Introduction to Parallel Programming for Multicore/Manycore Clusters

Part B1: FVM Code (ICCG)

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Files on PC

Files on WEB:

http://nkl.cc.u-tokyo.ac.jp/files/multicore-f.tar

```
>$ tar xvf multicore-f.tar
>$ cd multicore-f
```

Please confirm that following directories are created:

L1 L2

PC

Odyssey

- Background
  - Finite Volume Method
  - Preconditioned Iterative Solvers
- ICCG Solver for Poisson Equations
  - How to run
    - Data Structure
  - Program
    - Initialization
    - Coefficient Matrices
    - ICCG

Target of the Class

- Material: ICCG solver for sparse matrices derived from FVM applications (Finite Volume Method).
- Parallelization on a single node of Oakbridge-CX (OBCX) using OpenMP
  - Data Placement
  - Reordering

- Keywords
  - Finite Volume Method (FVM)
  - Sparse Matrices
  - ICCG Method

Target Application

- 3D Poisson Equation/Poisson's Equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

- Finite Volume Method (FVM)
  - Arbitrary Shape Meshes, Cell-Centered
  - "Direct" Finite Difference Method
- Boundary Conditions (B.C.) etc.
  - Dirichlet B.C., Volume Flux
- Preconditioned Iterative Solvers
  - Conjugate Gradient + Preconditioner

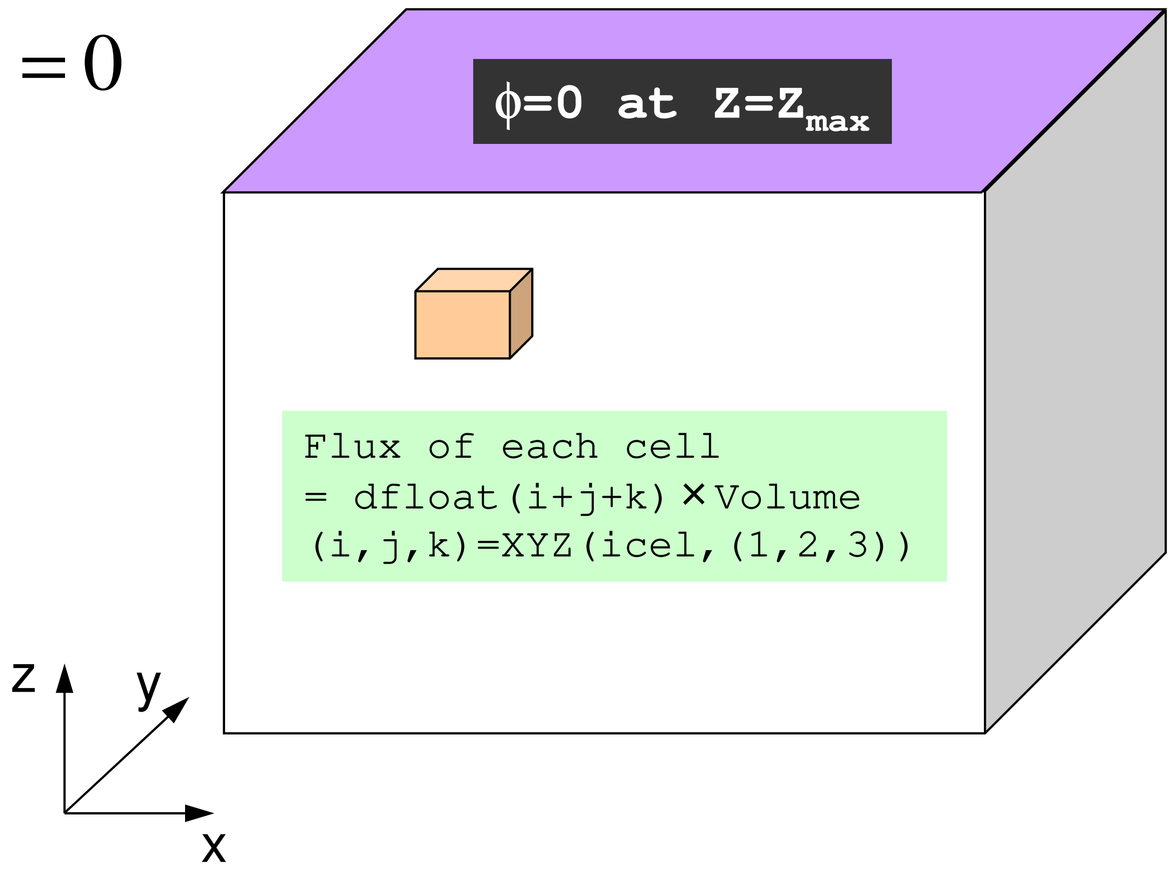
Target Problem: Variables are defined at cell-center's

Poisson Equation/
Poisson's Equation

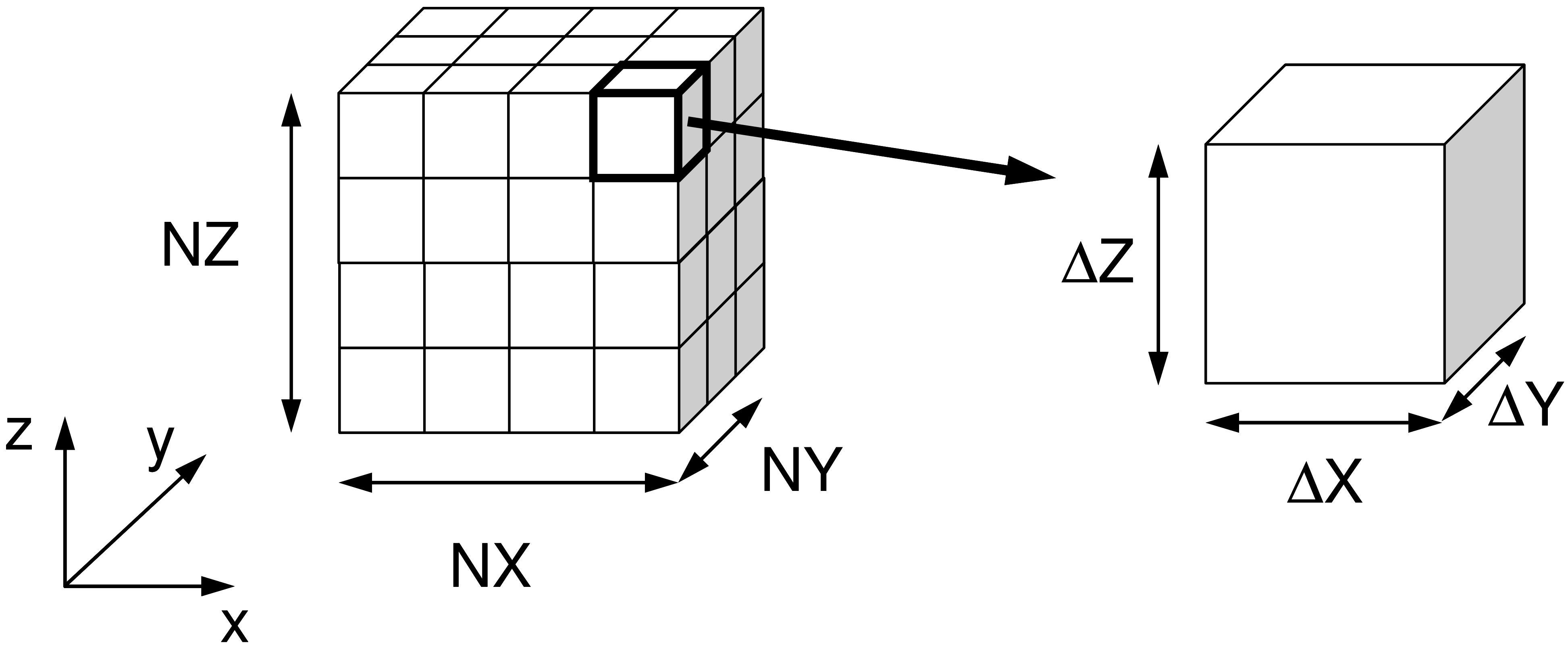
$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

Boundary Conditions (B.C.) etc.

