

formula:

$$(f, g)_{\mathcal{D}} = \sum_{i=1}^N (f, g)_i \quad (\text{D.31})$$

$$(f, g)_i = \int_{x_{i-1/2}}^{x_{i+1/2}} f \cdot g \, dx \quad (\text{D.32})$$

$$(f, g)_{E_h^i} = \sum_{i=1}^{N-1} (f, g)_{i+1/2} \quad (\text{D.33})$$

$$(f, g)_{i+1/2} = f_{i+1/2} g_{i+1/2} \quad (\text{D.34})$$

$$(f, g)_{i+1/2}^R = f_{i+1/2}^R g_{i+1/2}^R \quad (\text{D.35})$$

$$(f, g)_{i+1/2}^L = f_{i+1/2}^L g_{i+1/2}^L \quad (\text{D.36})$$

$$[\phi]_{i+1/2} = \phi_{i+1/2}^R - \phi_{i+1/2}^L \quad (\text{D.37})$$

$$[\phi^*]_{i+1/2} = \phi_{i+1/2}^{*R} - \phi_{i+1/2}^{*L} \quad (\text{D.38})$$

$$[Dd_x \phi]_{i+1/2} = \left[D \frac{d\phi}{dx} \right]_{i+1/2}^R - \left[D \frac{d\phi}{dx} \right]_{i+1/2}^L \quad (\text{D.39})$$

$$[Dd_x \phi^*]_{i+1/2} = \left[D \frac{d\phi^*}{dx} \right]_{i+1/2}^R - \left[D \frac{d\phi^*}{dx} \right]_{i+1/2}^L \quad (\text{D.40})$$

$$\{Dd_x \phi\}_{i+1/2} = \frac{1}{2} \left(\left[D \frac{d\phi}{dx} \right]_{i+1/2}^R + \left[D \frac{d\phi}{dx} \right]_{i+1/2}^L \right) \quad (\text{D.41})$$

$$\{Dd_x \phi^*\}_{i+1/2} = \frac{1}{2} \left(\left[D \frac{d\phi^*}{dx} \right]_{i+1/2}^R + \left[D \frac{d\phi^*}{dx} \right]_{i+1/2}^L \right) \quad (\text{D.42})$$

We copy the multi-dimensional diffusion conforming form to here:

$$\begin{aligned}
b_{DCF}(\Phi, \Phi^*) = & (\sigma_a \Phi, \Phi^*)_{\mathcal{D}} + (D\vec{\nabla}\Phi, \vec{\nabla}\Phi^*)_{\mathcal{D}} \\
& + \frac{1}{4}([\Phi], [\Phi^*])_{E_h^i} + ([\Phi], \{\{D\partial_n \Phi^*\}\})_{E_h^i} + (\{\{D\partial_n \Phi\}\}, [\Phi^*])_{E_h^i} \\
& + \frac{1}{4}(\Phi, \Phi^*)_{\partial\mathcal{D}^d} - \frac{1}{2}(\Phi, D\partial_n \Phi^*)_{\partial\mathcal{D}^d} - \frac{1}{2}(D\partial_n \Phi, \Phi)_{\partial\mathcal{D}^d} \\
& - \frac{9}{16}([D\vec{\nabla}\Phi], [D\vec{\nabla}\Phi^*])_{E_h^i} - \frac{9}{16}([D\partial_n \Phi], [D\partial_n \Phi^*])_{E_h^i} \\
& - \frac{9}{16}(D\vec{\nabla}\Phi, D\vec{\nabla}\Phi^*)_{\partial\mathcal{D}^d} - \frac{9}{16}(D\partial_n \Phi, D\partial_n \Phi^*)_{\partial\mathcal{D}^d}
\end{aligned} \tag{D.43}$$

$$l_{DCF}(\Phi^*) = (Q_0, \Phi^*)_{\mathcal{D}} + (J^{inc}, \Phi^*)_{\partial\mathcal{D}^d} - (\vec{\Upsilon}^{inc}, D\vec{\nabla}\Phi^*)_{\partial\mathcal{D}^d}$$

