Discretization of the Diffusion Term

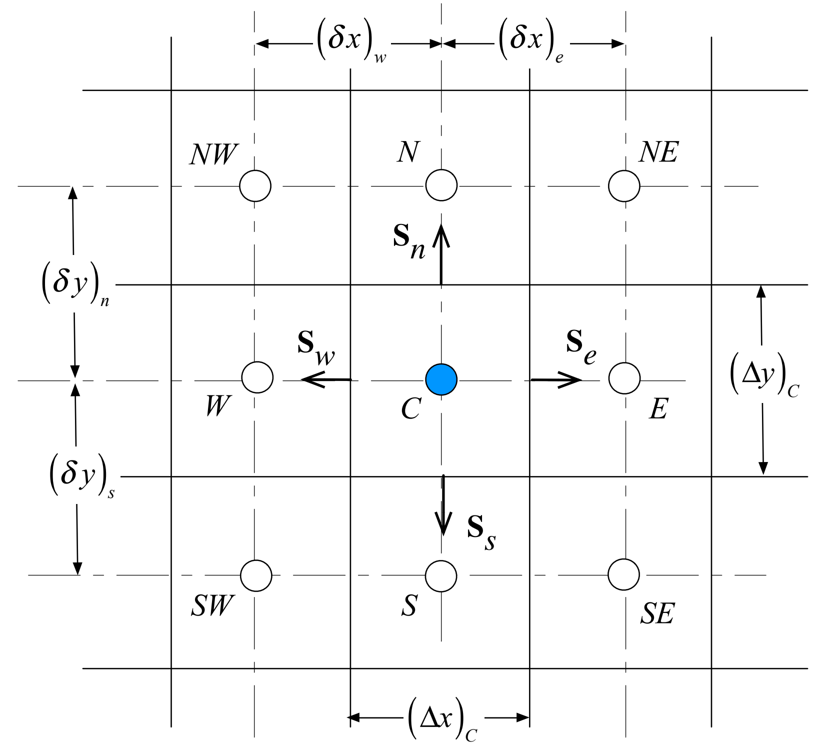
Chapter 08

Diffusion Equation

$$-\nabla \cdot \left(\Gamma \nabla \phi\right) = Q$$

$$\sum_{f\sim nb(C)} \left(-\Gamma^{\phi} \nabla \phi\right)_f \cdot \mathbf{S}_f = Q_C^{\phi} V_C$$

$$\left(-\Gamma^{\phi} \nabla \phi\right)_e \cdot \mathbf{S}_e + \left(-\Gamma^{\phi} \nabla \phi\right)_w \cdot \mathbf{S}_w$$
$$+\left(-\Gamma^{\phi} \nabla \phi\right)_n \cdot \mathbf{S}_n + \left(-\Gamma^{\phi} \nabla \phi\right)_s \cdot \mathbf{S}_s = Q_C^{\phi} V_C$$



$$\mathbf{S_e} = +(\Delta y)_e\,\mathbf{i} = \|\mathbf{S_e}\|\mathbf{i} = S_e\mathbf{i}$$
$$\mathbf{S}_w = -(\Delta y)_w\,\mathbf{i} = -\|\mathbf{S}_w\|\mathbf{i} = -S_w\mathbf{i}$$
$$\mathbf{S}_n = +(\Delta x)_n\,\mathbf{j} = \|\mathbf{S}_n\|\mathbf{j} = S_n\mathbf{j}$$
$$\mathbf{S}_s = -(\Delta x)_s\,\mathbf{j} = -\|\mathbf{S}_s\|\mathbf{j} = -S_s\mathbf{j}$$

$$J_e^{\phi,D} = -\left(\Gamma^{\phi} \nabla \phi\right)_e \cdot \mathbf{S}_e$$
$$= -\Gamma_e^{\phi} S_e \left(\frac{\partial \phi}{\partial x}\mathbf{i} + \frac{\partial \phi}{\partial y}\mathbf{j}\right)_e \cdot \mathbf{i}$$
$$= -\Gamma_e^{\phi} (\Delta y)_e \left(\frac{\partial \phi}{\partial x}\right)_e$$

$$J_e^{\phi,D} = FluxT_e = FluxC_e\phi_C + FluxF_e\phi_F + FluxV_e$$

2D Cartesian

$$\left(\frac{\partial\phi}{\partial x}\right)_e = \frac{\phi_E-\phi_C}{(\delta x)_e}$$

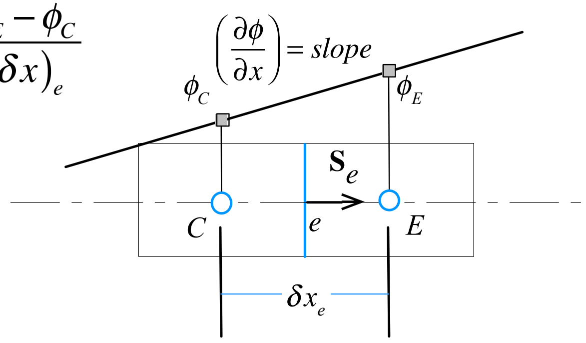


Figure 8.2 Interpolation profile at face e and slope of gradient.