- Volume Flux
- $\phi = 0$ @ $Z = Z_{max}$



3D Structured Mesh
Internal data structure is “unstructured”



Volume Flux f

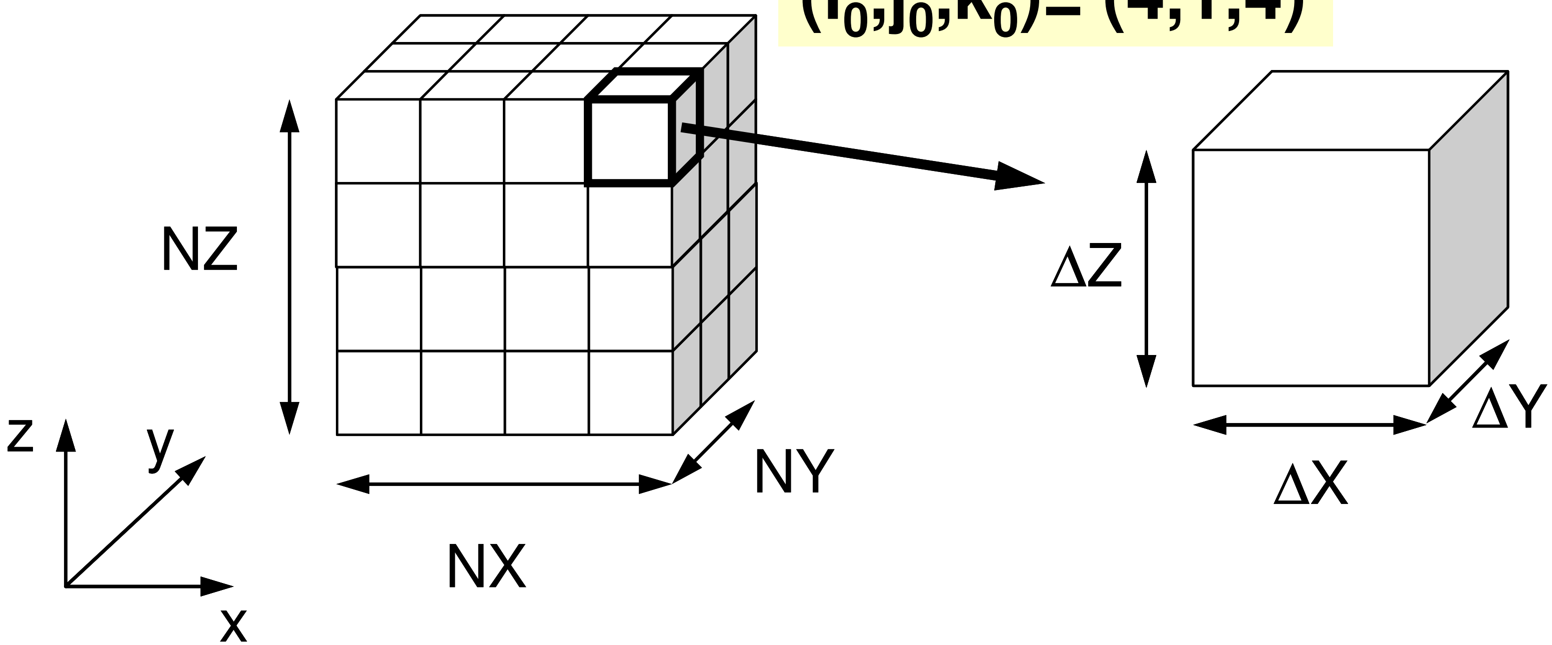
$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

$$f = dfloat(i_0 + j_0 + k_0)$$

$$i_0 = XYZ(icel, 1),$$
$$j_0 = XYZ(icel, 2),$$
$$k_0 = XYZ(icel, 3)$$

$XYZ(icel, k)$ (k=1,2,3)
Index for location of finite-difference mesh in X-/Y-/Z-axis.

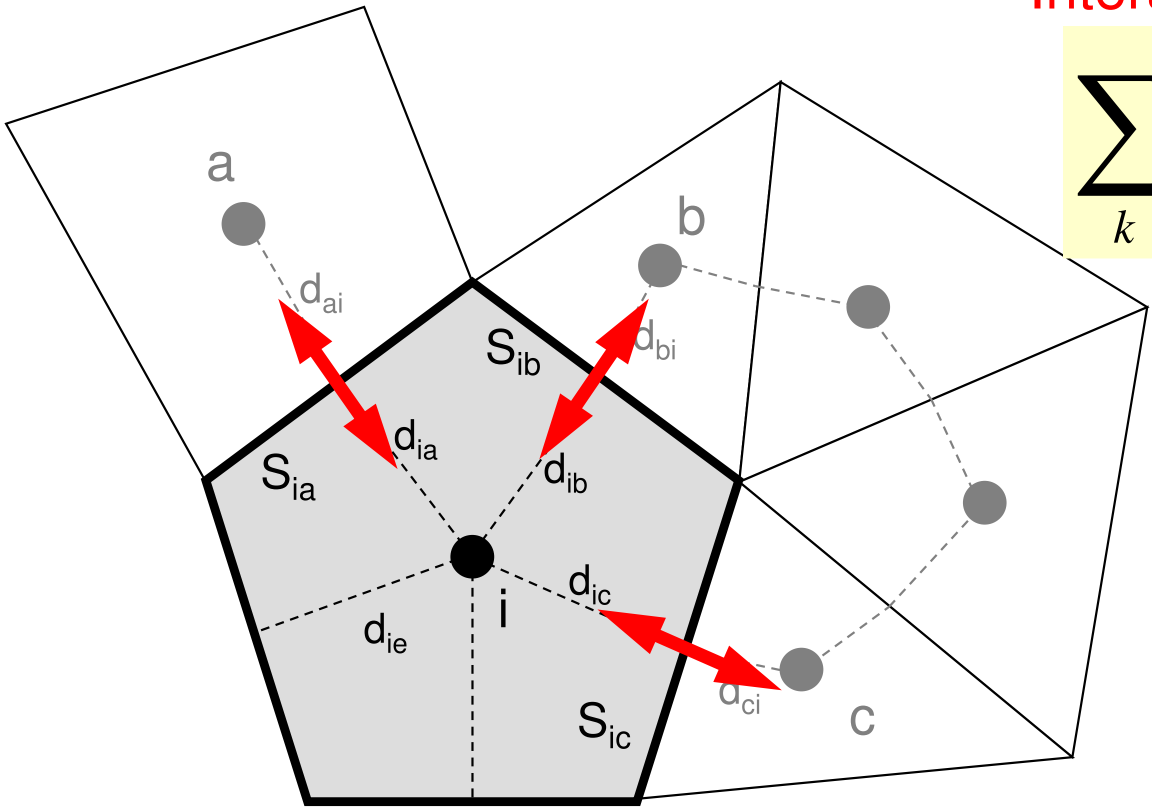
$(i_0, j_0, k_0) = (4,1,4)$



Poisson Equation by Finite Volume Method (FVM)