where

$$\begin{aligned}
J^{inc} &= \sum_{\vec{\Omega}_m \cdot \vec{n}(\vec{r}_b) < 0} w_m \left| \vec{\Omega}_m \cdot \vec{n}(\vec{r}_b) \right| \Psi_m^{inc} \\
\vec{\Upsilon}^{inc} &= - \sum_{\vec{\Omega}_m \cdot \vec{n}(\vec{r}_b) < 0} 3w_m \vec{\Omega}_m \left| \vec{\Omega}_m \cdot \vec{n}(\vec{r}_b) \right| \Psi_m^{inc}
\end{aligned} \tag{D.44}$$

We can see that, with following

$$D\vec{\nabla}\Phi = Dd_x\phi \tag{D.45}$$

$$D\partial_n \Phi = Dd_x\phi \quad \text{on } E_h^i \tag{D.46}$$

$$D\partial_n \Phi = Dd_x\phi \quad \text{on } x_{N+1/2} \tag{D.47}$$

$$D\partial_n \Phi = -Dd_x\phi \quad \text{on } x_{1/2} \tag{D.48}$$

We can obtain the 1-D form from the multi-dimensional formula.

I will present a different way to assemble the system. Let us consider two element

adjacent with each other noted with 1 for the left and 2 for the right.

$$\begin{aligned}
(\sigma_a \phi, \phi^*)_D &= \phi_1^{*T} \sigma_{a,1} \Delta x_1 \mathbf{M} \phi_1 + \phi_2^{*T} \sigma_{a,2} \Delta x_2 \mathbf{M} \phi_2 \\
(Dd_x \phi, d_x \phi^*)_D &= \phi_1^{*T} \frac{D_1}{\Delta x_1} \mathbf{S} \phi_1 + \phi_2^{*T} \frac{D_2}{\Delta x_2} \mathbf{S} \phi_2 \\
\frac{1}{4}([\phi], [\phi^*])_{E_h^i} &= \frac{1}{4}(\phi_{3/2}^R - \phi_{3/2}^L)(\phi_{3/2}^{*R} - \phi_{3/2}^{*L}) \\
&= \frac{1}{4}\phi_{3/2}^L \phi_{3/2}^{*L} + \frac{1}{4}\phi_{3/2}^R \phi_{3/2}^{*R} - \frac{1}{4}\phi_{3/2}^R \phi_{3/2}^{*L} - \frac{1}{4}\phi_{3/2}^L \phi_{3/2}^{*R} \\
&= \frac{1}{4}\phi_1^{*T} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \phi_1 + \frac{1}{4}\phi_2^{*T} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \phi_2 \\
&\quad - \frac{1}{4}\phi_1^{*T} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \phi_2 - \frac{1}{4}\phi_2^{*T} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \phi_1 \\
&= \phi_1^{*T} \mathbf{E}_{11}^1 \phi_1 + \phi_2^{*T} \mathbf{E}_{22}^1 \phi_2 + \phi_1^{*T} \mathbf{E}_{12}^1 \phi_2 + \phi_2^{*T} \mathbf{E}_{21}^1 \phi_1 \\
(\{Dd_x \phi\}, [\phi^*])_{E_h^i} &= \frac{1}{2} \left(\left[D \frac{d\phi}{dx} \right]_{3/2}^R + \left[D \frac{d\phi}{dx} \right]_{3/2}^L \right) (\phi_{3/2}^{*R} - \phi_{3/2}^{*L}) \\
&= -\frac{1}{2} \left[D \frac{d\phi}{dx} \right]_{3/2}^L \phi_{3/2}^{*L} + \frac{1}{2} \left[D \frac{d\phi}{dx} \right]_{3/2}^R \phi_{3/2}^{*R} \\
&\quad - \frac{1}{2} \left[D \frac{d\phi}{dx} \right]_{3/2}^R \phi_{3/2}^{*L} + \frac{1}{2} \left[D \frac{d\phi}{dx} \right]_{3/2}^L \phi_{3/2}^{*R} \\
&= -\frac{1}{2}\phi_1^{*T} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \frac{D_1}{\Delta x_1} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_1 + \frac{1}{2}\phi_2^{*T} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \frac{D_2}{\Delta x_2} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_2 \\
&\quad - \frac{1}{2}\phi_1^{*T} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \frac{D_2}{\Delta x_2} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_2 + \frac{1}{2}\phi_2^{*T} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \frac{D_1}{\Delta x_1} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_1 \\
&= \phi_1^{*T} \frac{D_1}{\Delta x_1} \mathbf{E}_{11}^2 \phi_1 + \phi_2^{*T} \frac{D_2}{\Delta x_2} \mathbf{E}_{22}^2 \phi_2 + \phi_1^{*T} \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^2 \phi_2 + \phi_2^{*T} \frac{D_1}{\Delta x_1} \mathbf{E}_{21}^2 \phi_1
\end{aligned}$$

