Linear Equations

$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$
$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$
$$\frac{\phi_{neib(icel,5)}-\phi_{icel}}{\Delta z}\Delta x\Delta y+\frac{\phi_{neib(icel,6)}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

$$\sum_k \frac{S_{icel-k}}{d_{icel-k}}\left(\phi_k-\phi_{icel}\right)=-f_{icel}V_i$$

$$-\left[\sum_k \frac{S_{icel-k}}{d_{icel-k}}\right]\phi_{icel}+\left[\sum_k \frac{S_{icel-k}}{d_{icel-k}}\phi_k\right]=-f_{icel}V_i \quad (icel=1,N)$$

Diagonal Off-Diagonal

→ $[A]\{\phi\}=\{f\}$

Solving Ux=y: Backward Substitution

$$\mathbf{Ux} = \mathbf{y} \iff \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$\begin{aligned} u_{nn} x_n &= y_n \\ u_{n-1,n-1} x_{n-1} + u_{n-1,n} x_n &= y_{n-1} \\ &\vdots \\ u_{11} x_1 + u_{12} x_2 + \cdots + u_{1n} x_n &= y_1 \end{aligned} \iff \begin{aligned} x_n &= y_n / u_{nn} \\ x_{n-1} &= (y_{n-1} - u_{n-1,n} x_n) / u_{n-1,n-1} \\ &\vdots \\ x_1 &= \left(y_1 - \sum_{i=2}^{n} u_{1j} x_j \right) / u_{11} \end{aligned}$$

Constructing Coefficient Matrix

Conservation for i-th mesh

$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

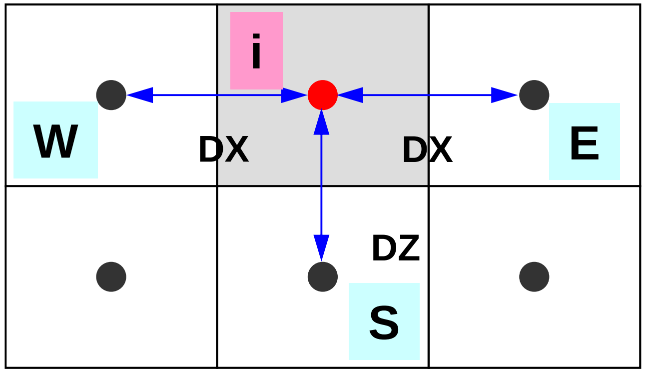
$$+\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k-\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_i=-V_i\dot{Q}_i$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal) **AL, AU (off-diag.)** **BFORCE (RHS)**

Dirichlet B.C.

$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\left(\phi_k-\phi_i\right)+V_i\dot{Q}_i=0$$



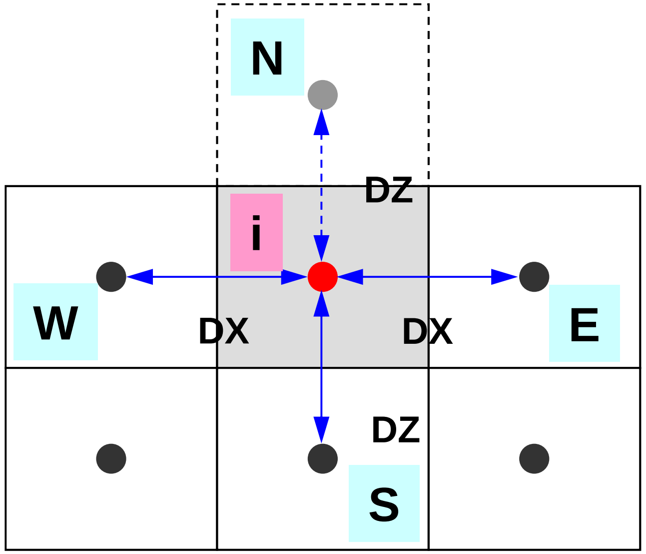
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal)

AL, AU (off-diag.)

BFORCE (RHS)

Dirichlet B.C.