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}+f=0$$

Conservation of Fluxes through Surfaces



Diffusion:
Interaction with Neighbors

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

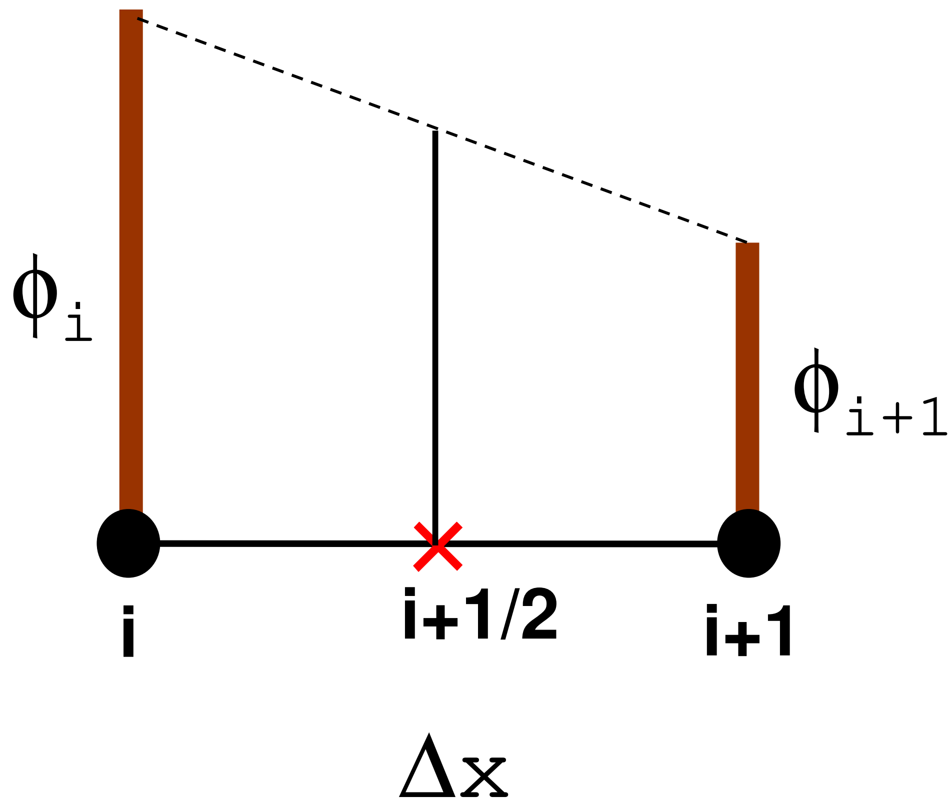
Volume Flux

```
Vi   : Volume
S    : Surface Area
dij  : Distance between
       Cell-Center &
       Surface
Q    : Volume Flux
```

Finite Difference Method (FDM)
（有限）差分法：巨視的微分
macroscopic differentiation

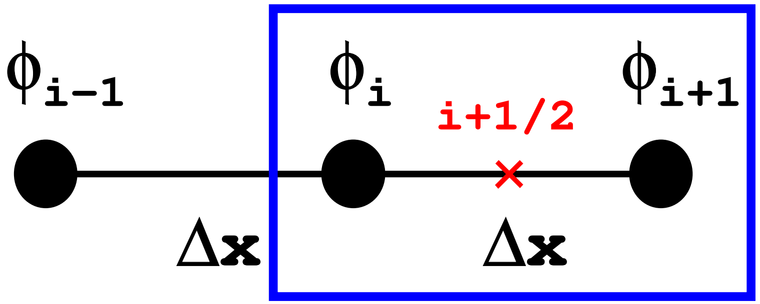
$$\left(\frac{d\phi}{dx}\right)_{i+1/2} \approx \frac{\phi_{i+1}-\phi_i}{\Delta x}$$

$$\left(\frac{d\phi}{dx}\right)_{i+1/2} = \lim_{\Delta x \to 0}\frac{\phi_{i+1}-\phi_i}{\Delta x}$$



2nd Order Differentiation in FDM Taylor Series Expansion

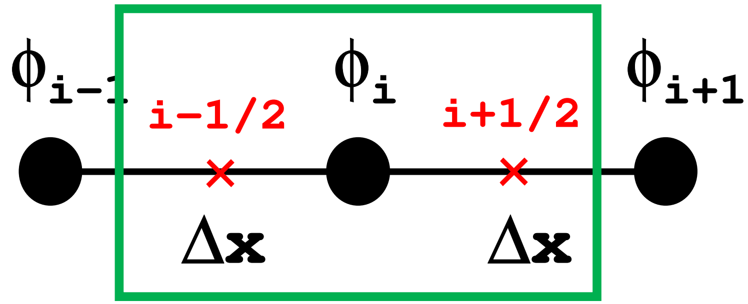
- **Approximate Derivative at × (center of *i* and *i+1*)**



$$\left(\frac{d\phi}{dx}\right)_{i+1/2} \approx \frac{\phi_{i+1}-\phi_i}{\Delta x}$$

$\Delta x \rightarrow 0$: Real Derivative

- **2nd-Order Diff. at *i***



$$\left(\frac{d^2\phi}{dx^2}\right)_i \approx \frac{\left(\frac{d\phi}{dx}\right)_{i+1/2}-\left(\frac{d\phi}{dx}\right)_{i-1/2}}{\Delta x} = \frac{\frac{\phi_{i+1}-\phi_i}{\Delta x}-\frac{\phi_i-\phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{\Delta x^2}$$

Poisson Equation by Finite Volume Method (FVM)

