:

$$\mathbf{S}_+\left(\mathbf{J}_{L,2}\vec{\phi}_2 + \mathbf{J}_{R,1}\vec{\phi}_1\right) + \mathbf{L}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_1 = \mathbf{M}\vec{Q}\,, \tag{31}$$

$$\mathbf{S}_-\left(\mathbf{J}_{L,N_{cell}}\vec{\phi}_{N_{cell}} + \mathbf{J}_{R,N_{cell}-1}\vec{\phi}_{N_{cell}-1}\right) + \mathbf{L}\vec{\phi}_{N_{cell}} + \widehat{\mathbf{M}}_{\sigma_a}\vec{\phi}_{N_{cell}} = \mathbf{M}\vec{Q}\,, \tag{32}$$

4 Alternative Use of Integration By Parts

$$B_i\left[\widehat{J}_{out} - \widehat{J}_{in}\right] \tag{33}$$

$$\left(B_i(1)J_{+,k,k+1/2} + B_i(-1)J_{-,k,k-1/2}\right) - \left(B_i(-1)J_{+,k-1,k-1/2} + B_i(1)J_{-,k+1,k-1/2}\right) \tag{34}$$

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

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

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

$$
\left. + B_i(1) \sum_{\substack{d=1\\ \mu_d<0}}^{N_{dir}} w_d\mu_d \sum_{j=1}^{N_P} \phi_{k+1,j} \left[\frac{B_j(-1)}{2} - \frac{2}{\Delta x_{k+1}} D_{k+1}(-1) \frac{dB_j}{ds}\bigg|_{s=-1} \right] \right) \tag{35}
$$

$$
\left(\mathbf{S}_+ \mathbf{J}_{R,k} \vec{\phi}_k + \mathbf{S}_- \mathbf{J}_{L,k} \vec{\phi}_k \right) - \left(\mathbf{S}_+ \mathbf{J}_{L,k+1} \vec{\phi}_{k+1} + \mathbf{S}_- \mathbf{J}_{R,k-1} \right) \vec{\phi}_{k-1} \tag{36}
$$

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.

6 MIP DSA

Start with Yaqi and Ragusa's Modified Interior Penalty (MIP) DSA equation:

$$
\begin{aligned}
b_{MIP}(\phi, \phi^*) = \quad & (\sigma_a \phi, \phi^*)_{\mathcal{D}} + \left(D \vec{\nabla} \phi, \vec{\nabla} \phi \right)_{\mathcal{D}} && \text{(37a)}\\
& + \left(\kappa_e \llbracket \phi \rrbracket , \llbracket \phi^* \rrbracket \right)_{E_h^i} && \text{(37b)}\\
& + \left(\llbracket \phi \rrbracket , \{\!\{ D \partial_n \phi^* \}\!\} \right)_{E_h^i} && \text{(37c)}\\
& + \left(\{\!\{ D \partial_n \phi \}\!\} , \llbracket \phi^* \rrbracket \right)_{E_h^i} && \text{(37d)}\\
& + (\kappa_e \phi, \phi^*)_{\partial \mathcal{D}^d} - \frac{1}{2} \left(\phi, D \partial_n \phi^* \right)_{\partial \mathcal{D}^d} && \text{(37e)}\\
& - \frac{1}{2} \left(D \partial_n \phi, \phi^* \right)_{\partial \mathcal{D}^d} \; . && \text{(37f)}
\end{aligned}
$$

Eq. (37) involves a series of integrals/evaluations over all cells and edges in the spatial domain. We will first consider the interior edges and integrals. Since all of the test functions, ϕ^* are only non-zero within a given spatial cell c, we define the terms of Eq. (37) by looking at the integrals in a single cell, c, with left and right edges $c-1/2$ and $c+1/2$, respectively. The volumetric integrals of Eq. (37a) are the simplest to calculate:

$$(\sigma_a \phi, \phi^*) = \frac{\Delta x_c}{2} \int_{-1}^{1} \sigma_a(s) \widetilde{\phi}(s) B_i(s)\ ds \tag{38}$$

and

$$\left(D\vec{\nabla}\phi, \vec{\nabla}\phi^* \right) = \frac{2}{\Delta x_c} \int_{-1}^{1} D(s) \frac{d\widetilde{\phi}}{ds} \frac{dB_i}{ds}\ ds\,. \tag{39}$$