$$\begin{aligned} FluxT_e &= -\Gamma_e^\phi(\Delta y)_e\frac{(\phi_E-\phi_C)}{\delta x_e} \\ &= \Gamma_e^\phi\frac{(\Delta y)_e}{\delta x_e}(\phi_C-\phi_E) \\ &= FluxC_e\phi_C + FluxF_e\phi_E + FluxV_e \end{aligned}$$

$$gDiff_e = \frac{(\Delta y)_e}{\delta x_e} = \frac{\|\mathbf{S}_e\|}{\|\mathbf{d}_{CE}\|} = \frac{S_e}{d_{CE}}$$

$$\begin{aligned} FluxC_e &= \Gamma_e^\phi gDiff_e \\ FluxF_e &= -\Gamma_e^\phi gDiff_e \\ FluxV_e &= 0 \end{aligned}$$

$$\begin{aligned} FluxT_w &= -\left(\Gamma^\phi\nabla\phi\right)_w\cdot\mathbf{S}_w \\ &= -\Gamma_w^\phi S_w\left(\frac{\partial\phi}{\partial x}\mathbf{i}+\frac{\partial\phi}{\partial y}\mathbf{j}\right)_w\cdot(-\mathbf{i}) \\ &= \Gamma_w^\phi S_w\left(\frac{\partial\phi}{\partial x}\right)_w \\ &= \Gamma_w^\phi S_w\frac{(\phi_C-\phi_W)}{(\delta x)_w} \\ &= FluxC_w\phi_C + FluxF_w\phi_W + FluxV_w \end{aligned}$$

$$\begin{aligned} FluxC_w &= \Gamma_w^\phi gDiff_w \\ FluxF_w &= -\Gamma_w^\phi gDiff_w \\ FluxV_w &= 0 \end{aligned}$$

Algebraic form

$$_P\phi_P + a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S = b_P$$

$$\begin{aligned}
a_E &= FluxF_e = -\Gamma_e^\phi gDiff_e \\
a_W &= FluxF_w = -\Gamma_w^\phi gDiff_w \\
a_N &= FluxF_n = -\Gamma_n^\phi gDiff_n \\
a_S &= FluxF_s = -\Gamma_s^\phi gDiff_s \\
a_C &= FluxC_e + FluxC_w + FluxC_n + FluxC_s \\
&= -\left(a_E + a_W + a_N + a_S\right) \\
b_C &= Q_C^\phi V_C - \left(FluxV_e + FluxV_w + FluxV_n + FluxV_s\right)
\end{aligned}$$

$$a_C\phi_C + \sum_{F\sim NB(C)} a_F\phi_F = b_C$$

$$\begin{aligned}
a_F &= FluxF_f = -\Gamma_f^\phi gDiff_f \\
a_C &= \sum_{f\sim nb(C)} FluxC_f \\
b_C &= Q_C^\phi V_C - \sum_{f\sim nb(C)} FluxV_f
\end{aligned}$$

Properties of the Discretized Equation

The Zero Sum Rule

With a zero source term $-\nabla\cdot\left(\Gamma^{\phi}\nabla\phi\right)=0$

if ϕ is a solution then $\phi + constant$ should also be a solutions to the equation

$$\left.\begin{aligned}&a_C\phi_C+\sum_{F\sim NB(C)}a_F\phi_F=0\\&a_C\left(\phi_C+constant\right)+\sum_{F\sim NB(C)}a_F\left(\phi_F+constant\right)=0\end{aligned}\right\}\Rightarrow a_C+\sum_{F\sim NB(C)}a_F=0$$

The Opposite Signs Rule

$$\sum_{F\sim NB(C)}\frac{a_F}{a_C}=-1$$

BC: Dirichlet

$$FluxT_b = -\Gamma_b^\phi (\nabla\phi)_b \cdot \mathbf{S}_b$$
$$= -\Gamma_b^\phi \frac{\|\mathbf{S}_b\|}{\|\mathbf{d}_{Cb}\|}(\phi_b - \phi_C)$$
$$= FluxC_b \phi_C + FluxV_b$$

$$\phi_b = \phi_{specified}$$

$$FluxC_b = \Gamma_b^\phi gDiff_b = a_b$$
$$FluxV_b = -\Gamma_b^\phi gDiff_b \phi_b = -a_b \phi_b$$

$$gDiff_b = \frac{S_b}{d_{CB}}$$

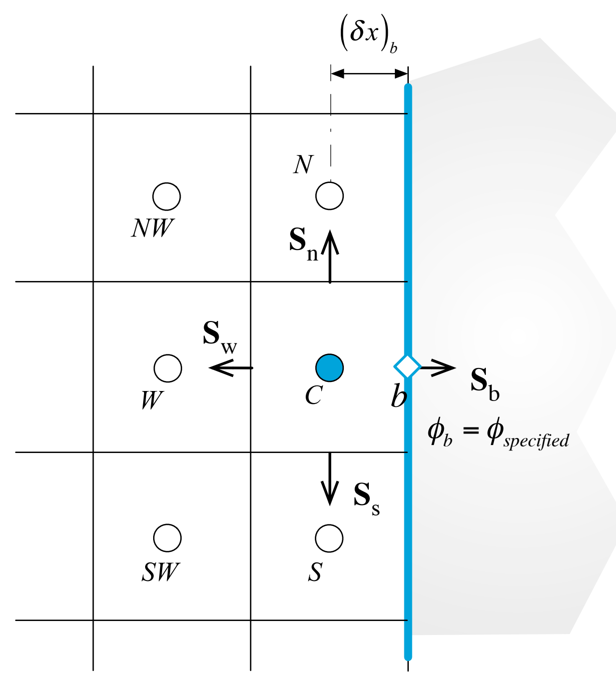


Figure 8.3 Value specified boundary condition.