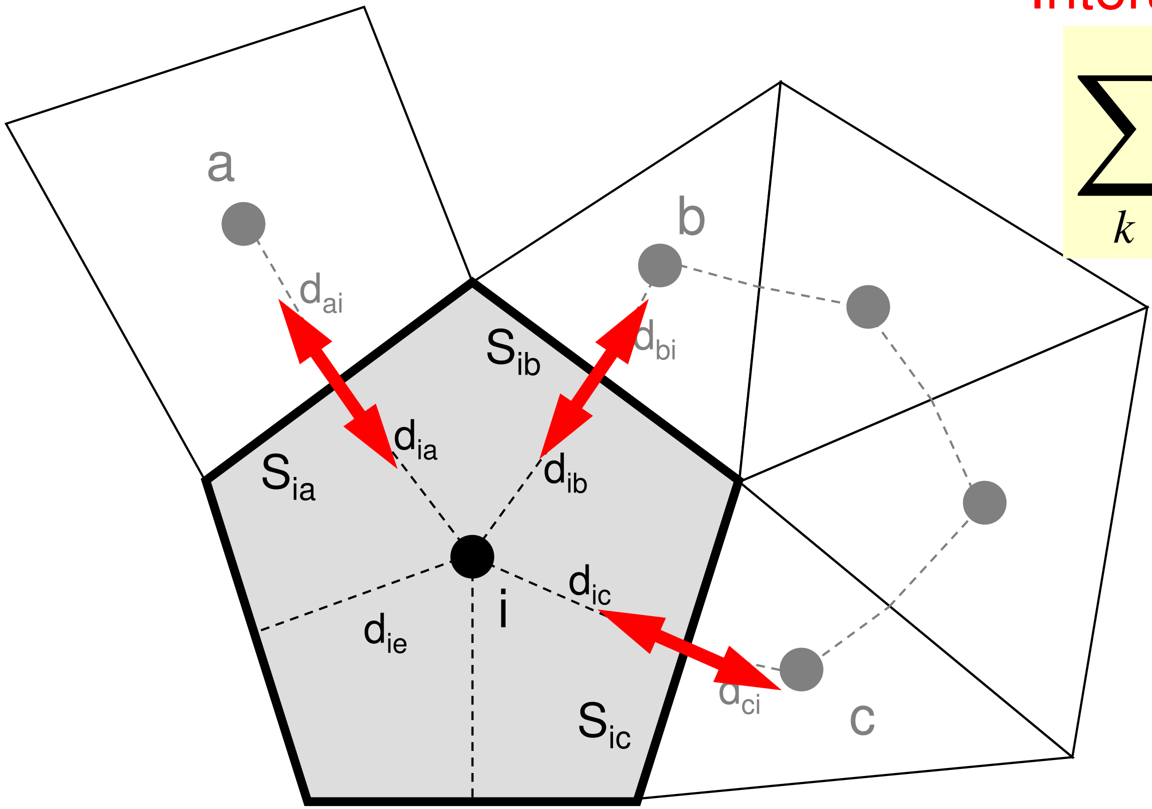
$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

Conservation of Fluxes through Surfaces

Diffusion:
Interaction with Neighbors

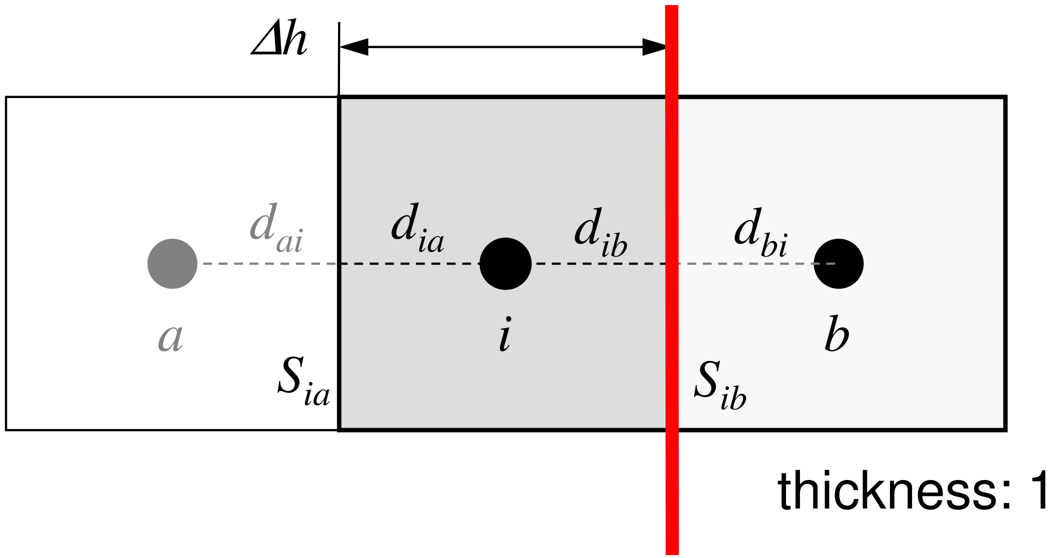
$$\sum_k \frac{S_{ik}}{d_{ik} + d_{ki}} \left(\phi_k - \phi_i\right) + V_i \dot{Q}_i = 0$$

Volume Flux




```
V_i  : Volume
S    : Surface Area
d_ij : Distance between
       Cell-Center &
       Surface
Q    : Volume Flux
```

Comparison with 1D FDM (1/3)



Δh x Δh Square Mesh

Surface Area: $S_{ik} = \Delta h$

Volume: $V_i = \Delta h^2$

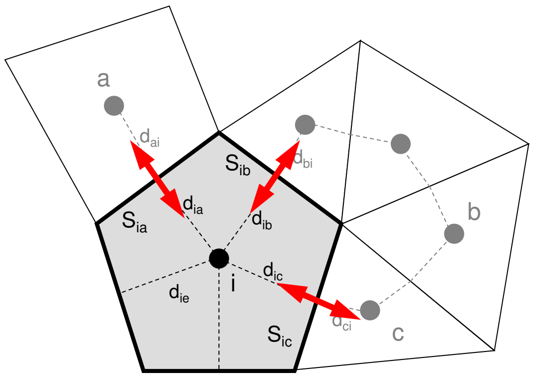
Distance (Ctr.-Suf): $d_{ij} = \Delta h/2$

Flux through this surface: Qs_{ib}

$$Qs_{ib} = -\frac{\phi_b - \phi_i}{d_{ib} + d_{bi}} \cdot S_{ib}$$

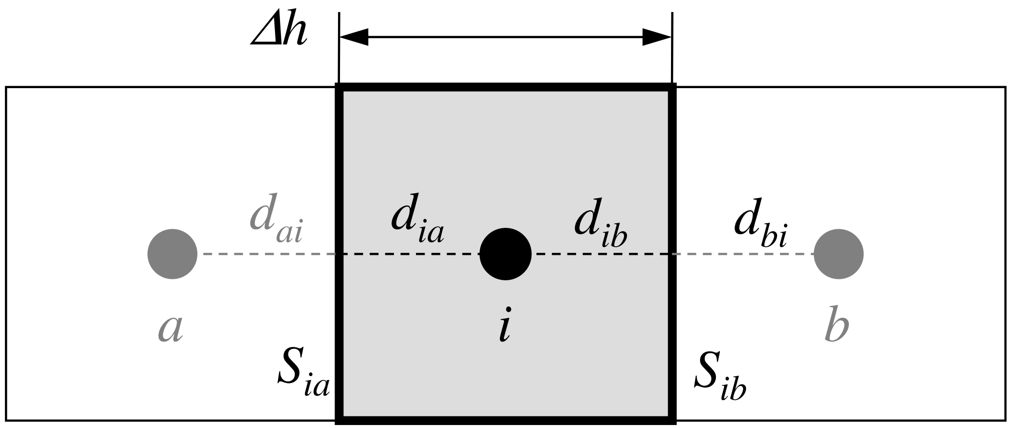
Fourier's Law

Flux through a surface
= - (gradient of potential)



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

Comparison with 1D FDM (2/3)