While Eq. (37c) - Eq. (37d) are defined as edge integrations, because B_i(s), which are the ϕ^* test functions, are only non-zero within a single cell, then $\{\!\{\phi^*\}\!\}$ and $[\![\phi^*]\!]$ are only non zero on edges $c-1/2$ and $c+1/2$ when B_i is defined is non-zero in cell c. Considering the left edge, $c-1/2$ first, $(\kappa_e [\![\phi]\!], [\![\phi^*]\!])$ is:

$$\left(\kappa_{c-1/2} [\![\phi]\!], [\![\phi^*]\!]\right)_{c-1/2} = \kappa_{c-1/2} \left(\widetilde{\phi}_c \Big|_{s=-1} - \widetilde{\phi}_{c-1} \Big|_{s=1} \right) (B_i(-1) - 0)\ . \tag{40}$$

The next term, $([\![\phi]\!], \{\!\{D\partial_n \phi^*\}\!\})$:

$$([\![\phi]\!], \{\!\{D\partial_n \phi^*\}\!\})_{c-1/2} = \left(\widetilde{\phi}_c \Big|_{s=-1} - \widetilde{\phi}_{c-1} \Big|_{s=1} \right) \frac{1}{2} \left(0 + \frac{2D_c}{\Delta x_c} \frac{dB_i}{ds} \Big|_{s=-1} \right)\ . \tag{41}$$

The Eq. (37d) term is:

$$(\{\!\{D\partial_n \phi\}\!\}, [\![\phi^*]\!])_{c-1/2} = \frac{1}{2} \left(\frac{2D_{c-1}}{\Delta x_{c-1}} \frac{d\widetilde{\phi}_{c-1}}{ds} \Big|_{s=1} + \frac{2D_c}{\Delta x_c} \frac{d\widetilde{\phi}_c}{ds} \Big|_{s=-1} \right) (B_i(-1) - 0)\ . \tag{42}$$

In Eq. (40), $\kappa_{c-1/2}$ is defined as:

$$\kappa_{c-1/2} = \max\left(\frac{1}{4}, \kappa_{c-1/2}^{IP} \right)\,, \tag{43}$$

and $\kappa_{c-1/2}^{IP}$ is defined as:

$$\kappa_{c-1/2}^{IP} = p_c(p_c+1) \frac{D_c}{\Delta x_c} \Big|_{s=-1} + p_{c-1}(p_{c-1}+1) \frac{D_{c-1}}{\Delta x_{c-1}} \Big|_{s=1}\,, \tag{44}$$

where p_c is the DFEM trial space degree in cell c. We now define the right edge terms quickly:

$$\left(\kappa_{c+1/2} [\![\phi]\!], [\![\phi^*]\!]\right)_{c+1/2} = \kappa_{c+1/2} \left(\widetilde{\phi}_{c+1} \Big|_{s=-1} - \widetilde{\phi}_c \Big|_{s=1} \right) (0 - B_i(1)) \tag{45}$$

$$([\![\phi]\!], \{\!\{D\partial_n \phi^*\}\!\})_{c+1/2} = \left(\widetilde{\phi}_{c+1} \Big|_{s=-1} - \widetilde{\phi}_c \Big|_{s=1} \right) \frac{1}{2} \left(0 + \frac{2D_c}{\Delta x_c} \frac{dB_i}{ds} \Big|_{s=1} \right) \tag{46}$$

$$(\{\!\{D\partial_n \phi\}\!\}, [\![\phi^*]\!])_{c+1/2} = \frac{1}{2} \left(\frac{2D_c}{\Delta x_c} \frac{d\widetilde{\phi}_c}{ds} \Big|_{s=1} + \frac{2D_{c+1}}{\Delta x_{c+1}} \frac{d\widetilde{\phi}_{c+1}}{ds} \Big|_{s=-1} \right) (0 - B_i(1)) \tag{47}$$

In the above, we have implicitly assumed that the edge normal vector, $\vec{n}$ is oriented in the $+x$ direction. On the cell interior, this orientation is arbitrary, so long as it is consistent. However, on the global boundaries, the edge normal vector must be oriented outward. On the left boundary, this is in the $-x$ direction, and on the right boundary, in $+x$ direction.