$$a_C \phi_C + a_W \phi_W + a_N \phi_N + a_S \phi_S = b_C$$
$$a_E = 0$$
$$a_W = FluxF_w = -\Gamma_w^\phi gDiff_w$$
$$a_N = FluxF_n = -\Gamma_n^\phi gDiff_n$$
$$a_S = FluxF_s = -\Gamma_s^\phi gDiff_s$$
$$a_C = FluxC_b + \sum_{f\sim nb(C)} FluxC_f = FluxC_b + (FluxC_w + FluxC_n + FluxC_s)$$

$$b_C = Q_C^\phi V_C - \left(FluxV_b + \sum_{f\sim nb(C)} FluxV_f \right)$$

BC: Von Newmann

$$\mathbf{J}_b^{\phi,D} \cdot \mathbf{S}_b = -\left(\Gamma^{\phi}\nabla\phi\right)_b \cdot \|\mathbf{S}_b\| \mathbf{i} = q_b \|\mathbf{S}_b\|$$
$$= FluxC_b \phi_C + FluxV_b$$

$$-\left(\Gamma^{\phi}\nabla\phi\right)_b \cdot \mathbf{i} = q_b$$

$$FluxC_b = 0$$
$$FluxV_b = q_b S_b$$
$$= q_b (\Delta y)_C$$

$$a_C\phi_C + a_W\phi_W + a_N\phi_N + a_S\phi_S = b_C$$

$$a_E = 0$$
$$a_W = FluxF_w = -\Gamma_w^{\phi} gDiff_w$$
$$a_N = FluxF_n = -\Gamma_n^{\phi} gDiff_n$$
$$a_S = FluxF_s = -\Gamma_s^{\phi} gDiff_s$$
$$a_C = \sum_{f\sim nb(C)} FluxC_f = -\left(a_W + a_N + a_S\right)$$

$$b_C = Q_C^{\phi} V_C - \left(FluxV_b + \sum_{f\sim nb(C)} FluxV_f \right)$$

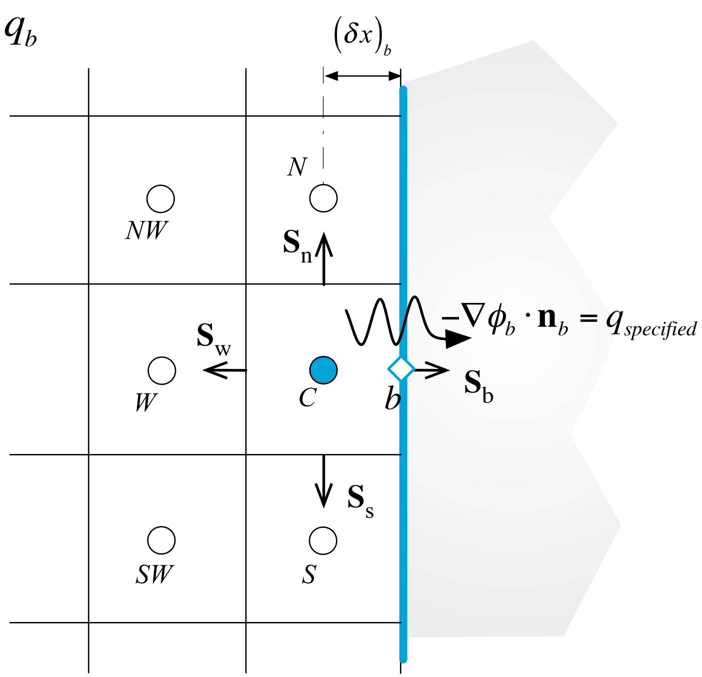


Figure 8.4 flux specified boundary condition.

BC: Mixed

$$\mathbf{J}_b^{\phi,D}\cdot\mathbf{S}_b = -\left(\Gamma^\phi\nabla\phi\right)_b\cdot\mathbf{i}S_b = -h_\infty\left(\phi_\infty-\phi_b\right)(\Delta y)_C$$

$$-\Gamma_b^\phi S_b\left(\frac{\phi_b-\phi_C}{\delta x_b}\right) = -h_\infty\left(\phi_\infty-\phi_b\right)S_b$$

$$\phi_b = \frac{h_\infty\phi_\infty+\left(\Gamma_b^\phi/\delta x_b\right)\phi_C}{h_\infty+\left(\Gamma_b^\phi/\delta x_b\right)}$$

$$\mathbf{J}_b^{\phi,D}\cdot\mathbf{S}_b = -\underbrace{\left[\frac{h_\infty\left(\Gamma_b^\phi/\delta x_b\right)}{h_\infty+\left(\Gamma_b^\phi/\delta x_b\right)}S_b\right]}_{R_{eq}}\left(\phi_\infty-\phi_C\right)$$

$$= FluxC_b\phi_C + FluxV_b$$

$$FluxC_b = R_{eq}$$

$$FluxV_b = -R_{eq}\phi_\infty$$

$$a_C\phi_C + a_W\phi_W + a_N\phi_N + a_S\phi_S = b_C$$

$$a_E = 0$$

$$a_W = FluxF_w = -\Gamma_w^\phi gDiff_w$$

$$a_N = FluxF_n = -\Gamma_n^\phi gDiff_n$$

$$a_S = FluxF_s = -\Gamma_s^\phi gDiff_s$$

$$a_C = FluxC_b + \sum_{f\sim nb(C)} FluxC_f = \left(FluxC_b + FluxC_w + FluxC_n + FluxC_s\right)$$