Δh x Δh Square Mesh

Surface Area: $S_{ik}= \Delta h$

Volume: $V_i = \Delta h^2$

Distance (Ctr.-Suf): $d_{ij}=\Delta h/2$

thickness: 1

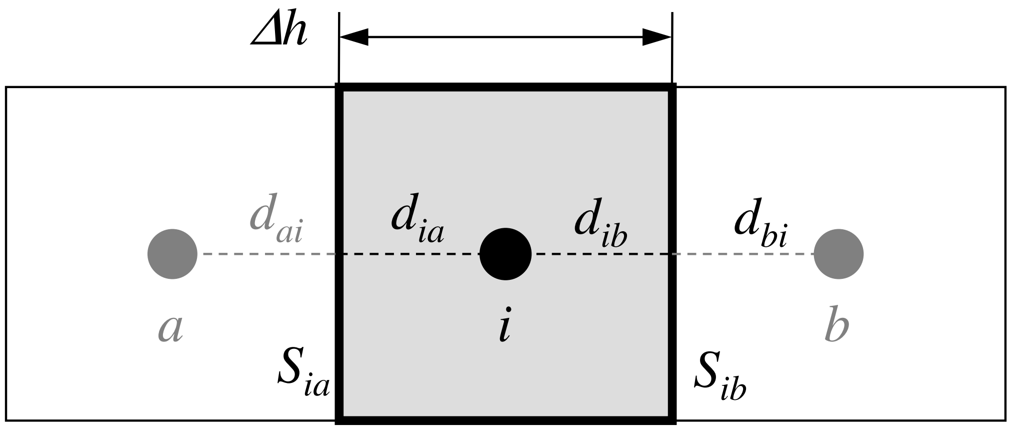
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

Divided by V_i:

$$\frac{1}{V_i}\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+\dot{Q}_i=0$$

considering this part

Comparison with 1D FDM (3/3)



thickness: 1

Δh x Δh Square Mesh

Surface Area: $S_{ik} = \Delta h$

Volume: $V_i = \Delta h^2$

Distance (Ctr.-Suf): $d_{ij} = \Delta h/2$

$$\frac{1}{V_i}\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k - \phi_i) = \frac{1}{(\Delta h)^2}\sum_{k=a,b}\frac{\Delta h}{\frac{\Delta h}{2}+\frac{\Delta h}{2}}(\phi_k - \phi_i)$$

$$= \frac{1}{(\Delta h)^2}\sum_{k=a,b}\frac{\Delta h}{\frac{\Delta h}{2}+\frac{\Delta h}{2}}(\phi_k - \phi_i) = \frac{1}{(\Delta h)^2}\sum_{k=a,b}\frac{\Delta h}{\Delta h}(\phi_k - \phi_i) = \frac{1}{(\Delta h)^2}\sum_{k=a,b}(\phi_k - \phi_i)$$

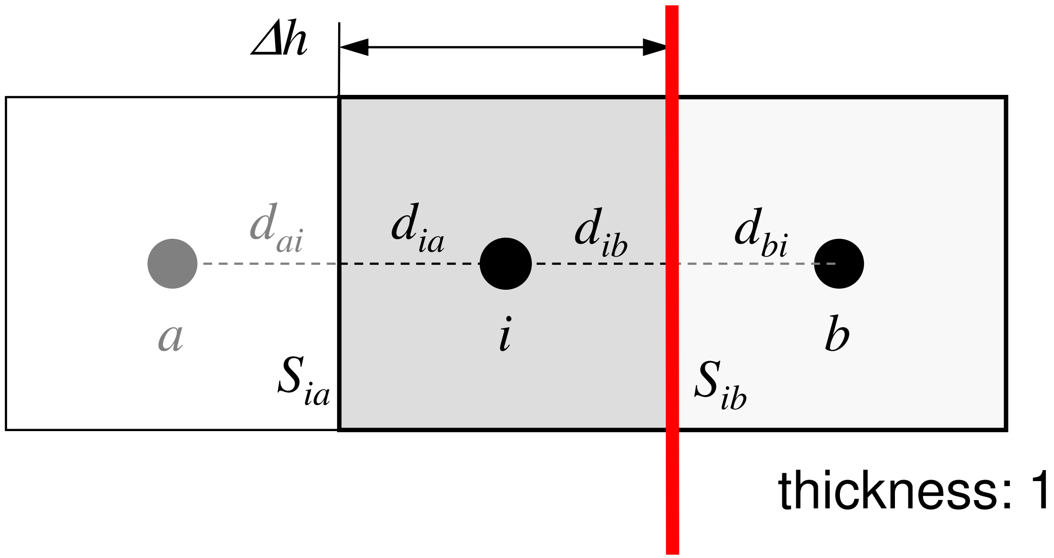
$$= \frac{1}{(\Delta h)^2}(\phi_a - \phi_i) + \frac{1}{(\Delta h)^2}(\phi_b - \phi_i) = \boxed{\frac{\phi_a - 2\phi_i + \phi_b}{(\Delta h)^2}}$$

for i-th cell
linear equations

Heat Equation (1/3)

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+Q=0$$

λ: Thermal Conductivity



Δh x Δh Square Mesh

Surface Area: $S_{ik}=\Delta h$

Volume: $V_i=\Delta h^2$

Distance (Ctr.-Suf): $d_{ij}=\Delta h/2$

Heat Flux through this surface: Qs_{ib}

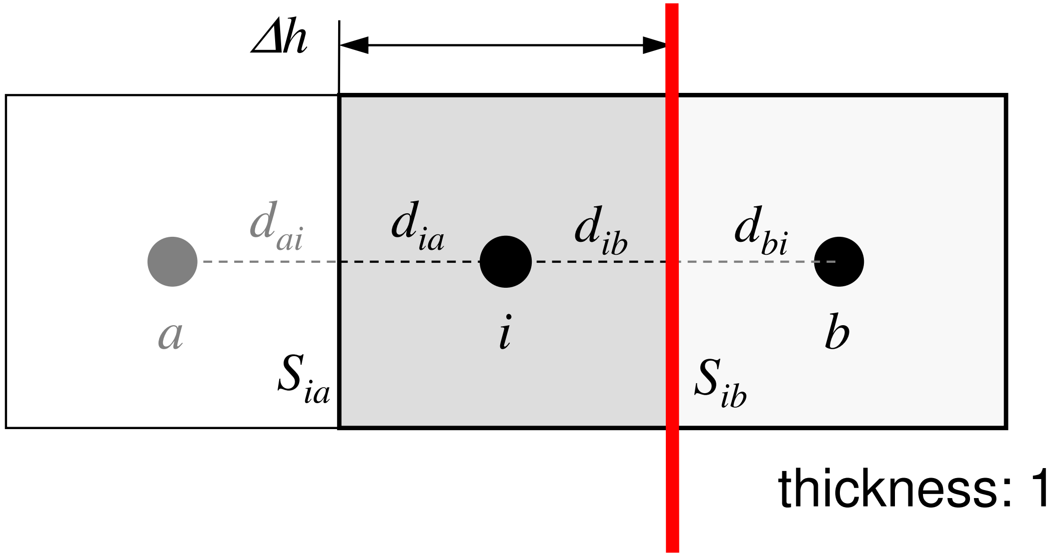
$$Qs_{ib}=-\lambda\frac{T_b-T_i}{\Delta h}\cdot S_{ib}$$

$$\lambda_i=\lambda_b=\lambda$$

Heat Equation (2/3)