It is possible to consider the MIP equations in matrix form within each cell. First, let us define the following $N_P \times N_P$ diagonal matrices:

$$\mathbf{B}_{L,ii} = B_i(-1) \tag{48}$$

$$\mathbf{B}_{R,ii} = B_i(1) \tag{49}$$

$$\widehat{\mathbf{B}}_{L,ii} = \left.\frac{dB_i}{ds}\right|_{s=-1} \tag{50}$$

$$\widehat{\mathbf{B}}_{R,ii} = \left.\frac{dB_i}{ds}\right|_{s=1} . \tag{51}$$

We also define the following $N_P \times N_P$ matrices:

$$\begin{aligned}
\mathbf{P}_{L,i} &= \begin{bmatrix} B_1(-1) & B_2(-1) & \dots & B_{N_P}(-1) \end{bmatrix} \\
\mathbf{P}_{R,i} &= \begin{bmatrix} B_1(1) & B_2(1) & \dots & B_{N_P}(1) \end{bmatrix} \\
\widehat{\mathbf{P}}_{L,i} &= \begin{bmatrix} \left.\frac{dB_1}{ds}\right|_{s=-1} & \left.\frac{dB_2}{ds}\right|_{s=-1} & \dots & \left.\frac{dB_{N_P}}{ds}\right|_{s=-1} \end{bmatrix} . \\
\widehat{\mathbf{P}}_{R,i} &= \begin{bmatrix} \left.\frac{dB_1}{ds}\right|_{s=1} & \left.\frac{dB_2}{ds}\right|_{s=1} & \dots & \left.\frac{dB_{N_P}}{ds}\right|_{s=1} \end{bmatrix}
\end{aligned} \tag{52}$$

We note that $\mathbf{P}_L$ and $\mathbf{P}_R$ have only N_P non-zero entries if there are interpolation points located at $s = \pm 1$. The volumetric MIP moment equations, Eq. (38) and Eq. (39) become:

$$\frac{\Delta x_c}{2} \mathbf{R}_{\sigma_a} \vec{\phi}_c + \frac{2}{\Delta x_c} \mathbf{L}_D \vec{\phi}_c \,, \tag{53}$$

where:

$$\mathbf{R}_{\sigma_a,ij} = \int_{-1}^{1} \sigma_a(s) B_i(s) B_j(s) \; ds \tag{54}$$

$$\mathbf{L}_{D,ij} = \int_{-1}^{1} D(s) \frac{dB_i}{ds} \frac{dB_j}{ds} \; ds \,. \tag{55}$$

The left edge terms, Eq. (40) - Eq. (42) are:

$$\left(\kappa_{c+1/2} \left[\!\left[\phi\right]\!\right], \left[\!\left[\phi^*\right]\!\right]\right)_{c-1/2} = \kappa_{c-1/2} \mathbf{B}_L \mathbf{P}_L \vec{\phi}_c - \kappa_{c-1/2} \mathbf{B}_L \mathbf{P}_R \vec{\phi}_{c-1} \tag{56}$$

$$\left(\left[\!\left[\phi\right]\!\right], \left\{\!\!\left\{D \partial_n \phi^*\right\}\!\!\right\}\right)_{c-1/2} = \left.\frac{D_c}{\Delta x_c}\right|_{s=-1} \widehat{\mathbf{B}}_L \left[\mathbf{P}_L \vec{\phi}_c - \mathbf{P}_R \vec{\phi}_{c-1}\right] \tag{57}$$

$$\left(\left\{\!\!\left\{D \partial_n \phi\right\}\!\!\right\}, \left[\!\left[\phi^*\right]\!\right]\right)_{c-1/2} = \; . \tag{58}$$

