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:

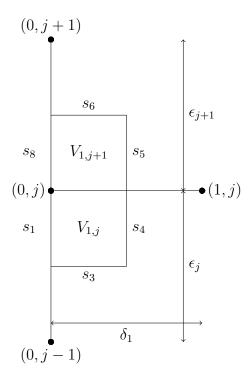
$$-\frac{\partial}{\partial x}D(x,y)\frac{\partial}{\partial x}\phi(x,y) - \frac{\partial}{\partial y}D(x,y)\frac{\partial}{\partial y}\phi(x,y) + \Sigma_a(x,y)\phi(x,y) = S(x,y)$$

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:

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

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 .

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

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

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

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

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:

$$\int \int dx dy \ \Sigma_{a}(x,y)\phi(x,y) = \left[\phi_{0,j}\left(\Sigma_{a,1,j}V_{1,j} + \Sigma_{a,1,j+1}V_{1,j+1}\right) \equiv \Sigma_{a,0j}^{*}\right],$$
$$\int \int dx dy \ S(x,y) = \left[S_{1,j}V_{1,j} + S_{1,j+1}V_{1,j+1} \equiv S_{0j}^{*}\right].$$

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

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

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

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

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

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

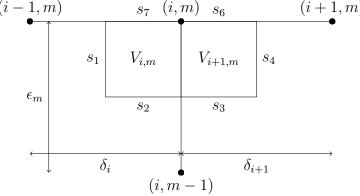
$$a_{0,j}^{*,0j} = \Sigma_{a,0j}^* - \left(a_{1,j}^{0j} + a_{0,j-1}^{*,0j} + a_{0,j+1}^{*,0j}\right).$$

TOP

The top boundary condition is:

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

$$s_7 \quad (i,m) \quad s_6 \qquad (i+1,m)$$



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 .

$$\frac{\partial}{\partial \hat{n}} \phi(\vec{r}) = \frac{\phi_{i-1,m} - \phi_{i,m}}{\delta_i} \quad \text{on } S_1$$

$$= \frac{\phi_{i+1,m} - \phi_{i,m}}{\delta_{i+1}} \quad \text{on } S_4$$

$$= \frac{\phi_{i,m-1} - \phi_{i,m}}{\epsilon_m} \quad \text{on } S_2, S_3$$

$$= 0 \quad \text{on } S_7, S_6$$

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:

$$\int \int dx dy \ \Sigma_a(x,y)\phi(x,y) = \left[\phi_{n,j}\left(\Sigma_{a,i,m}V_{i,m} + \Sigma_{a,i+1,m}V_{i+1,m}\right) \equiv \Sigma_{a,im}^*\right],$$
$$\int \int dx dy \ S(x,y) = \left[S_{i,m}V_{i,m} + S_{i+1,m}V_{i+1,m} \equiv S_{im}^*\right].$$

Collecting all of the terms and separating them, we get a 4-point difference equation for i = 1, ..., 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 how change to become

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

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

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

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