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+Q=0$$

λ: Thermal Conductivity



Δh x Δh Square Mesh

Surface Area: $S_{ik}=\Delta h$

Volume: $V_i=\Delta h^2$

Distance (Ctr.-Suf): $d_{ij}=\Delta h/2$

Heat Flux through this surface: Qs_{ib}

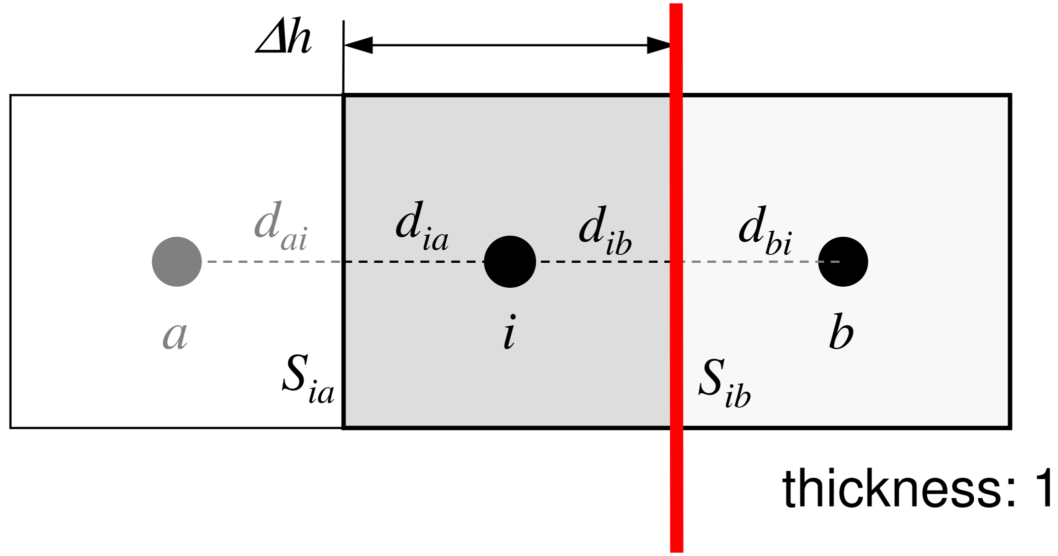
$$Qs_{ib}=-\lambda\frac{T_b-T_i}{\frac{\Delta h}{2}+\frac{\Delta h}{2}}\cdot S_{ib}=-\frac{T_b-T_i}{\left[\left(\frac{\Delta h}{2}\right)/\lambda\right]+\left[\left(\frac{\Delta h}{2}\right)/\lambda\right]}\cdot S_{ib}$$

$$\lambda_i=\lambda_b=\lambda$$

Heat Equation (3/3)

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+Q=0$$

λ: Thermal Conductivity



Δh x Δh Square Mesh

Surface Area: $S_{ik} = \Delta h$

Volume: $V_i = \Delta h^2$

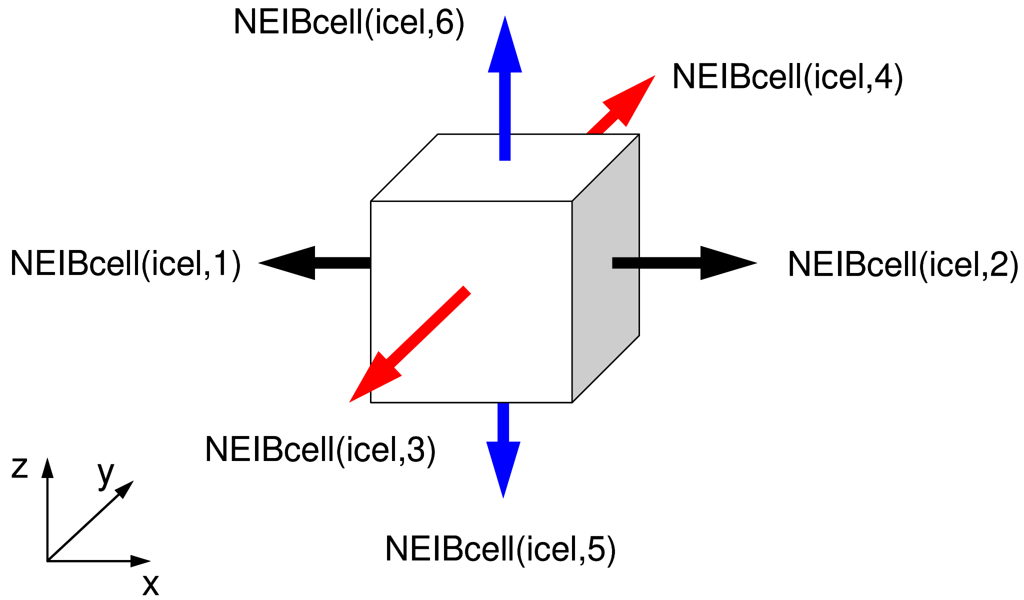
Distance (Ctr.-Suf): $d_{ij} = \Delta h/2$

Heat Flux through this surface: Qs_{ib}

$$Qs_{ib} = -\frac{T_b - T_i}{\left[\left(\frac{\Delta h}{2}\right)/\lambda_i\right]+\left[\left(\frac{\Delta h}{2}\right)/\lambda_b\right]}\cdot S_{ib}$$

$$\lambda_i \neq \lambda_b$$

in 3D



$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

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

Linear Equations

$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

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

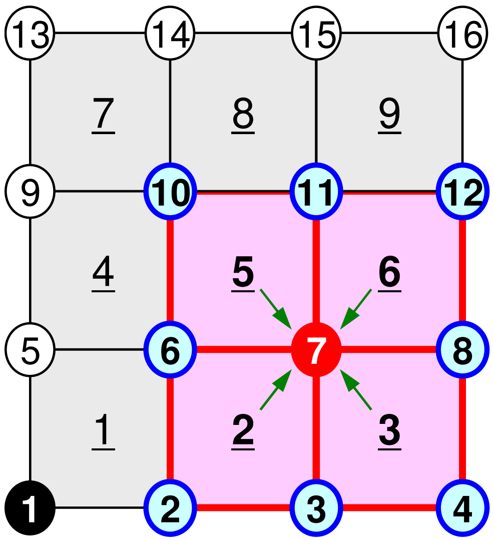
$$\sum_k \frac{S_{icel-k}}{d_{icel-k}}\left(\phi_k-\phi_{icel}\right)=-f_{icel}V_i$$

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

Diagonal　　Off-Diagonal

→ $[A]\{\phi\}=\{f\}$

Sparse Coef. Matrix in FEM
Many "0's"



$$[K]\{\Phi\}=\{F\}$$

$$
\begin{bmatrix}
D & X & & & X & X & & & & & & & & & & \\
X & D & X & & X & X & X & & & & & & & & & \\
& X & D & X & & X & X & X & & & & & & & & \\
& & X & D & & & X & X & & & & & & & & \\
X & X & & & D & X & & & X & X & & & & & & \\
X & X & X & & X & D & X & & X & X & X & & & & & \\
& X & X & X & & X & D & X & & X & X & X & & & & \\
& & X & X & & & X & D & & & X & X & & & & \\
& & & & X & X & & & D & X & & & X & X & & \\
& & & & X & X & X & & X & D & X & & X & X & X & \\
& & & & & X & X & X & & X & D & X & & X & X & X \\
& & & & & & X & X & & & X & D & & & X & X \\
& & & & & & & & X & X & & & D & X & & \\
& & & & & & & & X & X & X & & X & D & X & \\
& & & & & & & & & X & X & X & & X & D & X \\
& & & & & & & & & & X & X & & & X & D
\end{bmatrix}
\begin{Bmatrix}
\Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \\ \Phi_9 \\ \Phi_{10} \\ \Phi_{11} \\ \Phi_{12} \\ \Phi_{13} \\ \Phi_{14} \\ \Phi_{15} \\ \Phi_{16}
\end{Bmatrix}
=
\begin{Bmatrix}
F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \\ F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \\ F_{16}
\end{Bmatrix}
$$