$$\begin{aligned}
([\phi], \{Dd_x \phi^*\})_{E_h^i} &= \frac{1}{2}(\phi_{3/2}^R - \phi_{3/2}^L) \left(\left[D \frac{d\phi^*}{dx} \right]_{3/2}^R + \left[D \frac{d\phi^*}{dx} \right]_{3/2}^L \right) \\
&= -\frac{1}{2} \left[D \frac{d\phi^*}{dx} \right]_{3/2}^L \phi_{3/2}^L + \frac{1}{2} \left[D \frac{d\phi^*}{dx} \right]_{3/2}^R \phi_{3/2}^R \\
&\quad + \frac{1}{2} \left[D \frac{d\phi^*}{dx} \right]_{3/2}^L \phi_{3/2}^R - \frac{1}{2} \left[D \frac{d\phi^*}{dx} \right]_{3/2}^R \phi_{3/2}^L \\
&= -\frac{1}{2} \frac{D_1}{\Delta x_1} \phi_1^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \phi_1 + \frac{1}{2} \frac{D_2}{\Delta x_2} \phi_2^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \phi_2 \\
&\quad - \frac{1}{2} \frac{D_1}{\Delta x_1} \phi_1^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \phi_2 + \frac{1}{2} \frac{D_2}{\Delta x_2} \phi_2^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \phi_1 \\
&= \phi_1^{*T} \frac{D_1}{\Delta x_1} \mathbf{E}_{11}^{2T} \phi_1 + \phi_2^{*T} \frac{D_2}{\Delta x_2} \mathbf{E}_{22}^{2T} \phi_2 + \phi_1^{*T} \frac{D_1}{\Delta x_1} \mathbf{E}_{21}^{2T} \phi_2 + \phi_2^{*T} \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^{2T} \phi_1
\end{aligned}$$