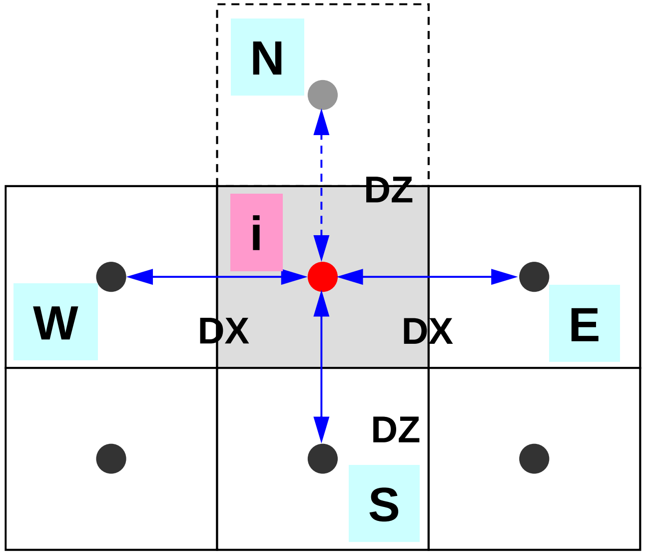
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal) **AL, AU (off-diag.)** **BFORCE (RHS)**

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+\frac{\phi_N-\phi_i}{\Delta z}\Delta x\Delta y=-V_i\dot{Q}_i, \quad \phi_N=-\phi_i$$

Dirichlet B.C.



$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\left(\phi_k-\phi_i\right)+V_i\dot{Q}_i=0$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal)

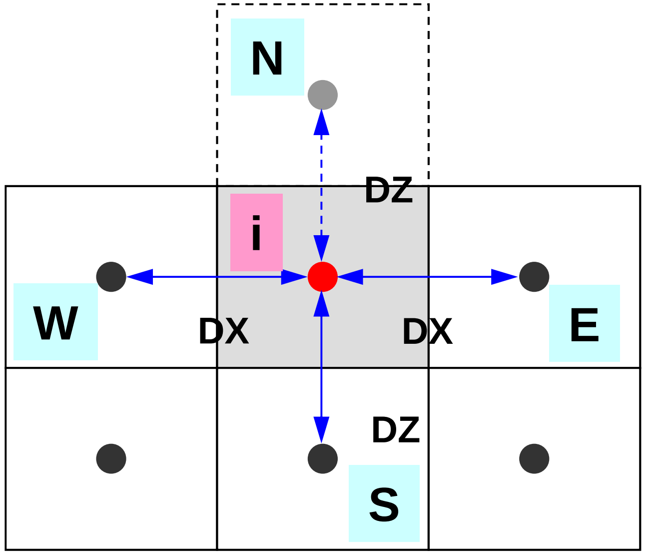
AL, AU (off-diag.)

BFORCE (RHS)

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+\frac{\phi_N-\phi_i}{\Delta z}\Delta x\Delta y=-V_i\dot{Q}_i, \quad \phi_N=-\phi_i$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+\frac{-\phi_i-\phi_i}{\Delta z}\Delta x\Delta y=-V_i\dot{Q}_i$$

Dirichlet B.C.



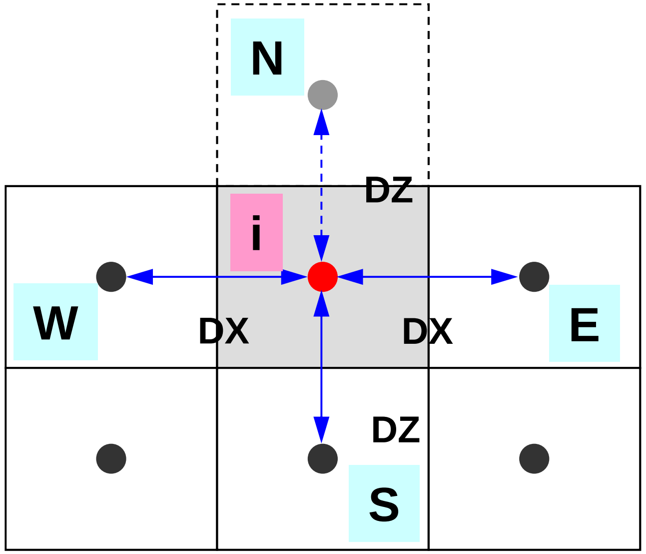
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal) **AL, AU (off-diag.)** **BFORCE (RHS)**

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+\frac{-2\phi_i}{\Delta z}\Delta x\Delta y=+V_i\dot{Q}_i$$

Dirichlet B.C.