The right edge terms are:

$$\left(\kappa_{c+1/2} \left[\!\left[\phi\right]\!\right], \left[\!\left[\phi^*\right]\!\right]\right)_{c+1/2} = \tag{59}$$

$$\left(\left[\!\left[\phi\right]\!\right], \left\{\!\!\left\{D \partial_n \phi^*\right\}\!\!\right\}\right)_{c+1/2} = \tag{60}$$

$$\left(\left\{\!\!\left\{D \partial_n \phi\right\}\!\!\right\}, \left[\!\left[\phi^*\right]\!\right]\right)_{c+1/2} = \; . \tag{61}$$

$$\kappa_{c-1/2}\mathbf{B}_L\left(\mathbf{P}_L\vec{\phi}_c - \mathbf{P}_R\vec{\phi}_{c-1}\right) + \left.\frac{D_c}{\Delta x_c}\right|_{s=-1}\widehat{\mathbf{B}}_L\left(\mathbf{P}_L\vec{\phi}_c - \mathbf{P}_R\vec{\phi}_{c-1}\right)$$
$$+ \mathbf{B}_L\left(\left.\frac{D_{c-1}}{\Delta x_{c-1}}\right|_{s=1}\widehat{\mathbf{P}}_R\vec{\phi}_{c-1} + \left.\frac{D_c}{\Delta x_c}\right|_{s=-1}\widehat{\mathbf{P}}_L\vec{\phi}_c\right). \quad (62)$$

The right edge terms are:

$$-\kappa_{c+1/2}\mathbf{B}_R\left(\mathbf{P}_L\vec{\phi}_{c+1} - \mathbf{P}_R\vec{\phi}_c\right) + \left.\frac{D_c}{\Delta x_c}\right|_{s=1}\widehat{\mathbf{B}}_R\left(\mathbf{P}_L\vec{\phi}_{c+1} - \mathbf{P}_R\vec{\phi}_c\right)$$
$$- \mathbf{B}_R\left(\left.\frac{D_c}{\Delta x_c}\right|_{s=1}\widehat{\mathbf{P}}_R\vec{\phi}_c + \left.\frac{D_{c+1}}{\Delta x_{c+1}}\right|_{s=-1}\widehat{\mathbf{P}}_L\vec{\phi}_{c+1}\right). \quad (63)$$

Combining Eq. (53), Eq. (62), and Eq. (63) and simplifying we have:

$$-\left[\kappa_{c-1/2}\mathbf{B}_L\mathbf{P}_R + \frac{D_c}{\Delta x_c}\Big|_{s=-1}\widehat{\mathbf{B}}_L\mathbf{P}_R - \left.\frac{D_{c-1}}{\Delta x_{c-1}}\right|_{s=1}\mathbf{B}_L\widehat{\mathbf{P}}_R\right]\vec{\phi}_{c-1}$$
$$+\left[\frac{\Delta x_c}{2}\mathbf{R}_{\sigma_a} + \frac{2}{\Delta x_c}\mathbf{L}_D + \kappa_{c-1/2}\mathbf{B}_L\mathbf{P}_L + \left.\frac{D_c}{\Delta x_c}\right|_{s=-1}\left(\widehat{\mathbf{B}}_L\mathbf{P}_L + \mathbf{B}_L\widehat{\mathbf{P}}_L\right)\dots\right.$$
$$\left. + \kappa_{c+1/2}\mathbf{B}_R\mathbf{P}_R - \left.\frac{D_c}{\Delta x_c}\right|_{s=1}\left(\widehat{\mathbf{B}}_R\mathbf{P}_R + \mathbf{B}_R\widehat{\mathbf{P}}_R\right)\right]\vec{\phi}_c$$
$$-\left[\kappa_{c+1/2}\mathbf{B}_R\mathbf{P}_L - \left.\frac{D_c}{\Delta x_c}\right|_{s=1}\widehat{\mathbf{B}}_R\mathbf{P}_L + \left.\frac{D_{c+1}}{\Delta x_{c+1}}\right|_{s=-1}\mathbf{B}_R\widehat{\mathbf{P}}_L\right]\vec{\phi}_{c+1}. \quad (64)$$