$$b_C = Q_C^\phi V_C - \left(FluxV_b + \sum_{f=nb(C)} FluxV_f\right)$$

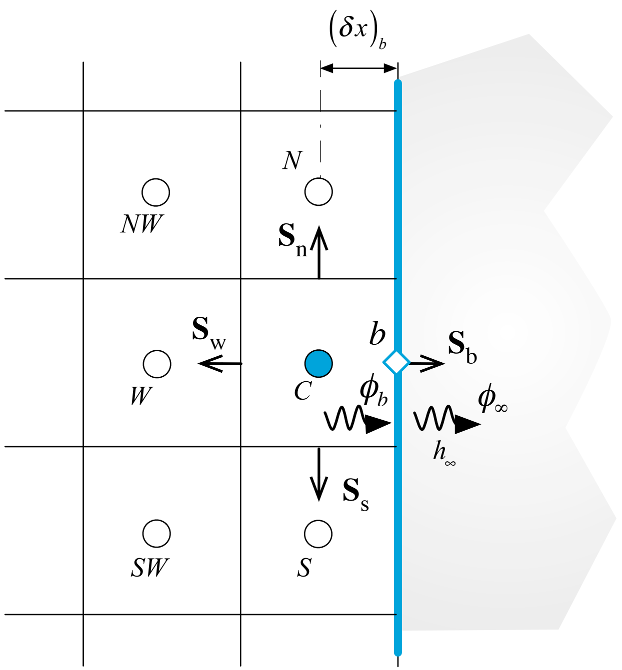
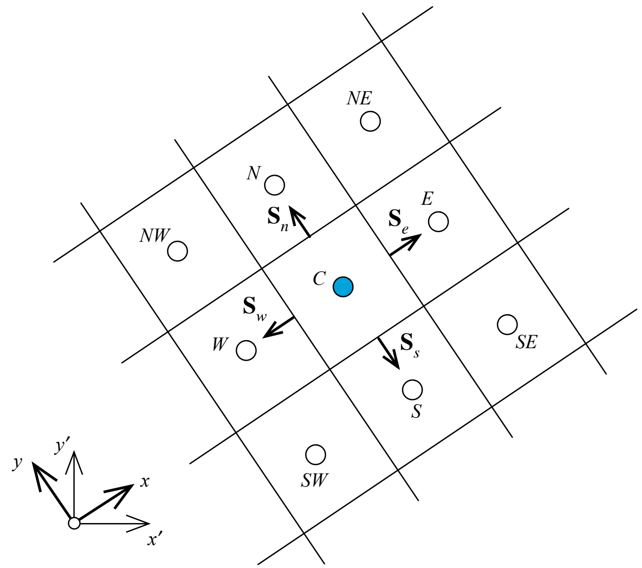
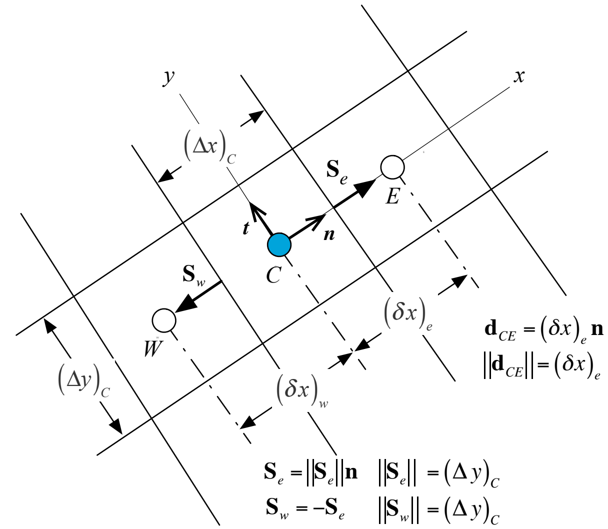


Figure 8.5 Mixed type boundary condition.

Orthogonal Non-Cartesian Grids





$$\nabla \cdot \mathbf{J}^D = Q$$

$$\sum_{\sim f=nb(P)} -(\Gamma \nabla \phi)_f \cdot \mathbf{S}_f = Q_P V_P$$

$$\mathbf{J}_\mathbf{e}^\mathbf{D} \cdot \mathbf{S}_\mathbf{e} = -\Gamma_e (\nabla \phi . \mathbf{n})_e S_e = -\Gamma_e \left(\frac{\partial \phi}{\partial n} \right)_e S_e \qquad (\nabla \phi . \mathbf{n})_e = \left(\frac{\partial \phi}{\partial n} \right)_e \qquad \left(\frac{\partial \phi}{\partial n} \right)_e = \frac{\phi_E - \phi_P}{\delta x'_{PE}}$$

Non-Orthogonal Grids

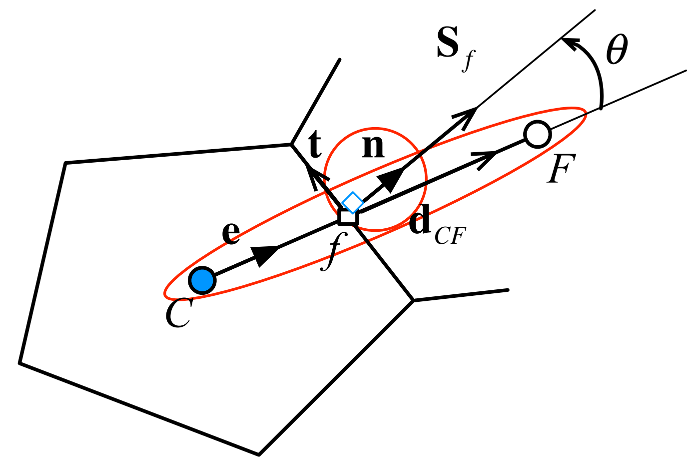
$$(\nabla\phi\cdot\mathbf{n})_f = \left(\frac{\partial\phi}{\partial n}\right)_f \neq \frac{\phi_F-\phi_C}{\|\mathbf{r}_F-\mathbf{r}_C\|} = \frac{\phi_F-\phi_C}{d_{CF}}$$

$$(\nabla\phi\cdot e)_f = \left(\frac{\partial\phi}{\partial e}\right)_f = \frac{\phi_F-\phi_C}{\|\mathbf{r}_F-\mathbf{r}_C\|} = \frac{\phi_F-\phi_C}{d_{CF}}$$

$$(\nabla\phi)_f\cdot\mathbf{S}_f = \underbrace{(\nabla\phi)_f\cdot\overbrace{\mathbf{E}_f}^{E_f\mathbf{e}}}_{\text{orthogonal-like contribution}} + \underbrace{(\nabla\phi)_f\cdot\mathbf{T}}_{\text{non-orthogonal like contribution}}$$

$$= E_f\left(\frac{\partial\phi}{\partial e}\right)_f + (\nabla\phi)_f\cdot\mathbf{T}_f$$

