

Derive the matrix expressions each reflecting boundary in the 2-D diffusion equation formulation derived with the finite volume method and describe the associated equations.

In 2-D:

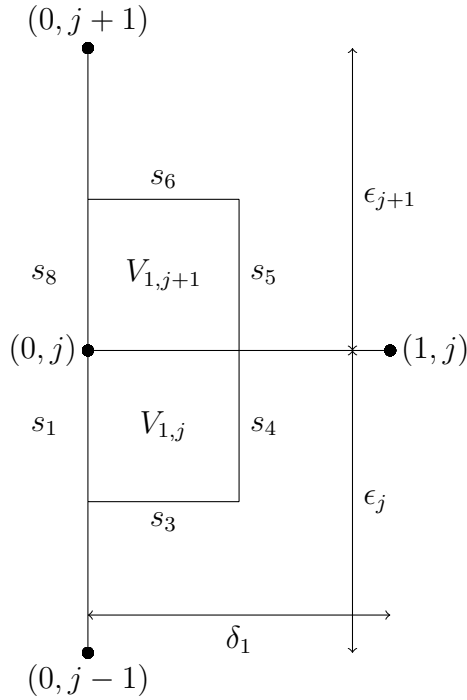
$$-\frac{\partial}{\partial x}D(x,y)\frac{\partial}{\partial x}\phi(x,y) - \frac{\partial}{\partial y}D(x,y)\frac{\partial}{\partial y}\phi(x,y) + \Sigma_a(x,y)\phi(x,y) = S(x,y)$$

with  $x \in [0, a]$  and  $y \in [0, b]$ .

## LEFT

The left side boundary condition is:

$$\frac{\partial}{\partial x}\phi(x,y)|_{x=0} = 0$$



To implement the boundary condition, we integrate in the first half-cell, so from  $x = 0$  to  $x = \delta_1/2$ .

Recall that when we considered the streaming term we converted the volume integral into a surface integral:

$$\begin{aligned} & - \int_V d\vec{r} [\nabla \cdot (D(\vec{r})\nabla\phi(\vec{r}))] \\ & = - \int_S d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}}\phi(\vec{r}) \end{aligned}$$

and we defined the partial derivative w.r.t. direction on each surface. We now have two fewer surfaces (no  $s_2$  or  $s_7$ ), and we apply the zero current boundary condition to  $s_1$  and  $s_8$ .

$$\begin{aligned} \frac{\partial}{\partial \hat{n}}\phi(\vec{r}) &= \frac{\phi_{0,j-1} - \phi_{0,j}}{\epsilon_j} && \text{on } S_3 \\ &= \frac{\phi_{0,j+1} - \phi_{0,j}}{\epsilon_{j+1}} && \text{on } S_6 \\ &= \frac{\phi_{1,j} - \phi_{0,j}}{\delta_1} && \text{on } S_4, S_5 \\ &= 0 && \text{on } S_1, S_8 \end{aligned}$$

We then use the midpoint rule for the integration and integrate along each surface. Recall that the physics values are cell-centered while the flux is edge-centered. The two terms that are different are for the top and bottom of the cell:

$$\begin{aligned}
-\int_{S_3} d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \frac{\phi_{0,j} - \phi_{0,j-1}}{\epsilon_j} \left( \frac{D_{1,j} \delta_1}{2} \right) \\
-\int_{S_6} d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \frac{\phi_{0,j+1} - \phi_{0,j}}{\epsilon_{j+1}} \left( \frac{D_{1,j+1} \delta_1}{2} \right) \\
S_1 + S_8 &= 0, \\
S_4 + S_5 &= \frac{\phi_{1,j} - \phi_{0,j}}{\delta_1} \left( \frac{D_{1,j} \epsilon_j + D_{1,j+1} \epsilon_{j+1}}{2} \right).
\end{aligned}$$

The absorption and streaming terms now become:

$$\begin{aligned}
\int \int dx dy \Sigma_a(x, y) \phi(x, y) &= \boxed{\phi_{0,j} (\Sigma_{a,1,j} V_{1,j} + \Sigma_{a,1,j+1} V_{1,j+1}) \equiv \Sigma_{a,0j}^*}, \\
\int \int dx dy S(x, y) &= \boxed{S_{1,j} V_{1,j} + S_{1,j+1} V_{1,j+1} \equiv S_{0j}^*}.
\end{aligned}$$

Collecting all of the terms and separating them, we get a 4-point difference equation for  $i = 0; j = 1, \dots, m-1$ :

$$\boxed{a_{1,j}^{0j} \phi_{1,j} + a_{0,j-1}^{*,0j} \phi_{0,j-1} + a_{0,j+1}^{*,0j} \phi_{0,j+1} + a_{0,j}^{*,0j} \phi_{0,j} = S_{0j}^*}$$

