

|                                             |  |
|---------------------------------------------|--|
| 1. The Discretisation Scheme .....          |  |
| 1.1. Discretisation in the bulk .....       |  |
| 1.2. Discretisation at the boundaries ..... |  |
| 1.2.1. At the Eastern boundary: .....       |  |
| 1.2.2. At the Western Boundary .....        |  |
| 1.2.3. At the Southern Boundary .....       |  |
| 1.2.4. At the Northern Boundary .....       |  |
| 2. Summary of equations .....               |  |
| 3. Using the code .....                     |  |

## 1. The Discretisation Scheme

Consider a general equation:

$$k\phi + \vec{\nabla} \cdot (C_y \phi \hat{j} + C_z \phi \hat{k}) + \vec{\nabla} \cdot \left( D_y \frac{\partial \phi}{\partial y} \hat{j} + D_z \frac{\partial \phi}{\partial z} \hat{k} \right) = S$$

where,

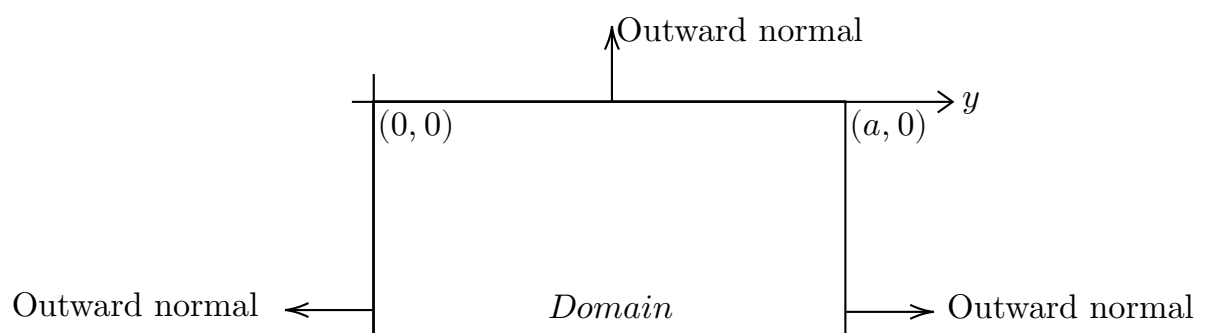
$$\vec{\nabla} = \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}$$

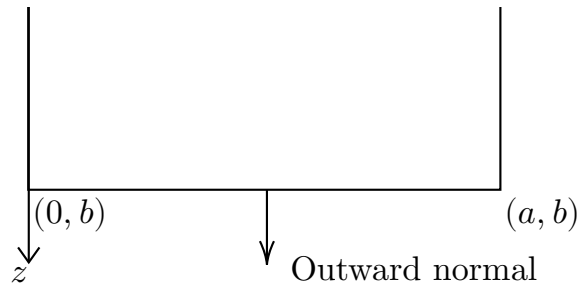
This equation is subject to boundary conditions:

$$\alpha\phi + \beta \frac{\partial \phi}{\partial n} = G$$

at the walls. The direction  $n$  the outward normal. Thus,

$$\begin{aligned} \frac{\partial \phi}{\partial n} &= -\frac{\partial \phi}{\partial y} \text{ at } y = 0 \\ \frac{\partial \phi}{\partial n} &= +\frac{\partial \phi}{\partial y} \text{ at } y = a \\ \frac{\partial \phi}{\partial n} &= -\frac{\partial \phi}{\partial z} \text{ at } z = 0 \\ \frac{\partial \phi}{\partial n} &= +\frac{\partial \phi}{\partial z} \text{ at } z = b \end{aligned}$$