$$= E_f\frac{\phi_F-\phi_C}{d_{CF}} + (\nabla\phi)_f\cdot\mathbf{T}_f$$



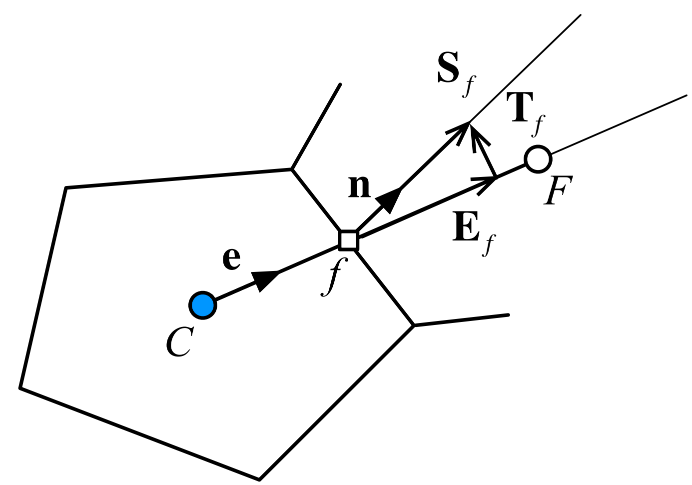
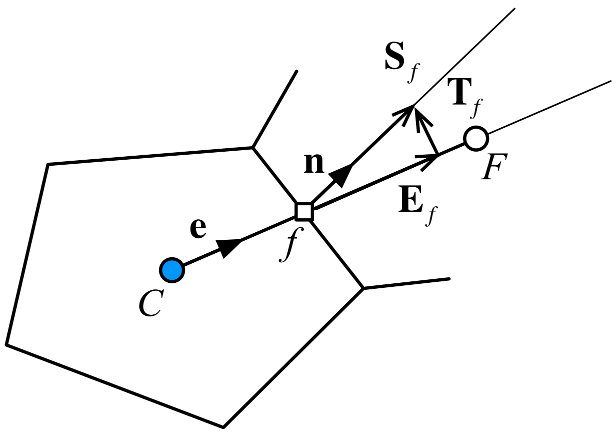
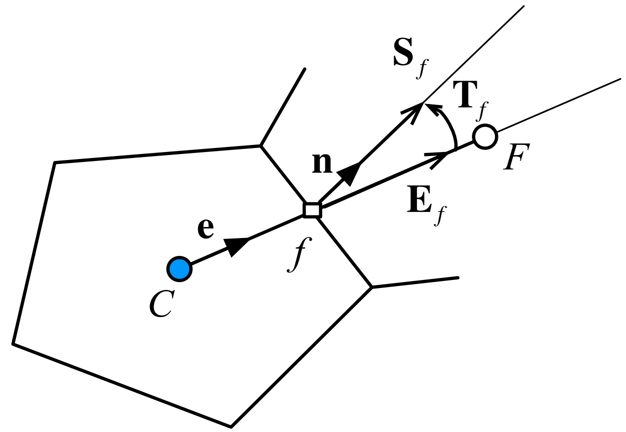


Figure 8.9 Decomposing $\mathbf{S}_f$ via the minimum correction approach.

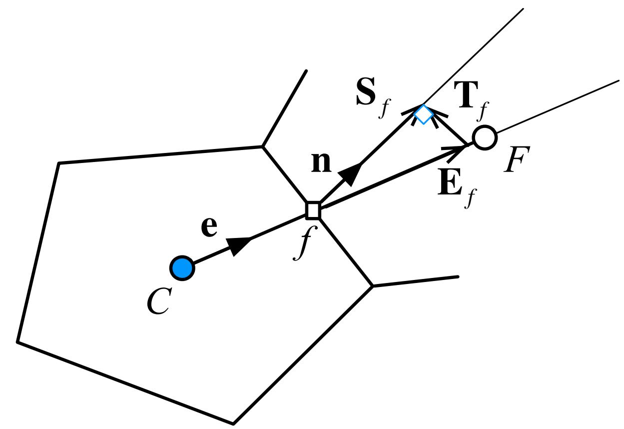
E Computation



$$\mathbf{E}_f = \left(\frac{S_f}{\cos\theta}\right)\mathbf{e} = \left(\frac{S_f^2}{S_f\cos\theta}\right)\mathbf{e} = \frac{\mathbf{S}_f\cdot\mathbf{S}_f}{\mathbf{e}\cdot\mathbf{S}_f}\mathbf{e}$$



$$\mathbf{E}_f = S_f\mathbf{e}$$



$$\mathbf{E}_f = \left(\mathbf{e}\cdot\mathbf{S}_f\right)\mathbf{e} = \left(S_f\cos\theta\right)\mathbf{e}$$

$$(\nabla\phi)_f\cdot\mathbf{T}_f = (\nabla\phi)_f\cdot\left(\mathbf{S}_f - \mathbf{E}_f\right)$$

$$= \begin{cases} (\nabla\phi)_f\cdot(\mathbf{n} - \cos\theta\mathbf{e})S_f & \textit{minimum correction} \\ (\nabla\phi)_f\cdot(\mathbf{n} - \mathbf{e})S_f & \textit{normal correction} \\ (\nabla\phi)_f\cdot\left(\mathbf{n} - \dfrac{1}{\cos\theta}\mathbf{e}\right)S_f & \textit{over-relaxed} \end{cases}$$