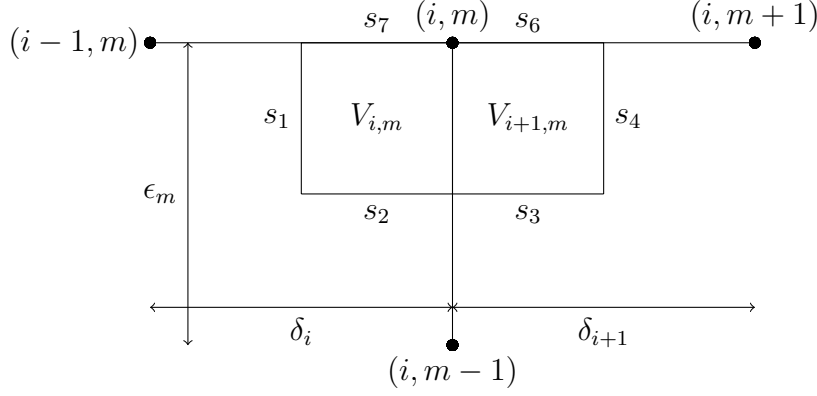
Recall: the lower index is the cell to which you are coupling, and the upper index is which cell you are in. The coefficients now change to become

$$\begin{aligned}
a_{1,j}^{0j} &= -\frac{D_{1,j} \epsilon_j + D_{1,j+1} \epsilon_{j+1}}{2\delta_1} \\
a_{0,j-1}^{*,0j} &= -\frac{D_{1,j} \delta_1}{2\epsilon_j} \\
a_{0,j+1}^{*,0j} &= -\frac{D_{1,j+1} \delta_1}{2\epsilon_{j+1}} \\
a_{0,j}^{*,0j} &= \Sigma_{a,0j}^* - (a_{1,j}^{0j} + a_{0,j-1}^{*,0j} + a_{0,j+1}^{*,0j}).
\end{aligned}$$

## TOP

The top boundary condition is:

$$\frac{\partial}{\partial y} \phi(x, y) \Big|_{y=b} = 0$$



To implement the boundary condition, we integrate in the last half-cell, so from  $y = \epsilon_m/2$  to  $y = b$ .

Recall that when we considered the streaming term we converted the volume integral into a surface integral:

$$\begin{aligned} & - \int_V d\vec{r} [\nabla \cdot (D(\vec{r}) \nabla \phi(\vec{r}))] \\ & = - \int_S d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) \end{aligned}$$

and we defined the partial derivative w.r.t. direction on each surface. We now have two fewer surfaces (no  $s_8$  or  $s_5$ ), and we apply the zero current boundary condition to  $s_7$  and  $s_6$ .

$$\begin{aligned} \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \frac{\phi_{i-1,m} - \phi_{i,m}}{\delta_i} && \text{on } S_1 \\ &= \frac{\phi_{i+1,m} - \phi_{i,m}}{\delta_{i+1}} && \text{on } S_4 \\ &= \frac{\phi_{i,m-1} - \phi_{i,m}}{\epsilon_m} && \text{on } S_2, S_3 \\ &= 0 && \text{on } S_7, S_6 \end{aligned}$$

We then use the midpoint rule for the integration and integrate along each surface. Recall that the physics values are cell-centered while the flux is edge-centered. The two terms that

are different are for the left and right of the cell:

$$\begin{aligned} - \int_{S_1} d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \frac{\phi_{i,m} - \phi_{i-1,m}}{\delta_i} \left( \frac{D_{i,m} \epsilon_m}{2} \right) \\ - \int_{S_4} d\vec{S} D(\vec{r}) \frac{\partial}{\partial \hat{n}} \phi(\vec{r}) &= \frac{\phi_{i+1,m} - \phi_{i,m}}{\delta_{i+1}} \left( \frac{D_{i+1,m} \epsilon_m}{2} \right) \end{aligned}$$

The absorption and streaming terms now become:

$$\begin{aligned} \int \int dxdy \Sigma_a(x, y) \phi(x, y) &= \boxed{\phi_{n,j} (\Sigma_{a,i,m} V_{i,m} + \Sigma_{a,i+1,m} V_{i+1,m}) \equiv \Sigma_{a,im}^*}, \\ \int \int dxdy S(x, y) &= \boxed{S_{i,m} V_{i,m} + S_{i+1,m} V_{i+1,m} \equiv S_{im}^*}. \end{aligned}$$

Collecting all of the terms and separating them, we get a 4-point difference equation for  $i = 1, \dots, n-1, j = m$ :

$$\boxed{a_{i-1,m}^{*,im} \phi_{i-1,m} + a_{i,m-1}^{*,im} \phi_{i,m-1} + a_{i+1,m}^{*,im} \phi_{i+1,m} + a_{i,m}^{*,im} \phi_{i,m} = S_{im}^*}$$

Recall: the lower index is the cell to which you are coupling, and the upper index is which cell you are in. The coefficients now change to become

$$\begin{aligned} a_{i-1,m}^{*,im} &= -\frac{D_{i,m} \epsilon_m}{2\delta_i} \\ a_{i,m-1}^{*,im} &= -\frac{D_{i,m} \delta_i + D_{i+1,m} \delta_{i+1}}{2\epsilon_m} \\ a_{i+1,m}^{*,im} &= -\frac{D_{i+1,m} \epsilon_m}{2\delta_{i+1}} \\ a_{n,j}^{*,im} &= \Sigma_{a,im} - (a_{i-1,m}^{*,im} + a_{i,m-1}^{*,im} + a_{i+1,m}^{*,im}). \end{aligned}$$