$$\begin{aligned}
-\frac{9}{8}([Dd_x \phi], [Dd_x \phi^*])_{E_h^i} &= -\frac{9}{8} \left(\left[D \frac{d\phi}{dx} \right]_{3/2}^R - \left[D \frac{d\phi}{dx} \right]_{3/2}^L \right) \left(\left[D \frac{d\phi^*}{dx} \right]_{3/2}^R - \left[D \frac{d\phi^*}{dx} \right]_{3/2}^L \right) \\
&= -\frac{9}{8} \left[D \frac{d\phi}{dx} \right]_{3/2}^L \left[D \frac{d\phi^*}{dx} \right]_{3/2}^L - \frac{9}{8} \left[D \frac{d\phi}{dx} \right]_{3/2}^R \left[D \frac{d\phi^*}{dx} \right]_{3/2}^R \\
&\quad + \frac{9}{8} \left[D \frac{d\phi}{dx} \right]_{3/2}^R \left[D \frac{d\phi^*}{dx} \right]_{3/2}^L + \frac{9}{8} \left[D \frac{d\phi}{dx} \right]_{3/2}^L \left[D \frac{d\phi^*}{dx} \right]_{3/2}^R \\
&= -\frac{9}{8} \frac{D_1}{\Delta x_1} \phi_1^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \frac{D_1}{\Delta x_1} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_1 - \frac{9}{8} \frac{D_2}{\Delta x_2} \phi_2^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \frac{D_2}{\Delta x_2} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_2 \\
&\quad + \frac{9}{8} \frac{D_1}{\Delta x_1} \phi_1^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \frac{D_2}{\Delta x_2} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_2 + \frac{9}{8} \frac{D_2}{\Delta x_2} \phi_2^{*T} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \frac{D_1}{\Delta x_1} \begin{bmatrix} -1 & 1 \end{bmatrix} \phi_1 \\
&= \phi_1^{*T} \left(\frac{D_1}{\Delta x_1} \right)^2 \mathbf{E}_{11}^3 \phi_1 + \phi_2^{*T} \left(\frac{D_2}{\Delta x_2} \right)^2 \mathbf{E}_{22}^3 \phi_2 \\
&\quad + \phi_1^{*T} \frac{D_1}{\Delta x_1} \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^3 \phi_2 + \phi_2^{*T} \frac{D_1}{\Delta x_1} \frac{D_2}{\Delta x_2} \mathbf{E}_{21}^3 \phi_1
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{M} &= \frac{1}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \\
\mathbf{S} &= \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\
\mathbf{E}_{11}^1 &= \frac{1}{4} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \\
\mathbf{E}_{22}^1 &= \frac{1}{4} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\
\mathbf{E}_{12}^1 &= -\frac{1}{4} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix} \\
\mathbf{E}_{21}^1 &= -\frac{1}{4} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix} \\
\mathbf{E}_{11}^2 = \mathbf{E}_{12}^2 &= -\frac{1}{2} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix} \\
\mathbf{E}_{22}^2 = \mathbf{E}_{21}^2 &= \frac{1}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix} \\
\mathbf{E}_{11}^3 = \mathbf{E}_{22}^3 &= -\frac{9}{8} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} = \frac{9}{8} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \\
\mathbf{E}_{12}^3 = \mathbf{E}_{21}^3 &= \frac{9}{8} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} = \frac{9}{8} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}
\end{aligned}$$

Note that $\mathbf{E}_{12}^1 = \mathbf{E}_{21}^{1T}$. So the final system without the boundary treatment is

$$\begin{bmatrix} \phi_1^* & \phi_2^* \end{bmatrix} \mathbf{A} \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \quad (\text{D.49})$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \quad (\text{D.50})$$

$$\mathbf{A}_{11} = \sigma_{a,1} \Delta x_1 \mathbf{M} + \frac{D_1}{\Delta x_1} \mathbf{S} + \mathbf{E}_{11}^1 + \frac{D_1}{\Delta x_1} (\mathbf{E}_{11}^2 + \mathbf{E}_{11}^{2T}) + \left(\frac{D_1}{\Delta x_1}\right)^2 \mathbf{E}_{11}^3 \quad (\text{D.51})$$

$$\mathbf{A}_{12} = \mathbf{E}_{12}^1 + \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^2 + \frac{D_1}{\Delta x_1} \mathbf{E}_{21}^{2T} + \frac{D_1}{\Delta x_1} \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^3 \quad (\text{D.52})$$

$$\mathbf{A}_{21} = \mathbf{E}_{21}^1 + \frac{D_1}{\Delta x_1} \mathbf{E}_{21}^2 + \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^{2T} + \frac{D_1}{\Delta x_1} \frac{D_2}{\Delta x_2} \mathbf{E}_{21}^3 \quad (\text{D.53})$$

$$\mathbf{A}_{22} = \sigma_{a,2} \Delta x_2 \mathbf{M} + \frac{D_2}{\Delta x_2} \mathbf{S} + \mathbf{E}_{22}^1 + \frac{D_2}{\Delta x_2} (\mathbf{E}_{22}^2 + \mathbf{E}_{22}^{2T}) + \left(\frac{D_2}{\Delta x_2}\right)^2 \mathbf{E}_{22}^3 \quad (\text{D.54})$$