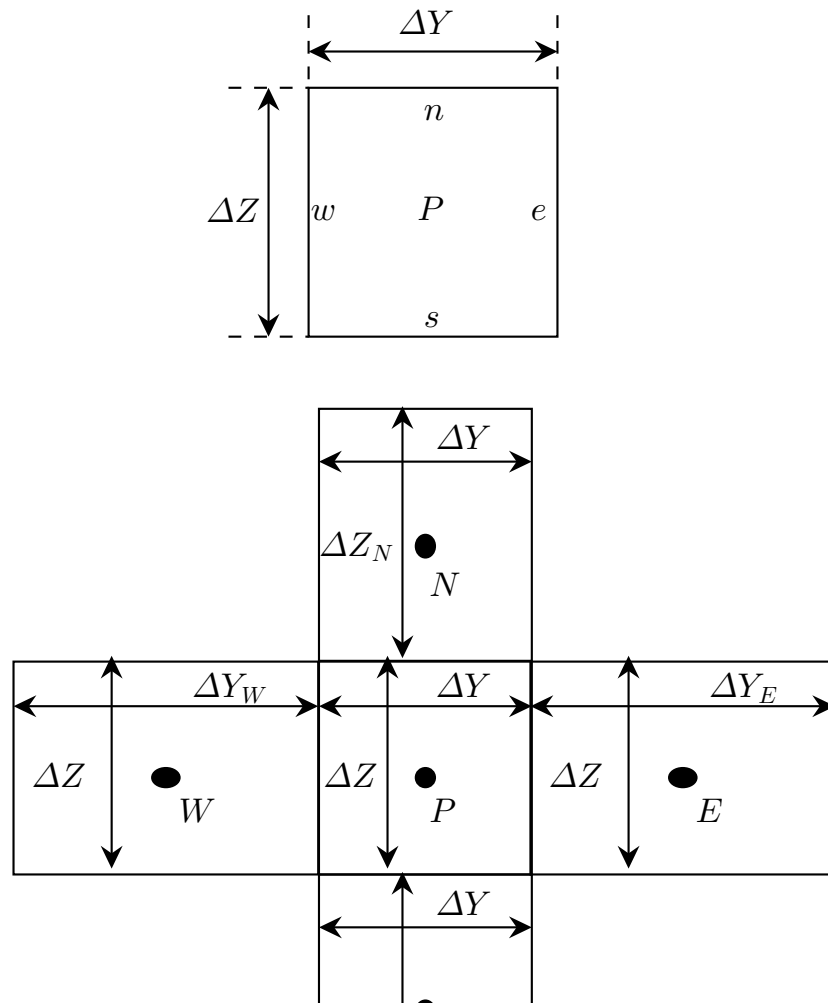


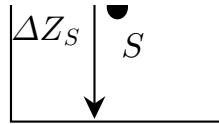
Expanding eq. (1), and setting  $k = S = 0$ ,

$$\left( \frac{\partial C_y \phi}{\partial y} + \frac{\partial C_z \phi}{\partial z} \right) + \left( \frac{\partial}{\partial y} D_y \frac{\partial \phi}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial \phi}{\partial z} \right) = 0$$

### 1.1. Discretisation in the bulk

Consider a typical cell as shown below





Integrating eq. (3) on this cell, we get

$$\left( \frac{\partial C_y \phi}{\partial y} + \frac{\partial C_z \phi}{\partial z} \right) + \left( \frac{\partial}{\partial y} D_y \frac{\partial \phi}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial \phi}{\partial z} \right) = 0$$

$$\left( \frac{\Delta Z (C_{y,e} \phi_e - C_{y,w} \phi_w)}{\Delta Y \Delta Z} + \frac{\Delta Y (C_{z,s} \phi_s - C_{z,n} \phi_n)}{\Delta Y \Delta Z} \right) +$$

$$\left( \frac{\Delta Z \left( D_{y,e} \frac{\partial \phi}{\partial y} \Big|_e - D_{y,w} \frac{\partial \phi}{\partial y} \Big|_w \right)}{\Delta Y \Delta Z} + \frac{\Delta Y \left( D_{z,s} \frac{\partial \phi}{\partial z} \Big|_s - D_{z,n} \frac{\partial \phi}{\partial z} \Big|_n \right)}{\Delta Y \Delta Z} \right) = 0$$

Where,

$$\phi_e = \frac{\Delta Y_E \phi_P + \Delta Y \phi_E}{\Delta Y_E + \Delta Y}$$

$$\phi_w = \frac{\Delta Y_W \phi_P + \Delta Y \phi_W}{\Delta Y_W + \Delta Y}$$

$$\phi_s = \frac{\Delta Z_S \phi_P + \Delta Z \phi_S}{\Delta Z_S + \Delta Z}$$

$$\phi_n = \frac{\Delta Z_N \phi_P + \Delta Z \phi_N}{\Delta Z_N + \Delta Z}$$

$$\frac{\partial \phi}{\partial y} \Big|_e = \frac{2(\phi_E - \phi_P)}{\Delta Y_E + \Delta Y}$$

$$\frac{\partial \phi}{\partial y} \Big|_w = \frac{2(\phi_P - \phi_W)}{\Delta Y_W + \Delta Y}$$