Treatment of Non-Orthogonal Term

$$
\begin{aligned}
\sum_{f\sim nb(C)} \left(\mathbf{J}_f^{\phi,D}\cdot\mathbf{S}_f\right) &= \sum_{f\sim nb(C)} \left(-\left(\Gamma^{\phi}\nabla\phi\right)_f\cdot\left(\mathbf{E}_f+\mathbf{T}_f\right)\right) \\
&= \underbrace{\sum_{f\sim nb(C)} \left(-\left(\Gamma^{\phi}\nabla\phi\right)_f\cdot\mathbf{E}_f\right)}_{\substack{Orthogonal \\ Linearizeable \\ Part}} + \underbrace{\sum_{f\sim nb(C)} \left(-\left(\Gamma^{\phi}\nabla\phi\right)_f\cdot\mathbf{T}_f\right)}_{\substack{Non-Orthogonal \\ Non-Linearizeable \\ Part}} \\
&= \sum_{f\sim nb(C)} \left(-\Gamma_f^{\phi}E_f\frac{\left(\phi_F-\phi_C\right)}{d_{CF}}\right) + \sum_{f\sim nb(C)} \left(-\left(\Gamma^{\phi}\nabla\phi\right)_f\cdot\mathbf{T}_f\right) \\
&= \sum_{f\sim nb(C)} \Gamma_f^{\phi}gDiff_f\left(\phi_C-\phi_F\right) + \sum_{f\sim nb(C)} \left(-\left(\Gamma^{\phi}\nabla\phi\right)_f\cdot\mathbf{T}_f\right) \\
&= \left(\sum_{f\sim nb(C)} FluxC_f\right)\phi_C + \sum_{f\sim nb(C)} \left(FluxF_f\phi_F\right) + \sum_{f\sim nb(C)} \left(FluxV_f\right)
\end{aligned}
$$

$$
gDiff_f = \frac{E_f}{d_{CF}}
$$

Discretized Equation

$$a_C\phi_C + \sum_{F\sim NB(C)} a_F\phi_F = b_C$$

$$a_F = FluxF_f = -\Gamma_f^{\phi} gDiff_f$$

$$a_C = \sum_{f\sim nb(C)} FluxC_f = -\sum_{f\sim nb(C)} FluxF_f = \sum_{f\sim nb(C)} \Gamma_f^{\phi} gDiff_f$$

$$b_C = Q_C^{\phi}V_C - \sum_{f\sim nb(C)}\left(FluxV_f\right) = S_C^{\phi}V_C + \sum_{f\sim nb(C)}\left(\left(\Gamma^{\phi}\nabla\phi\right)_f \cdot \mathbf{T}_f\right)$$

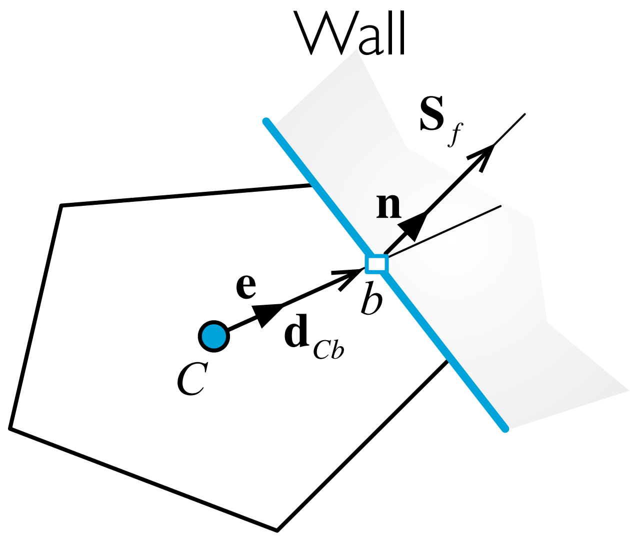
Boundary Conditions

BC: Temperature Specified

$$\mathbf{J}_b^{\phi,D}\cdot\mathbf{S_b} = -\Gamma_b^{\phi}\left(\nabla\phi\right)_b\cdot\mathbf{S_b} = -\Gamma_b^{\phi}\left(\nabla\phi\right)_b\cdot\left(\mathbf{E_b}+\mathbf{T_b}\right)$$

$$= -\Gamma_b^{\phi}\left(\frac{\phi_b-\phi_C}{d_{Pb}}\right)E_b - \Gamma_b^{\phi}\left(\nabla\phi\right)_b\cdot\mathbf{T_b}$$

$$= FluxC_b\phi_C + FluxV_b$$



$$FluxC_b = \Gamma_b^{\phi} gDiff_b$$

$$FluxV_b = -\Gamma_b^{\phi} gDiff_b\phi_b - \Gamma_b^{\phi}\left(\nabla\phi\right)_b\cdot\mathbf{T_b}$$

$$gDiff_b = \frac{E_b}{d_{Pb}}$$

$$a_F = FluxF_f \qquad a_C = \sum_{f\sim nb(C)} FluxC_f + FluxC_b$$

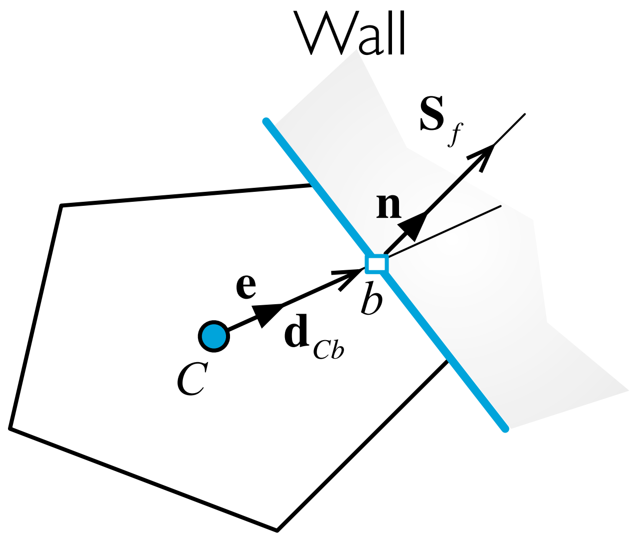
$$b_C = Q_C^{\phi}V_C - FluxV_b - \sum_{f\sim nb(C)} FluxV_f$$