Matrix \mathbf{A} is symmetric. If there is another cell on the right of cell 2 denoted with 3, the resulting matrix will be

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{0} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{A}_{23} \\ \mathbf{0} & \mathbf{A}_{32} & \mathbf{A}_{33} \end{bmatrix} \quad (\text{D.55})$$

where

$$\mathbf{A}_{11} = \sigma_{a,1} \Delta x_1 \mathbf{M} + \frac{D_1}{\Delta x_1} \mathbf{S} + \mathbf{E}_{11}^1 + \frac{D_1}{\Delta x_1} (\mathbf{E}_{11}^2 + \mathbf{E}_{11}^{2T}) + \left(\frac{D_1}{\Delta x_1}\right)^2 \mathbf{E}_{11}^3 \quad (\text{D.56})$$

$$\mathbf{A}_{12} = \mathbf{E}_{12}^1 + \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^2 + \frac{D_1}{\Delta x_1} \mathbf{E}_{21}^{2T} + \frac{D_1}{\Delta x_1} \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^3 \quad (\text{D.57})$$

$$\mathbf{A}_{21} = \mathbf{E}_{21}^1 + \frac{D_1}{\Delta x_1} \mathbf{E}_{21}^2 + \frac{D_2}{\Delta x_2} \mathbf{E}_{12}^{2T} + \frac{D_1}{\Delta x_1} \frac{D_2}{\Delta x_2} \mathbf{E}_{21}^3 \quad (\text{D.58})$$

$$\begin{aligned} \mathbf{A}_{22} = & \sigma_{a,2} \Delta x_2 \mathbf{M} + \frac{D_2}{\Delta x_2} \mathbf{S} + \mathbf{E}_{22}^1 + \frac{D_2}{\Delta x_2} (\mathbf{E}_{22}^2 + \mathbf{E}_{22}^{2T}) + \left(\frac{D_2}{\Delta x_2}\right)^2 \mathbf{E}_{22}^3 + \mathbf{E}_{11}^1 + \\ & \frac{D_2}{\Delta x_2} (\mathbf{E}_{11}^2 + \mathbf{E}_{11}^{2T}) + \left(\frac{D_2}{\Delta x_2}\right)^2 \mathbf{E}_{11}^3 \end{aligned} \quad (\text{D.59})$$

$$\mathbf{A}_{32} = \mathbf{E}_{21}^1 + \frac{D_2}{\Delta x_2} \mathbf{E}_{21}^2 + \frac{D_3}{\Delta x_3} \mathbf{E}_{12}^{2T} + \frac{D_2}{\Delta x_2} \frac{D_3}{\Delta x_3} \mathbf{E}_{21}^3 \quad (\text{D.60})$$

$$\mathbf{A}_{33} = \sigma_{a,3} \Delta x_3 \mathbf{M} + \frac{D_3}{\Delta x_3} \mathbf{S} + \mathbf{E}_{22}^1 + \frac{D_3}{\Delta x_3} (\mathbf{E}_{22}^2 + \mathbf{E}_{22}^{2T}) + \left(\frac{D_3}{\Delta x_3}\right)^2 \mathbf{E}_{22}^3 \quad (\text{D.61})$$

This is one way where we basically are considering a bunch of small 2-by-2 system and then summing them together. We can also consider each cell with two side vertices, i.e., each row of the global system. 11 is right self-coupling, 22 is left self-coupling, 12 is right vertex coupling, 21 is left vertex coupling. This way is better in multi-dimensional situation.

$$\mathbf{E}_{11} = \mathbf{E}_R \quad (\text{D.62})$$

$$\mathbf{E}_{22} = \mathbf{E}_L \quad (\text{D.63})$$

$$\mathbf{E}_{12} = \mathbf{E}_{RC} \quad (\text{D.64})$$

$$\mathbf{E}_{21} = \mathbf{E}_{LC} \quad (\text{D.65})$$

APPENDIX E

PRECONDITIONED CG METHOD WITH EISENSTAT TRICK