$$\frac{\partial \phi}{\partial z} \Big|_s = \frac{2(\phi_S - \phi_P)}{\Delta Z_S + \Delta Z}$$

$$\frac{\partial \phi}{\partial z} \Big|_n = \frac{2(\phi_P - \phi_N)}{\Delta Z_N + \Delta Z}$$

$$C_{y,e} = \frac{\Delta Y_E C_{y,P} + \Delta Y C_{y,E}}{\Delta Y_E + \Delta Y}$$

$$C_{y,w} = \frac{\Delta Y_W C_{y,P} + \Delta Y C_{y,W}}{\Delta Y_W + \Delta Y}$$

$$C_{z,s} = \frac{\Delta Z_S C_{z,P} + \Delta Z C_{z,S}}{\Delta Z_S + \Delta Z}$$

$$C_{z,n} = \frac{\Delta Z_N C_{z,P} + \Delta Z C_{z,N}}{\Delta Z_N + \Delta Z}$$

$$\frac{\Delta Y_E + \Delta Y}{D_{y,e}} = \frac{\Delta Y_E}{D_{y,E}} + \frac{\Delta Y}{D_{y,P}}$$

$$\frac{\Delta Y_W + \Delta Y}{D_{y,w}} = \frac{\Delta Y_W}{D_{y,W}} + \frac{\Delta Y}{D_{y,P}}$$

$$\frac{\Delta Z_E + \Delta Z}{D_{y,e}} = \frac{\Delta Z_E}{D_{y,E}} + \frac{\Delta Z}{D_{y,P}}$$

$$\frac{\Delta Z_W + \Delta YZ}{D_{y,w}} = \frac{\Delta Y_W}{D_{y,W}} + \frac{\Delta Z}{D_{y,P}}$$

Expanding eq. 5,

$$\begin{aligned} & \frac{\Delta Z \left( \frac{C_{y,e} \Delta Y_E}{\Delta Y_E + \Delta Y} \phi_P + \frac{C_{y,e} \Delta Y}{\Delta Y_E + \Delta Y} \phi_E - \frac{C_{y,w} \Delta Y_W}{\Delta Y_W + \Delta Y} \phi_P - \frac{C_{y,w} \Delta Y}{\Delta Y_W + \Delta Y} \phi_W \right)}{\Delta Y \Delta Z} + \\ & \frac{\Delta Y \left( \frac{C_{z,s} \Delta Z_S}{\Delta Z_S + \Delta Z} \phi_P + \frac{C_{z,s} \Delta Z}{\Delta Z_S + \Delta Z} \phi_S - \frac{C_{z,n} \Delta Z_N}{\Delta Z_N + \Delta Z} \phi_P - \frac{C_{z,n} \Delta Z}{\Delta Z_N + \Delta Z} \phi_N \right)}{\Delta Y \Delta Z} + \\ & \frac{\Delta Z \left( \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} \phi_E - \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} \phi_P - \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \phi_P + \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \phi_W \right)}{\Delta Y \Delta Z} + \\ & \frac{\Delta Y \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} \phi_S - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} \phi_P - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \phi_P + \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \phi_N \right)}{\Delta Y \Delta Z} = 0 \end{aligned}$$

This may be written as

$$N_{Bulk} \phi_N + E_{Bulk} \phi_E + W_{Bulk} \phi_W + S_{Bulk} \phi_S + P_{Bulk} \phi_P = R_{Bulk}$$

where,

$$\begin{aligned}
N_{Bulk} &= \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} - \frac{C_{z,n} \Delta Z}{\Delta Z_N + \Delta Z} \right) \\
E_{Bulk} &= \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} + \frac{C_{y,e} \Delta Y}{\Delta Y_E + \Delta Y} \right) \\
W_{Bulk} &= \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} - \frac{C_{y,w} \Delta Y}{\Delta Y_W + \Delta Y} \right) \\
S_{Bulk} &= \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} + \frac{C_{z,s} \Delta Z}{\Delta Z_S + \Delta Z} \right) \\
P_{Bulk} &= \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{C_{z,s} \Delta Z_S}{\Delta Z_S + \Delta Z} - \frac{C_{z,n} \Delta Z_N}{\Delta Z_N + \Delta Z} - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \right) \\
&\quad + \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{C_{y,e} \Delta Y_E}{\Delta Y_E + \Delta Y} - \frac{C_{y,w} \Delta Y_W}{\Delta Y_W + \Delta Y} - \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} - \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \right) \\
R_{Bulk} &= 0
\end{aligned}$$