$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\left(\phi_k-\phi_i\right)+V_i\dot{Q}_i=0$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal)

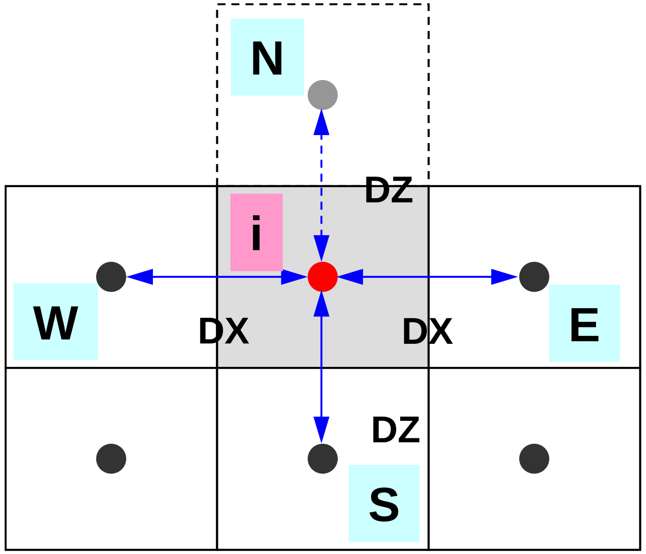
AL, AU (off-diag.)

BFORCE (RHS)

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+\frac{-2\phi_i}{\Delta z}\Delta x\Delta y=+V_i\dot{Q}_i$$

$$\left[-\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}-\frac{2}{\Delta z}\Delta x\Delta y\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+=-V_i\dot{Q}_i$$

Dirichlet B.C.



$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\left(\phi_k-\phi_i\right)+V_i\dot{Q}_i=0$$

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal) | **AL, AU (off-diag.)** | **BFORCE (RHS)**

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right.$$

```
do ib= 1, ZmaxCELtot
  icel= ZmaxCEL(ib)
  coef= 2.d0 * RDZ * ZAREA
  D(icel)= D(icel) - coef
enddo
```

$$\left[-\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}-\frac{2}{\Delta z}\Delta x\Delta y\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+=-V_i\dot{Q}_i$$

Forward/Backward Substitution for Incomplete Modified Cholesky Fact.

```
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Y)= W(i,R)
      enddo

      do i= 1, N
        WVAL= W(i,Y)
        do k= indexL(i-1)+1, indexL(i)
          WVAL= WVAL - AL(k) * W(itemL(k),Y)
        enddo
        W(i,Y)= WVAL * W(i,DD)
      enddo

      do i= N, 1, -1
        SW  = 0.0d0
        do k= indexU(i-1)+1, indexU(i)
          SW= SW + AU(k) * W(itemU(k),Z)
        enddo
        W(i,Z)= W(i,Y) - W(i,DD) * SW
      enddo
!C===
```

$$W(i,DD) = 1/l_{ii} = d_{ii}$$

$$(L)\{y\} = \{r\}$$

$$\begin{bmatrix} l_{11} & 0 & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} & 0 \\ l_{51} & l_{52} & l_{53} & l_{54} & l_{55} \end{bmatrix}$$

$$(DL^T)\{z\} = \{y\}$$

$$\begin{bmatrix} 1 & l_{21}/l_{11} & l_{31}/l_{11} & l_{41}/l_{11} & l_{51}/l_{11} \\ 0 & 1 & l_{32}/l_{22} & l_{42}/l_{22} & l_{52}/l_{22} \\ 0 & 0 & 1 & l_{43}/l_{33} & l_{53}/l_{33} \\ 0 & 0 & 0 & 1 & l_{54}/l_{44} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Forward/Backward Substitution for Incomplete Modified Cholesky Fact.

$$W(i,DD) = 1/l_{ii} = d_{ii}$$

$$(L)\{z\} = \{z\}$$

$$\begin{bmatrix} l_{11} & 0 & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} & 0 \\ l_{51} & l_{52} & l_{53} & l_{54} & l_{55} \end{bmatrix}$$

$$(DL^T)\{z\} = \{z\}$$

$$\begin{bmatrix} 1 & l_{21}/l_{11} & l_{31}/l_{11} & l_{41}/l_{11} & l_{51}/l_{11} \\ 0 & 1 & l_{32}/l_{22} & l_{42}/l_{22} & l_{52}/l_{22} \\ 0 & 0 & 1 & l_{43}/l_{33} & l_{53}/l_{33} \\ 0 & 0 & 0 & 1 & l_{54}/l_{44} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

```
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do i= 1, N
        WVAL= W(i,Z)
        do k= indexL(i-1)+1, indexL(i)
          WVAL= WVAL -  AL(k) * W(itemL(k),Z)
        enddo
        W(i,Z)= WVAL * W(i,DD)
      enddo

      do i= N, 1, -1
        SW  = 0.0d0
        do k= indexU(i-1)+1, indexU(i)
          SW= SW + AU(k) * W(itemU(k),Z)
        enddo
        W(i,Z)= W(i,Z) - W(i,DD) * SW
      enddo
!C===
```