Coefficient Matrices for FVM are sparse

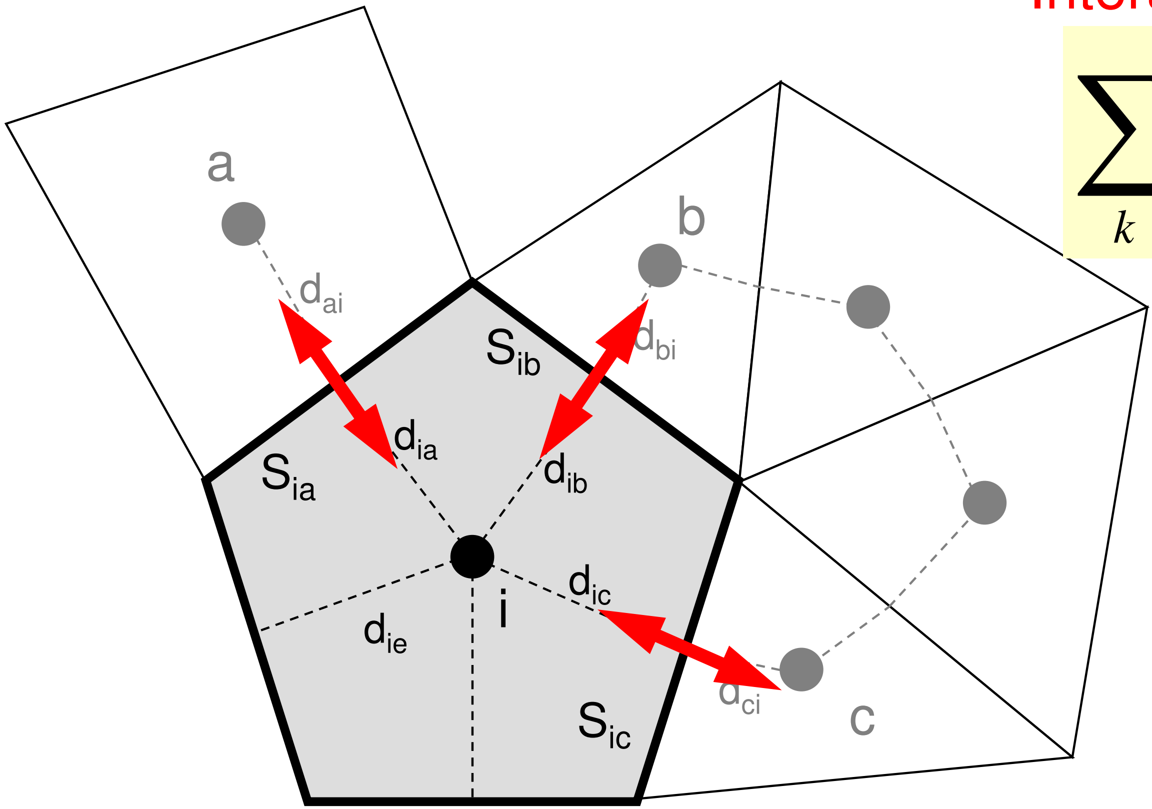
$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}+f=0$$

Only neighboring cells are considered

Diffusion:
Interaction with Neighbors

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

Volume Flux




```
Vi   : Volume
S    : Surface Area
dij  : Distance between
       Cell-Center &
       Surface
Q    : Volume Flux
```

Sparse Matrix for FVM

- Sparse Matrix
  - Many “0”’s
- Storing all components (e.g. A(i,j)) is not efficient for sparse matrices
  - A(i,j) is suitable for dense matrices

$$
\begin{bmatrix}
D & X & & & X & X & & & & & & & & & & \\
X & D & X & & X & X & X & & & & & & & & & \\
& X & D & X & & X & X & X & & & & & & & & \\
& & X & D & & & X & X & & & & & & & & \\
X & X & & & D & X & & & X & X & & & & & & \\
X & X & X & & X & D & X & & X & X & X & & & & & \\
& X & X & X & & X & D & X & & X & X & X & & & & \\
& & X & X & & & X & D & & & X & X & & & & \\
& & & & X & X & & & D & X & & & X & X & & \\
& & & & X & X & X & & X & D & X & & X & X & X & \\
& & & & & X & X & X & & X & D & X & & X & X & X \\
& & & & & & X & X & & & X & D & & & X & X \\
& & & & & & & & X & X & & & D & X & & \\
& & & & & & & & X & X & X & & X & D & X & \\
& & & & & & & & & X & X & X & & X & D & X \\
& & & & & & & & & & X & X & & & X & D
\end{bmatrix}
\begin{Bmatrix}
\Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \\ \Phi_9 \\ \Phi_{10} \\ \Phi_{11} \\ \Phi_{12} \\ \Phi_{13} \\ \Phi_{14} \\ \Phi_{15} \\ \Phi_{16}
\end{Bmatrix}
=
\begin{Bmatrix}
F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \\ F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \\ F_{16}
\end{Bmatrix}
$$

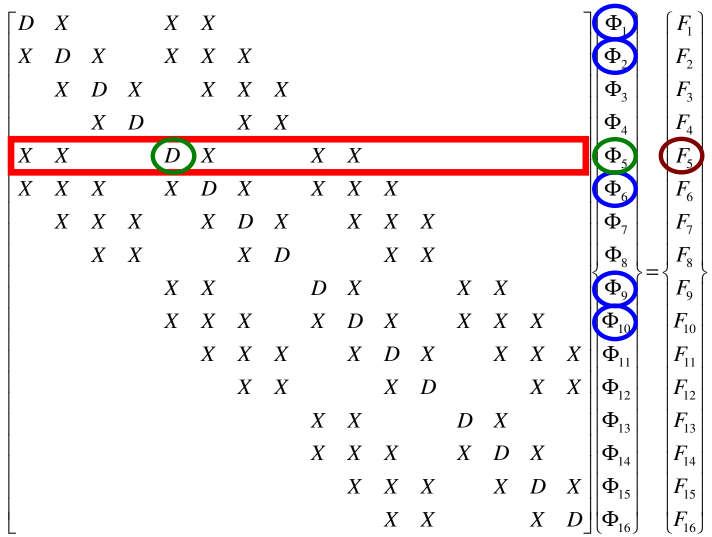
- Number of non-zero off-diagonal components is O(100) in FVM (only 6 in this case)
  - If number of unknowns is 10^8 :
    - A(i,j): $O(10^{16})$ words ~ $O(10^{17})$ bytes for DP: 100PB (400 x Odyssey)
    - Actual Non-zero Comp. : $O(10^9)$ words: 10GB (Odyssey: 32GB/node)
- Only (really) non-zero off-diag. components should be stored on memory

Mat-Vec. Multiplication for Sparse Matrix

Compressed Row Storage (CRS)

Diag (i)	Diagonal Components (REAL, i=1~N)
Index(i)	Number of Non-Zero Off-Diagonals at Each ROW (INT, i=0~N)
Item(k)	Non-Zero Off-Diagonal Components (Corresponding Column ID) (INT, k=1, index(N))
AMat(k)	Non-Zero Off-Diagonal Components (Value) (REAL, k=1, index(N))

```
{Y}= [A]{X}

do i= 1, N
  Y(i)= Diag(i)*X(i)
  do k= Index(i-1)+1, Index(i)
    Y(i)= Y(i) + Amat(k)*X(Item(k))
  enddo
enddo
```