## 1.2. Discretisation at the boundaries

### 1.2.1. At the Eastern boundary:

$$\begin{aligned}
\alpha \phi_e + \beta \left. \frac{\partial \phi}{\partial y} \right|_e &= G \\
\text{But } \left. \frac{\partial \phi}{\partial y} \right|_e &= \frac{2(\phi_e - \phi_P)}{\Delta Y} \\
\alpha \phi_e + \beta \frac{2(\phi_e - \phi_P)}{\Delta Y} &= G \\
\text{Solving for } \phi_e, \\
\phi_e &= \frac{G \Delta Y + 2\beta \phi_P}{\alpha \Delta Y + 2\beta} \\
\left. \frac{\partial \phi}{\partial y} \right|_e &= \frac{2(G - \alpha \phi_P)}{\alpha \Delta Y + 2\beta}
\end{aligned}$$

Substituting in (5),

$$\left( \frac{\Delta Z \left( C_{y,e} \frac{G\Delta Y + 2\beta\phi_P}{\alpha\Delta Y + 2\beta} - C_{y,w}\phi_w \right)}{\Delta Y\Delta Z} + \frac{\Delta Y(C_{z,s}\phi_s - C_{z,n}\phi_n)}{\Delta Y\Delta Z} \right) + \left( \frac{\Delta Z \left( 2D_{y,e} \frac{2(G - \alpha\phi_P)}{\alpha\Delta Y + 2\beta} - D_{y,w} \frac{\partial\phi}{\partial y} \Big|_w \right)}{\Delta Y\Delta Z} + \frac{\Delta Y \left( D_{z,s} \frac{\partial\phi}{\partial z} \Big|_s - D_{z,n} \frac{\partial\phi}{\partial y} \Big|_n \right)}{\Delta Y\Delta Z} \right) = 0$$

Expanding,

$$\begin{aligned} & \frac{\Delta Z \left( C_{y,e} \frac{G\Delta Y}{\alpha\Delta Y + 2\beta} + C_{y,e} \frac{2\beta}{\alpha\Delta Y + 2\beta} \phi_P - \frac{C_{y,w}\Delta Y_W}{\Delta Y_W + \Delta Y} \phi_P - \frac{C_{y,w}\Delta Y}{\Delta Y_W + \Delta Y} \phi_W \right)}{\Delta Y\Delta Z} + \\ & \frac{\Delta Y \left( \frac{C_{z,s}\Delta Z_S}{\Delta Z_S + \Delta Z} \phi_P + \frac{C_{z,s}\Delta Z}{\Delta Z_S + \Delta Z} \phi_S - \frac{C_{z,n}\Delta Z_N}{\Delta Z_N + \Delta Z} \phi_P - \frac{C_{z,n}\Delta Z}{\Delta Z_N + \Delta Z} \phi_N \right)}{\Delta Y\Delta Z} + \\ & \frac{\Delta Z \left( 2D_{y,e} \frac{G}{\alpha\Delta Y + 2\beta} - 2D_{y,e} \frac{\alpha}{\alpha\Delta Y + 2\beta} \phi_P - \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \phi_P + \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \phi_W \right)}{\Delta Y\Delta Z} + \\ & \frac{\Delta Y \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} \phi_S - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} \phi_P - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \phi_P + \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \phi_N \right)}{\Delta Y\Delta Z} = 0 \end{aligned}$$

This may be written as

$$N_{EB}\phi_N + E_{EB}\phi_E + W_{EB}\phi_W + S_{EB}\phi_S + P_{EB}\phi_P = R_{EB}$$

where,

$$\begin{aligned} N_{EB} &= \frac{\Delta Y}{\Delta Y\Delta Z} \left( \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} - \frac{C_{z,n}\Delta Z}{\Delta Z_N + \Delta Z} \right) \\ E_{EB} &= 0 \\ W_{EB} &= \frac{\Delta Z}{\Delta Y\Delta Z} \left( \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} - \frac{C_{y,w}\Delta Y}{\Delta Y_W + \Delta Y} \right) \\ S_{EB} &= \frac{\Delta Y}{\Delta Y\Delta Z} \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} + \frac{C_{z,s}\Delta Z}{\Delta Z_S + \Delta Z} \right) \\ P_{EB} &= \frac{\Delta Y}{\Delta Y\Delta Z} \left( \frac{C_{z,s}\Delta Z_S}{\Delta Z_S + \Delta Z} - \frac{C_{z,n}\Delta Z_N}{\Delta Z_N + \Delta Z} - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \right) \end{aligned}$$

$$+ \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{2\beta}{\alpha \Delta Y + 2\beta} \phi_P - \frac{C_{y,w} \Delta Y_W}{\Delta Y_W + \Delta Y} - 2D_{y,e} \frac{\alpha}{\alpha \Delta Y + 2\beta} - \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \right)$$

$$R_{EB} = - \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{G}{\alpha \Delta Y + 2\beta} \right)$$

