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.
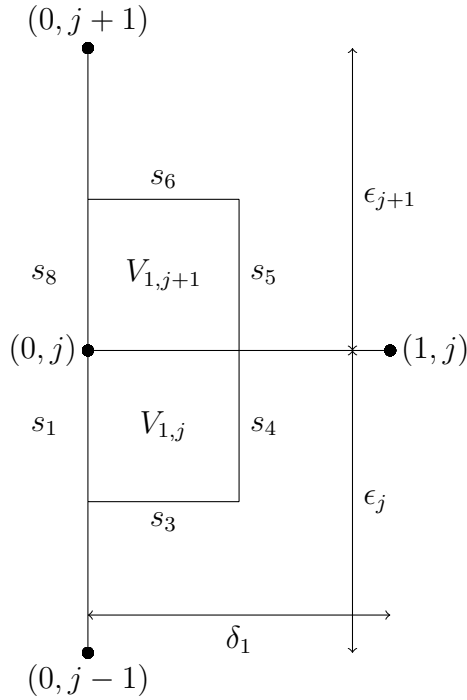In 2-D:

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

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

LEFT

The left side boundary condition is:

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

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:

$$-\int_V d\vec{r}\left[\nabla \cdot \left(D(\vec{r})\nabla\phi(\vec{r})\right)\right]$$

$$= -\int_S d\vec{S}\,D(\vec{r})\frac{\partial}{\partial\hat{n}}\phi(\vec{r})$$

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.

$$\frac{\partial}{\partial\hat{n}}\phi(\vec{r}) = \frac{\phi_{0,j-1} - \phi_{0,j}}{\epsilon_j} \qquad \text{on } S_3$$

$$= \frac{\phi_{0,j+1} - \phi_{0,j}}{\epsilon_{j+1}} \qquad \text{on } S_6$$

$$= \frac{\phi_{1,j} - \phi_{0,j}}{\delta_1} \qquad \text{on } S_4\,, S_5$$

$$= 0 \qquad \text{on } S_1\,, S_8$$

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:

$$-\int_{S_3} d\vec{S}\, D(\vec{r})\frac{\partial}{\partial \hat{n}}\phi(\vec{r}) = \frac{\phi_{0,j} - \phi_{0,j-1}}{\epsilon_j}\left(\frac{D_{1,j}\delta_1}{2}\right)$$

$$-\int_{S_6} d\vec{S}\, D(\vec{r})\frac{\partial}{\partial \hat{n}}\phi(\vec{r}) = \frac{\phi_{0,j+1} - \phi_{0,j}}{\epsilon_{j+1}}\left(\frac{D_{1,j+1}\delta_1}{2}\right)$$

$$S_1 + S_8 = 0\,,$$

$$S_4 + S_5 = \frac{\phi_{1,j} - \phi_{0,j}}{\delta_1}\left(\frac{D_{1,j}\epsilon_j + D_{1,j+1}\epsilon_{j+1}}{2}\right)\,.$$

The absorption and streaming terms now become:

$$\int\int dxdy\, \Sigma_a(x,y)\phi(x,y) = \boxed{\phi_{0,j}\left(\Sigma_{a,1,j}V_{1,j} + \Sigma_{a,1,j+1}V_{1,j+1}\right) \equiv \Sigma^*_{a,0j}}\,,$$

$$\int\int dxdy\, S(x,y) = \boxed{S_{1,j}V_{1,j} + S_{1,j+1}V_{1,j+1} \equiv S^*_{0j}}\,.$$

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

$$\boxed{a^{0j}_{1,j}\phi_{1,j} + a^{*,0j}_{0,j-1}\phi_{0,j-1} + a^{*,0j}_{0,j+1}\phi_{0,j+1} + a^{*,0j}_{0,j}\phi_{0,j} = S^*_{0j}}$$
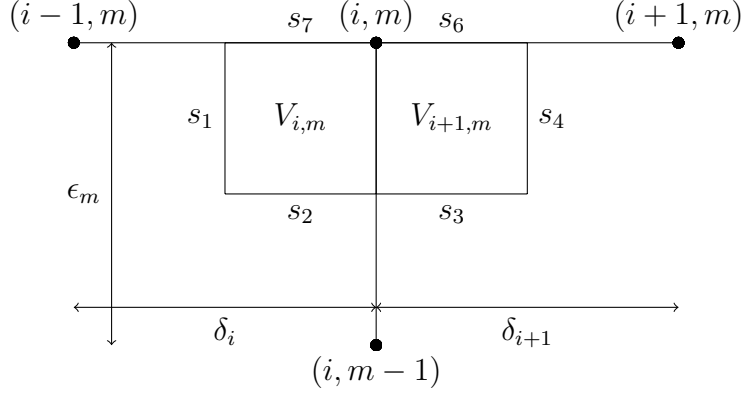
Recall: the lower index is the cell to which you are coupling, and the upper index is which cell you are in. The coefficients how change to become

$$a^{0j}_{1,j} = -\frac{D_{1,j}\epsilon_j + D_{1,j+1}\epsilon_{j+1}}{2\delta_1}$$

$$a^{*,0j}_{0,j-1} = -\frac{D_{1,j}\delta_1}{2\epsilon_j}$$

$$a^{*,0j}_{0,j+1} = -\frac{D_{1,j+1}\delta_1}{2\epsilon_{j+1}}$$

$$a^{*,0j}_{0,j} = \Sigma^*_{a,0j} - \left(a^{0j}_{1,j} + a^{*,0j}_{0,j-1} + a^{*,0j}_{0,j+1}\right)\,.$$

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 $y = b - \epsilon_m/2$ to $y = b$.

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

$$-\int_V d\vec{r}\left[\nabla \cdot \left(D(\vec{r})\nabla\phi(\vec{r})\right)\right]$$
$$= -\int_S d\vec{S}\, D(\vec{r})\frac{\partial}{\partial \hat{n}}\phi(\vec{r})$$

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:

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

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

The absorption and streaming terms now become:

$$\int\int dxdy\, \Sigma_a(x,y)\phi(x,y) = \boxed{\phi_{n,j}\left(\Sigma_{a,i,m}V_{i,m} + \Sigma_{a,i+1,m}V_{i+1,m}\right) \equiv \Sigma^*_{a,im}},$$

$$\int\int dxdy\, S(x,y) = \boxed{S_{i,m}V_{i,m} + S_{i+1,m}V_{i+1,m} \equiv S^*_{im}}.$$

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

$$\boxed{a^{*,im}_{i-1,m}\phi_{i-1,m} + a^{*,im}_{i,m-1}\phi_{i,m-1} + a^{*,im}_{i+1,m}\phi_{i+1,m} + a^{*,im}_{i,m}\phi_{i,m} = S^*_{im}}$$

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

$$a^{*,im}_{i-1,m} = -\frac{D_{i,m}\epsilon_m}{2\delta_i}$$

$$a^{*,im}_{i,m-1} = -\frac{D_{i,m}\delta_i + D_{i+1,m}\delta_{i+1}}{2\epsilon_m}$$

$$a^{*,im}_{i+1,m} = -\frac{D_{i+1,m}\epsilon_m}{2\delta_{i+1}}$$

$$a^{*,im}_{n,j} = \Sigma_{a,im} - \left(a^{*,im}_{i-1,m} + a^{*,im}_{i,m-1} + a^{*,im}_{i+1,m}\right).$$