The boundary cells have only one interior edge, but the boundary terms come into play. With this in mind, we handle the domain boundary terms of Eq. (37). Starting with the left boundary:

$$\left(\kappa_{1/2}\phi, \phi^*\right)_{1/2} = \kappa_{1/2}\left(\widetilde{\phi}_1(-1)\right)B_i(-1) \quad (65)$$
$$\frac{1}{2}\left(\phi, D\partial_n\phi^*\right)_{1/2} = \frac{1}{2}\widetilde{\phi}_1(-1)\left(-\frac{2D_1}{\Delta x_1}\left.\frac{dB_i}{ds}\right|_{s=-1}\right) \quad (66)$$
$$\frac{1}{2}\left(D\partial_n\phi, \phi^*\right)_{1/2} = \frac{1}{2}\left(-\frac{2D_1}{\Delta x_1}\left.\frac{d\widetilde{\phi}_1}{ds}\right|_{s=-1}\right)B_i(-1) \quad (67)$$
$$\kappa_{1/2} = \max\left(\frac{1}{4}, \kappa_{1/2}^{IP}\right) \quad (68)$$
$$\kappa_{1/2}^{IP} = 2p_1\frac{D_1(-1)}{\Delta x_1}. \quad (69)$$

The leftmost cell moment equations are:

$$\frac{\Delta x_1}{2}\int_{-1}^{1}\sigma_a(s)\widetilde{\phi}(s)B_i(s)\,ds + \frac{2}{\Delta x_1}\int_{-1}^{1}D(s)\frac{d\widetilde{\phi}}{ds}\frac{dB_i}{ds}\,ds$$
$$+\kappa_{3/2}\left(\widetilde{\phi}_2(-1) - \widetilde{\phi}_1(1)\right)(0 - B_i(1)) + \left(\widetilde{\phi}_2(-1) - \widetilde{\phi}_1(1)\right)\left(\frac{D_1}{2}\frac{2}{\Delta x_1}\left.\frac{dB_i}{ds}\right|_{s=1} + 0\right)$$
$$+\frac{1}{2}\left(\frac{2D_1}{\Delta x_1}\left.\frac{d\widetilde{\phi}_1}{ds}\right|_{s=1} + \frac{2D_2}{\Delta x_2}\left.\frac{d\widetilde{\phi}_2}{ds}\right|_{s=-1}\right)(0 - B_i(1)) + \kappa_{1/2}\widetilde{\phi}_1(-1)B_i(-1)$$
$$-\frac{1}{2}\widetilde{\phi}_1(-1)\left(-D_1\frac{2}{\Delta x_1}\left.\frac{dB_i}{ds}\right|_{s=-1}\right) - \frac{1}{2}\left(-\frac{2D_1}{\Delta x_1}\left.\frac{d\widetilde{\phi}_1}{ds}\right|_{s=-1}\right)B_i(-1). \quad (70)$$

Written in matrix form:

$$\left[\frac{\Delta x_1}{2}\mathbf{R}_{\sigma_a} + \frac{2}{\Delta x_1}\mathbf{L} + \kappa_{3/2}\mathbf{B}_R\mathbf{P}_R - \frac{D_1}{\Delta x_1}\bigg|_{s=1}\widehat{\mathbf{B}}_R\mathbf{P}_R - \frac{D_1}{\Delta x_1}\bigg|_{s=1}\mathbf{B}_R\widehat{\mathbf{P}}_R \ldots\right.$$

$$\left. +\kappa_{1/2}\mathbf{B}_L\mathbf{P}_L + \frac{D_1}{\Delta x_1}\bigg|_{s=-1}\widehat{\mathbf{B}}_L\mathbf{P}_L + \frac{D_1}{\Delta x_1}\bigg|_{s=-1}\mathbf{B}_L\widehat{\mathbf{P}}_L\right]\vec{\phi}_1$$

$$+\left[-\kappa_{3/2}\mathbf{B}_R\mathbf{P}_L + \frac{D_1}{\Delta x_1}\bigg|_{s=1}\widehat{\mathbf{B}}_R\mathbf{P}_L - \frac{D_2}{\Delta x_2}\bigg|_{s=-1}\mathbf{B}_R\widehat{\mathbf{P}}_L\right]\vec{\phi}_2 \quad (71)$$