Thus, we find that,

$$N_{EB} = N_{Bulk}$$

$$W_{EB} = W_{Bulk}$$

$$E_{EB} = 0$$

$$S_{EB} = S_{Bulk}$$

$$P_{EB} = P_{Bulk} + \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{2\beta}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} \right)$$

$$R_{EB} = R_{Bulk} - \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{G}{\alpha \Delta Y + 2\beta} \right)$$

### 1.2.2. At the Western Boundary

$$\alpha \phi_w - \beta \frac{\partial \phi}{\partial y} \Big|_w = G$$

$$\text{But } \frac{\partial \phi}{\partial y} \Big|_w = \frac{2(\phi_P - \phi_w)}{\Delta Y}$$

$$\alpha \phi_w + \beta \frac{2(\phi_w - \phi_P)}{\Delta Y} = G$$

Solving for  $\phi_w$ ,

$$\phi_w = \frac{G \Delta Y + 2\beta \phi_P}{\alpha \Delta Y + 2\beta}$$

$$\frac{\partial \phi}{\partial y} \Big|_w = \frac{2(G - \alpha \phi_P)}{\alpha \Delta Y + 2\beta}$$

Substituting in (5) and expanding,

$$\frac{\Delta Z \left( \frac{C_{y,e} \Delta Y_E}{\Delta Y_E + \Delta Y} \phi_P + \frac{C_{y,e} \Delta Y}{\Delta Y_E + \Delta Y} \phi_E - C_{y,w} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} - C_{y,w} \frac{2\beta}{\alpha \Delta Y + 2\beta} \phi_P \right)}{\Delta Y \Delta Z} +$$

$$\begin{aligned}
& \frac{\Delta Y \left( \frac{C_{z,s} \Delta Z_S}{\Delta Z_S + \Delta Z} \phi_P + \frac{C_{z,s} \Delta Z}{\Delta Z_S + \Delta Z} \phi_S - \frac{C_{z,n} \Delta Z_N}{\Delta Z_N + \Delta Z} \phi_P - \frac{C_{z,n} \Delta Z}{\Delta Z_N + \Delta Z} \phi_N \right)}{\Delta Y \Delta Z} + \\
& \frac{\Delta Z \left( \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} \phi_E - \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} \phi_P + 2D_{y,w} \frac{G}{\alpha \Delta Y + 2\beta} - 2D_{y,w} \frac{\alpha}{\alpha \Delta Y + 2\beta} \phi_P \right)}{\Delta Y \Delta Z} + \\
& \frac{\Delta Y \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} \phi_S - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} \phi_P - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \phi_P + \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \phi_N \right)}{\Delta Y \Delta Z} = 0
\end{aligned}$$

This may be written as

$$N_{WB} \phi_N + E_{WB} \phi_E + W_{WB} \phi_W + S_{WB} \phi_S + P_{WB} \phi_P = R_{WB}$$

where,

$$N_{WB} = \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} - \frac{C_{z,n} \Delta Z}{\Delta Z_N + \Delta Z} \right)$$

$$E_{WB} = \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} + \frac{C_{y,e} \Delta Y}{\Delta Y_E + \Delta Y} \right)$$

$$W_{WB} = 0$$

$$S_{WB} = \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} + \frac{C_{z,s} \Delta Z}{\Delta Z_S + \Delta Z} \right)$$

$$\begin{aligned}
P_{WB} = & \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{C_{z,s} \Delta Z_S}{\Delta Z_S + \Delta Z} - \frac{C_{z,n} \Delta Z_N}{\Delta Z_N + \Delta Z} - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \right) \\
& + \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{C_{y,e} \Delta Y_E}{\Delta Y_E + \Delta Y} - C_{y,w} \frac{2\beta}{\alpha \Delta Y + 2\beta} - \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} - 2D_{y,w} \frac{\alpha}{\alpha \Delta Y + 2\beta} \right)
\end{aligned}$$

$$R_{WB} = - \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{G}{\alpha \Delta Y + 2\beta} - C_{y,w} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} \right)$$