BC: Flux Specified

$$\underbrace{\left(-\Gamma\nabla\phi\right)_b \cdot \mathbf{n_b}}_{Specified\ Flux} = q_{b,specified}$$

$$\mathbf{J}_b^{\phi,D} \cdot \mathbf{S} = FluxC_b\phi_C + FluxV_b \qquad FluxC_b = 0$$

$$FluxV_f = q_{b,specified}$$



Under-Relaxation

Under-Relaxation

$$a_P\phi_P + \sum_{NB(P)} a_{NB}\phi_{NB} = b_P$$

$$\phi_P = \frac{-\sum\limits_{NB(P)} a_{NB}\phi_{NB} + b_P}{a_P}$$

$$\phi_P = \phi_P^* + \left(\frac{-\sum\limits_{NB(P)} a_{NB}\phi_{NB} + b_P}{a_P} - \phi_P^* \right)$$

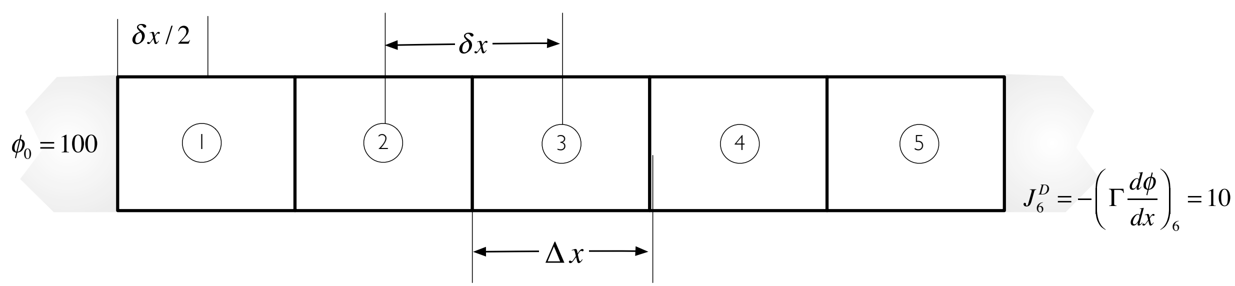
$$a_P \leftarrow \frac{a_P}{\lambda}$$

$$b_P \leftarrow b_P + \frac{(1-\lambda)a_P}{\lambda}\phi_P^*$$

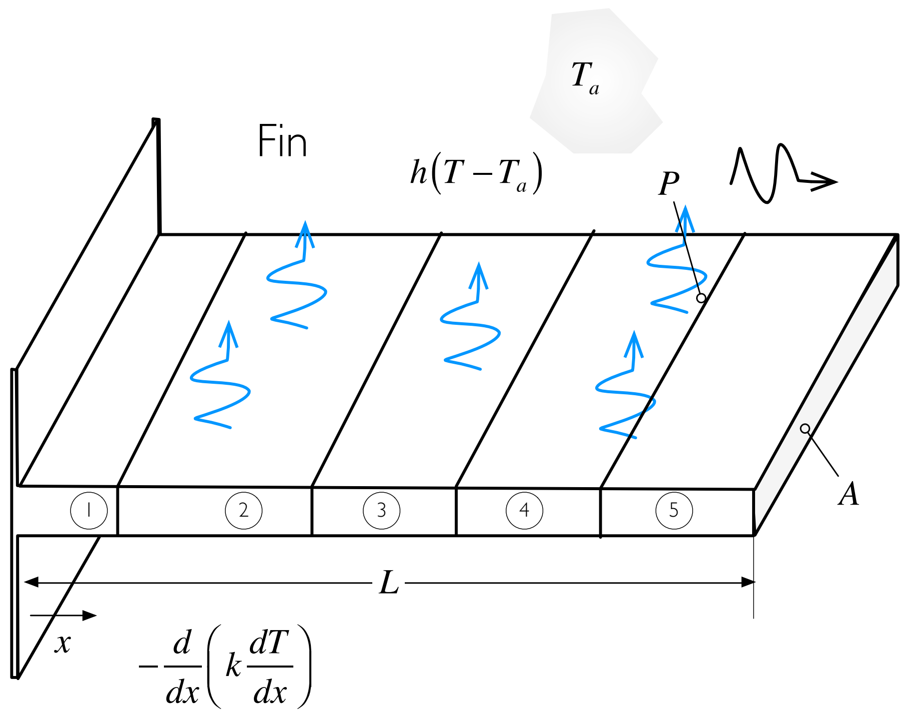
$$\phi_P = \phi_P^* + \lambda\left(\frac{-\sum\limits_{NB(P)} a_{NB}\phi_{NB} + b_P}{a_P} - \phi_P^* \right)$$

$$\frac{a_P}{\lambda}\phi_P + \sum_{NB(P)} a_{NB}\phi_{NB} = b_P + \frac{(1-\lambda)a_P}{\lambda}\phi_P^*$$