Now considering the rightmost cell, we first give the left edge terms:

$$\kappa_{N-1/2}\mathbf{B}_L\left(\mathbf{P}_L\vec{\phi}_N - \mathbf{P}_R\vec{\phi}_{N-1}\right) + \frac{D_N}{\Delta x_N}\bigg|_{s=-1}\widehat{\mathbf{B}}_L\left(\mathbf{P}_L\vec{\phi}_N - \mathbf{P}_R\vec{\phi}_{N-1}\right)$$

$$+\mathbf{B}_L\left(\frac{D_{N-1}}{\Delta x_{N-1}}\bigg|_{s=1}\widehat{\mathbf{P}}_R\vec{\phi}_{N-1} + \frac{D_N}{\Delta x_N}\bigg|_{s=-1}\widehat{\mathbf{P}}_L\vec{\phi}_N\right), \quad (72)$$

where N is the total number of mesh cells. The right boundary edge terms are:

$$\left(\kappa_{N+1/2}\phi, \phi^*\right)_{N+1/2} = \kappa_{N+1/2}\left(\widetilde{\phi}_N(1)\right)B_i(1) \quad (73)$$

$$\frac{1}{2}\left(\phi, D\partial_n\phi^*\right)_{N+1/2} = \frac{1}{2}\widetilde{\phi}_N(1)\left(\frac{2D_N}{\Delta x_N}\frac{dB_i}{ds}\bigg|_{s=1}\right) \quad (74)$$

$$\frac{1}{2}\left(D\partial_n\phi, \phi^*\right)_{N+1/2} = \frac{1}{2}\left(\frac{2D_N}{\Delta x_N}\frac{d\widetilde{\phi}_N}{ds}\bigg|_{s=1}\right)B_i(1) \quad (75)$$

$$\kappa_{N+1/2} = \max\left(\frac{1}{4}, \kappa_{N+1/2}^{IP}\right) \quad (76)$$

$$\kappa_{N+1/2}^{IP} = 2p_N\frac{D_N(1)}{\Delta x_N}, \quad (77)$$

Combing all of the edge and cell integral equations together, we have:

$$-\left[\kappa_{N-1/2}\mathbf{B}_L\mathbf{P}_R + \frac{D_N}{\Delta x_N}\bigg|_{s=-1}\widehat{\mathbf{B}}_L\mathbf{P}_R - \frac{D_{N-1}}{\Delta x_{N-1}}\bigg|_{s=1}\mathbf{B}_L\widehat{\mathbf{P}}_R\right]\vec{\phi}_{N-1}$$

$$\left[\frac{\Delta x_N}{2}\mathbf{R}_{\sigma_a} + \frac{2}{\Delta x_N}\mathbf{L}_D + \kappa_{N-1/2}\mathbf{B}_L\mathbf{P}_L + \frac{D_N}{\Delta x_N}\bigg|_{s=-1}\widehat{\mathbf{B}}_L\mathbf{P}_L + \frac{D_N}{\Delta x_N}\bigg|_{s=-1}\mathbf{B}_L\widehat{\mathbf{P}}_L \ldots\right.$$

$$\left.+\kappa_{N+1/2}\mathbf{B}_R\mathbf{P}_R - \frac{D_N}{\Delta x_N}\bigg|_{s=1}\widehat{\mathbf{B}}_R\mathbf{P}_R - \frac{D_N}{\Delta x_N}\bigg|_{s=1}\mathbf{B}_R\widehat{\mathbf{P}}_R\right]\vec{\phi}_N \quad (78)$$

References

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