Thus, we find that,

$$N_{WB} = N_{Bulk}$$

$$E_{WB} = E_{Bulk}$$

$$W_{WB} = 0$$

$$S_{WB} = S_{Bulk}$$



$$P_{WB} = P_{Bulk} + \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} - C_{y,w} \frac{2\beta}{\alpha \Delta Y + 2\beta} \right)$$

$$R_{WB} = R_{Bulk} - \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{G}{\alpha \Delta Y + 2\beta} - C_{y,w} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} \right)$$

### 1.2.3. At the Southern Boundary

Here, we use an analogy of the discretization at the eastern boundary, to directly write

$$\begin{aligned} N_{SB} &= N_{Bulk} \\ W_{SB} &= W_{Bulk} \\ E_{SB} &= E_{SB} \\ S_{SB} &= 0 \end{aligned}$$

$$P_{SB} = P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{2\beta}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} \right)$$

$$R_{SB} = R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{G}{\alpha \Delta Z + 2\beta} \right)$$

### 1.2.4. At the Northern Boundary

Here, we use an analogy of the discretization at the western boundary, to directly write

$$\begin{aligned} N_{NB} &= 0 \\ E_{NB} &= E_{Bulk} \\ W_{NB} &= W_{Bulk} \\ S_{NB} &= S_{Bulk} \end{aligned}$$

$$P_{NB} = P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} - C_{z,n} \frac{2\beta}{\alpha \Delta Z + 2\beta} \right)$$

$$R_{NB} = R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{G}{\alpha \Delta Z + 2\beta} - C_{z,n} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} \right)$$

## 2. Summary of equations

In the bulk,

$$N_{Bulk} = \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} - \frac{C_{z,n} \Delta Z}{\Delta Z_N + \Delta Z} \right)$$

$$\begin{aligned}
E_{Bulk} &= \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} + \frac{C_{y,e} \Delta Y}{\Delta Y_E + \Delta Y} \right) \\
W_{Bulk} &= \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} - \frac{C_{y,w} \Delta Y}{\Delta Y_W + \Delta Y} \right) \\
S_{Bulk} &= \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} + \frac{C_{z,s} \Delta Z}{\Delta Z_S + \Delta Z} \right) \\
P_{Bulk} &= \frac{\Delta Y}{\Delta Y \Delta Z} \left( \frac{C_{z,s} \Delta Z_S}{\Delta Z_S + \Delta Z} - \frac{C_{z,n} \Delta Z_N}{\Delta Z_N + \Delta Z} - \frac{2D_{z,s}}{\Delta Z_S + \Delta Z} - \frac{2D_{z,n}}{\Delta Z_N + \Delta Z} \right) \\
&+ \frac{\Delta Z}{\Delta Y \Delta Z} \left( \frac{C_{y,e} \Delta Y_E}{\Delta Y_E + \Delta Y} - \frac{C_{y,w} \Delta Y_W}{\Delta Y_W + \Delta Y} - \frac{2D_{y,e}}{\Delta Y_E + \Delta Y} - \frac{2D_{y,w}}{\Delta Y_W + \Delta Y} \right) \\
R_{Bulk} &= 0
\end{aligned}$$

Eastern Boundary:

$$\begin{aligned}
N_{EB} &= N_{Bulk} \\
W_{EB} &= W_{Bulk} \\
E_{EB} &= 0 \\
S_{EB} &= S_{Bulk}
\end{aligned}$$

$$\begin{aligned}
P_{EB} &= P_{Bulk} + \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{2\beta}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} \right) \\
R_{EB} &= R_{Bulk} - \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{G}{\alpha \Delta Y + 2\beta} \right)
\end{aligned}$$

Western Boundary:

$$\begin{aligned}
N_{WB} &= N_{Bulk} \\
E_{WB} &= E_{Bulk} \\
W_{WB} &= 0 \\
S_{WB} &= S_{Bulk}
\end{aligned}$$

$$\begin{aligned}
P_{WB} &= P_{Bulk} + \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} - C_{y,w} \frac{2\beta}{\alpha \Delta Y + 2\beta} \right) \\
R_{WB} &= R_{Bulk} - \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{G}{\alpha \Delta Y + 2\beta} - C_{y,w} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} \right)
\end{aligned}$$