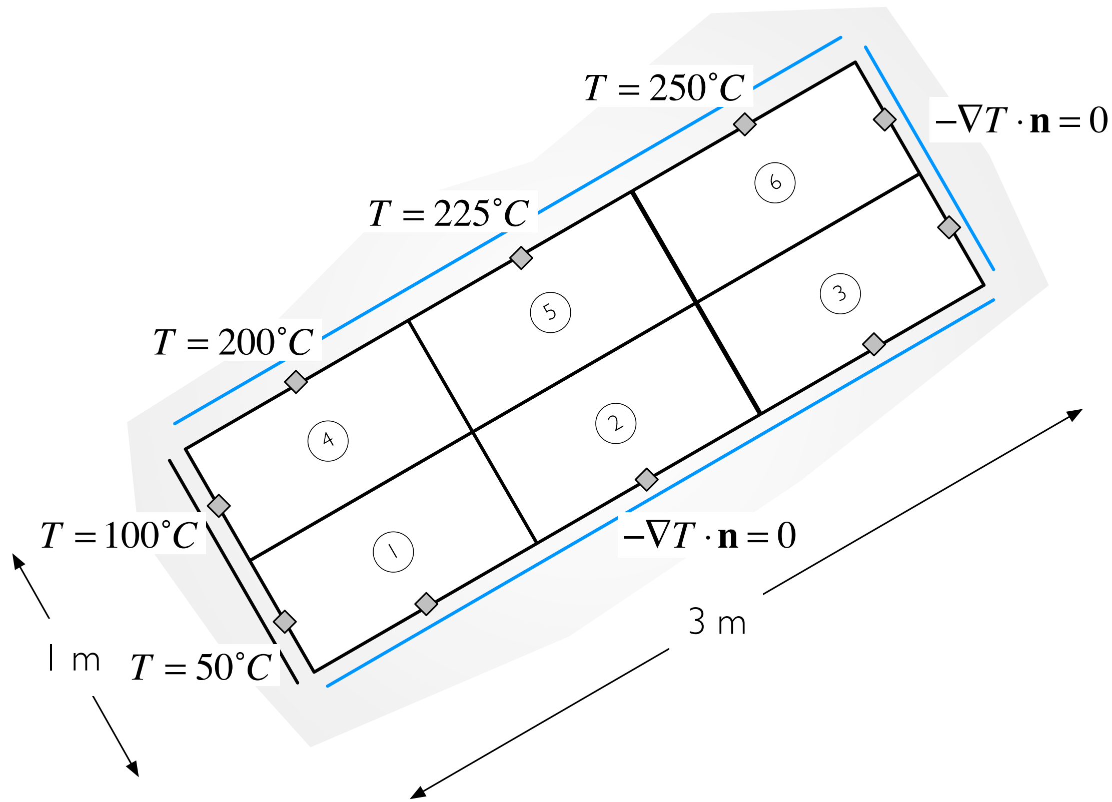
Exercises



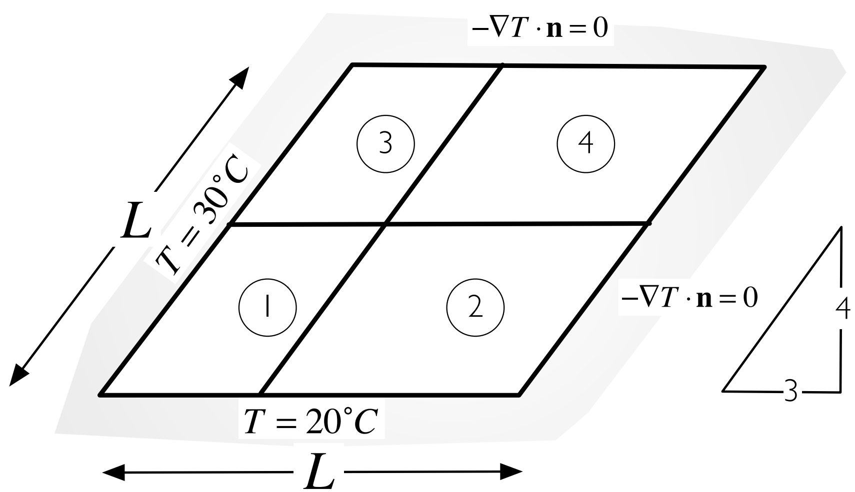
$\delta x/2$
δx
$\phi_0 = 100$
1
2
3
4
5
$J_6^D = -\left(\Gamma \frac{d\phi}{dx}\right)_6 = 10$
Δx

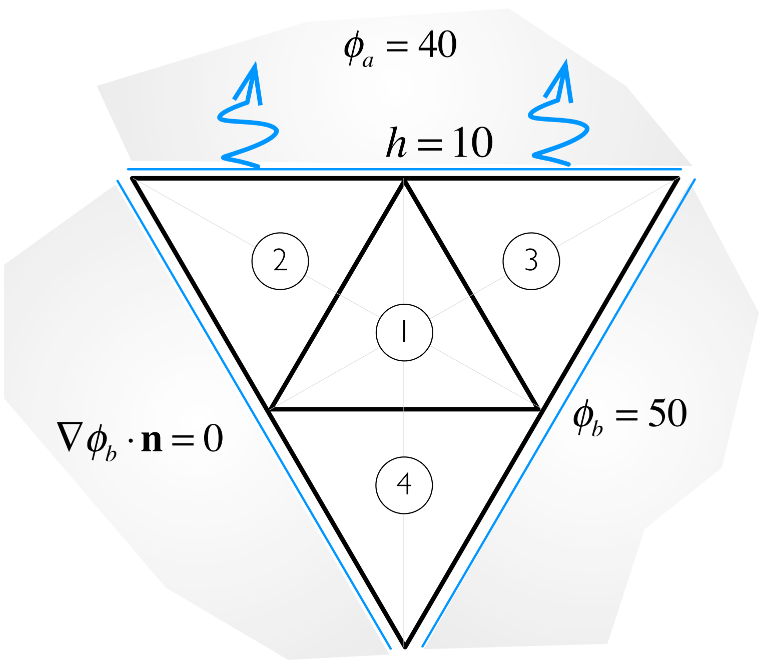


T_a
Fin
$h(T-T_a)$
P
1
2
3
4
5
A
L
x
$-\frac{d}{dx}\left(k\frac{dT}{dx}\right)$



$T = 250^\circ C$
$-\nabla T \cdot \mathbf{n} = 0$
$T = 225^\circ C$
$T = 200^\circ C$
6
5
3
4
2
1
$T = 100^\circ C$
$-\nabla T \cdot \mathbf{n} = 0$
3 m
1 m
$T = 50^\circ C$


$-\nabla T \cdot \mathbf{n} = 0$
3
4
L
$T = 30^\circ C$
1
2
$-\nabla T \cdot \mathbf{n} = 0$
4
3
$T = 20^\circ C$
L



$\phi_a = 40$
$h = 10$
2
3
1
4
$\phi_b = 50$
$\nabla \phi_b \cdot \mathbf{n} = 0$