Southern Boundary:

$$\begin{aligned}
N_{SB} &= N_{Bulk} \\
W_{SB} &= W_{Bulk}
\end{aligned}$$

$$\begin{aligned} E_{SB} &= E_{SB} \\ S_{SB} &= 0 \end{aligned}$$

$$\begin{aligned} P_{SB} &= P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{2\beta}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} \right) \\ R_{SB} &= R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{G}{\alpha \Delta Z + 2\beta} \right) \end{aligned}$$

Northern Boundary

$$\begin{aligned} N_{NB} &= 0 \\ E_{NB} &= E_{Bulk} \\ W_{NB} &= W_{Bulk} \\ S_{NB} &= S_{Bulk} \end{aligned}$$

$$\begin{aligned} P_{NB} &= P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} - C_{z,n} \frac{2\beta}{\alpha \Delta Z + 2\beta} \right) \\ R_{NB} &= R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{G}{\alpha \Delta Z + 2\beta} - C_{z,n} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} \right) \end{aligned}$$

North-Eastern Corner

$$\begin{aligned} N_{NE} &= 0 \\ E_{NE} &= 0 \\ W_{NE} &= W_{Bulk} \\ S_{NE} &= S_{Bulk} \end{aligned}$$

$$\begin{aligned} P_{NE} &= P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} - C_{z,n} \frac{2\beta}{\alpha \Delta Z + 2\beta} \right) \\ &\quad + \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{2\beta}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} \right) \\ R_{NE} &= R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{G}{\alpha \Delta Z + 2\beta} - C_{z,n} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} \right) \\ &\quad - \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{G}{\alpha \Delta Y + 2\beta} \right) \end{aligned}$$

North-Western Corner

$$\begin{aligned} N_{NW} &= 0 \\ E_{NW} &= E_{Bulk} \\ W_{NW} &= 0 \\ S_{NW} &= S_{Bulk} \end{aligned}$$

$$P_{NW} = P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} - C_{z,n} \frac{2\beta}{\alpha \Delta Z + 2\beta} \right) + \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} - C_{y,w} \frac{2\beta}{\alpha \Delta Y + 2\beta} \right)$$

$$R_{NW} = R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( 2D_{z,n} \frac{G}{\alpha \Delta Z + 2\beta} - C_{z,n} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} \right) - \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{G}{\alpha \Delta Y + 2\beta} - C_{y,w} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} \right)$$

South-Eastern Corner

$$N_{SE} = N_{Bulk}$$

$$W_{SE} = W_{Bulk}$$

$$E_{SE} = 0$$

$$S_{SE} = 0$$

$$P_{SE} = P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{2\beta}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} \right) + \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{2\beta}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} \right)$$

$$R_{SE} = R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{G}{\alpha \Delta Z + 2\beta} \right) - \frac{\Delta Z}{\Delta Y \Delta Z} \left( C_{y,e} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} + 2D_{y,e} \frac{G}{\alpha \Delta Y + 2\beta} \right)$$

South-Western Corner

$$N_{SW} = N_{Bulk}$$

$$W_{SW} = 0$$

$$E_{SW} = E_{SB}$$

$$S_{SW} = 0$$

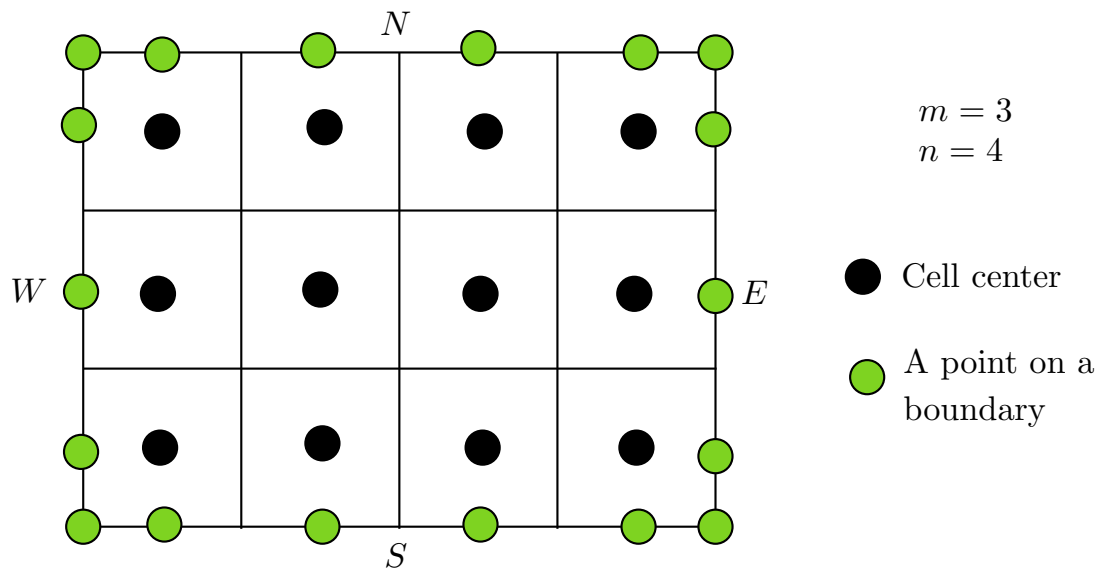
$$P_{SB} = P_{Bulk} + \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{2\beta}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{2\beta}{\Delta Z(\alpha \Delta Z + 2\beta)} \right) + \frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{2\beta}{\Delta Y(\alpha \Delta Y + 2\beta)} - C_{y,w} \frac{2\beta}{\alpha \Delta Y + 2\beta} \right)$$

$$R_{SB} = R_{Bulk} - \frac{\Delta Y}{\Delta Y \Delta Z} \left( C_{z,s} \frac{G \Delta Z}{\alpha \Delta Z + 2\beta} + 2D_{z,s} \frac{G}{\alpha \Delta Z + 2\beta} \right)$$

$$-\frac{\Delta Z}{\Delta Y \Delta Z} \left( 2D_{y,w} \frac{G}{\alpha \Delta Y + 2\beta} - C_{y,w} \frac{G \Delta Y}{\alpha \Delta Y + 2\beta} \right)$$

### 3. Using the code

Consider a  $m \times n$  grid of cells as shown below. There are  $(m + 2)$  and  $(n + 2)$  points on the boundaries



To use the code, create the following matrices

NB: A  $3 \times n$  matrix. Row 1: Value of  $\alpha$ , Row 2: Value of  $\beta$  and Row 3: Value of  $G$ , from eq. (different value of  $\alpha$ ,  $\beta$ , and  $G$  can be specified for each cell.

SB: A  $3 \times n$  matrix. Row 1: Value of  $\alpha$ , Row 2: Value of  $\beta$  and Row 3: Value of  $G$ , from eq. (different value of  $\alpha$ ,  $\beta$ , and  $G$  can be specified for each cell.

EB: A  $3 \times m$  matrix. Row 1: Value of  $\alpha$ , Row 2: Value of  $\beta$  and Row 3: Value of  $G$ , from eq. (different value of  $\alpha$ ,  $\beta$ , and  $G$  can be specified for each cell.

WB: A  $3 \times m$  matrix. Row 1: Value of  $\alpha$ , Row 2: Value of  $\beta$  and Row 3: Value of  $G$ , from eq. A different value of  $\alpha$ ,  $\beta$ , and  $G$  can be specified for each cell.

dY: A  $m \times n$  matrix specifying  $\Delta Y$  for each cell

dZ: A  $m \times n$  matrix specifying  $\Delta Z$  for each cell.

Dy: A  $(m + 2) \times (n + 2)$  matrix specifying the value of  $D_y$  at each cell center and each point the boundary

Dz: A  $(m + 2) \times (n + 2)$  matrix specifying the value of  $D_z$  at each cell center and each point the boundary

Cy: A  $(m + 2) \times (n + 2)$  matrix specifying the value of  $C_y$  at each cell center and each point the boundary

Cz: A  $(m + 2) \times (n + 2)$  matrix specifying the value of  $C_z$  at each cell center and each point the boundary

Finally, call

```
[N, E, W, S, P, R] = EqnWriter(Cy, Cz, Dy, Dz, dY, dZ, NB, EB, WB, SB)
```

Note: We have still solved only eq. (3), a simplified form of eq. (1). To solve eq. (1), simply add

```
P = P + k;
R = R + S;
```

where,

k: A  $m \times n$  matrix specifying  $k$  for each cell (from eq. (1))

S: A  $m \times n$  matrix specifying  $S$  for each cell (from eq. (1))

Finally, once can solve the system by simply calling

```
Soln = PentDiagSol(N, E, W, S, P, R)
```

Soln: A  $m \times n$  matrix giving  $\phi$  for each cell.

To get the value of  $\phi$  on the boundary, call

```
Soln_ext = BoundCond(NB,EB,WB,SB,dY,dZ,U)
```

Soln\_ext: A  $(m + 2) \times (n + 2)$  matrix giving  $\phi$  for each cell center and all points on the bound