Mat-Vec. Multiplication for Sparse Matrix

Compressed Row Storage (CRS)

```
{Q}=[A]{P}

for(i=0;i<N;i++){
        W[Q][i] = Diag[i] * W[P][i];
        for(k=Index[i];k<Index[i+1];k++){
                W[Q][i] += AMat[k]*W[P][Item[k]];
        }
}
```

Mat-Vec. Multiplication for Dense Matrix

Very Easy, Straightforward

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1,N-1} & a_{1,N} \\ a_{21} & a_{22} & & a_{2,N-1} & a_{2,N} \\ \cdots & & \cdots & & \cdots \\ a_{N-1,1} & a_{N-1,2} & & a_{N-1,N-1} & a_{N-1,N} \\ a_{N,1} & a_{N,2} & \cdots & a_{N,N-1} & a_{N,N} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N-1} \\ x_N \end{Bmatrix} = \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{Bmatrix}$$

```
{Y}= [A]{X}

do j= 1, N
  Y(j)= 0.d0
  do i= 1, N
    Y(j)= Y(j) + A(i,j)*X(i)
  enddo
enddo
```

Compressed Row Storage (CRS)

	1	2	3	4	5	6	7	8
1	1.1	2.4	0	0	3.2	0	0	0
2	4.3	3.6	0	2.5	0	3.7	0	9.1
3	0	0	5.7	0	1.5	0	3.1	0
4	0	4.1	0	9.8	2.5	2.7	0	0
5	3.1	9.5	10.4	0	11.5	0	4.3	0
6	0	0	6.5	0	0	12.4	9.5	0
7	0	6.4	2.5	0	0	1.4	23.1	13.1
8	0	9.5	1.3	9.6	0	3.1	0	51.3

Compressed Row Storage (CRS): Fortran

	1	2	3	4	5	6	7	8
1	1.1 ①	2.4 ②			3.2 ⑤			
2	4.3 ①	3.6 ②		2.5 ④		3.7 ⑥		9.1 ⑧
3			5.7 ③		1.5 ⑤		3.1 ⑦	
4		4.1 ②		9.8 ④	2.5 ⑤	2.7 ⑥		
5	3.1 ①	9.5 ②	10.4 ③		11.5 ⑤		4.3 ⑦	
6			6.5 ③			12.4 ⑥	9.5 ⑦	
7		6.4 ②	2.5 ③			1.4 ⑥	23.1 ⑦	13.1 ⑧
8		9.5 ②	1.3 ③	9.6 ④		3.1 ⑥		51.3 ⑧

```
N= 8
```

Diagonal Components

```
Diag(1)=  1.1
Diag(2)=  3.6
Diag(3)=  5.7
Diag(4)=  9.8
Diag(5)= 11.5
Diag(6)= 12.4
Diag(7)= 23.1
Diag(8)= 51.3
```

Compressed Row Storage (CRS)

	1	2	3	4	5	6	7	8
1	1.1 ①		2.4 ②			3.2 ⑤		
2	3.6 ②	4.3 ①			2.5 ④		3.7 ⑥		9.1 ⑧
3	5.7 ③					1.5 ⑤		3.1 ⑦	
4	9.8 ④		4.1 ②			2.5 ⑤	2.7 ⑥		
5	11.5 ⑤	3.1 ①	9.5 ②	10.4 ③				4.3 ⑦	
6	12.4 ⑥			6.5 ③				9.5 ⑦	
7	23.1 ⑦		6.4 ②	2.5 ③			1.4 ⑥		13.1 ⑧
8	51.3 ⑧		9.5 ②	1.3 ③	9.6 ④		3.1 ⑥		

Compressed Row Storage (CRS)

Row	Diag.					# Non-Zero Off-Diag.	index
							index(0)= 0
1	1.1 ①	2.4 ②	3.2 ⑤			2	index(1)= 2
2	3.6 ②	4.3 ①	2.5 ④	3.7 ⑥	9.1 ⑧	4	index(2)= 6
3	5.7 ③	1.5 ⑤	3.1 ⑦			2	index(3)= 8
4	9.8 ④	4.1 ②	2.5 ⑤	2.7 ⑥		3	index(4)= 11
5	11.5 ⑤	3.1 ①	9.5 ②	10.4 ③	4.3 ⑦	4	index(5)= 15
6	12.4 ⑥	6.5 ③	9.5 ⑦			2	index(6)= 17
7	23.1 ⑦	6.4 ②	2.5 ③	1.4 ⑥	13.1 ⑧	4	index(7)= 21
8	51.3 ⑧	9.5 ②	1.3 ③	9.6 ④	3.1 ⑥	4	index(8)= 25

NPLU= 25 (=index(N))

index(i-1)+1th~index(i)th
Non-Zero Off-Diag. Components corresponding to *i*-th row

Compressed Row Storage (CRS)

						# Non-Zero Off-Diag.	index(0)= 0
1	1.1 ①	2.4 ②,1	3.2 ⑤,2			2	index(1)= 2
2	3.6 ②	4.3 ①,3	2.5 ④,4	3.7 ⑥,5	9.1 ⑧,6	4	index(2)= 6
3	5.7 ③	1.5 ⑤,7	3.1 ⑦,8			2	index(3)= 8
4	9.8 ④	4.1 ②,9	2.5 ⑤,10	2.7 ⑥,11		3	index(4)= 11
5	11.5 ⑤	3.1 ①,12	9.5 ②,13	10.4 ③,14	4.3 ⑦,15	4	index(5)= 15
6	12.4 ⑥	6.5 ③,16	9.5 ⑦,17			2	index(6)= 17
7	23.1 ⑦	6.4 ②,18	2.5 ③,19	1.4 ⑥,20	13.1 ⑧,21	4	index(7)= 21
8	51.3 ⑧	9.5 ②,22	1.3 ③,23	9.6 ④,24	3.1 ⑥,25	4	index(8)= 25

NPLU= 25 (=index(N))

index(i-1)+1th~index(i)th
Non-Zero Off-Diag. Components corresponding to *i*-th row

Compressed Row Storage (CRS)

❶	1.1 ①	2.4 ②,1	3.2 ⑤,2		
❷	3.6 ②	4.3 ①,3	2.5 ④,4	3.7 ⑥,5	9.1 ⑧,6
❸	5.7 ③	1.5 ⑤,7	3.1 ⑦,8		
❹	9.8 ④	4.1 ②,9	2.5 ⑤,10	2.7 ⑥,11	
❺	11.5 ⑤	3.1 ①,12	9.5 ②,13	10.4 ③,14	4.3 ⑦,15
❻	12.4 ⑥	6.5 ③,16	9.5 ⑦,17		
❼	23.1 ⑦	6.4 ②,18	2.5 ③,19	1.4 ⑥,20	13.1 ⑧,21
❽	51.3 ⑧	9.5 ②,22	1.3 ③,23	9.6 ④,24	3.1 ⑥,25

```
Example:
item( 7)= 5, AMAT( 7)= 1.5
item(19)= 3, AMAT(19)= 2.5
```

Compressed Row Storage (CRS)

❶	1.1 ①	2.4 ②,1	3.2 ⑤,2		
❷	3.6 ②	4.3 ①,3	2.5 ④,4	3.7 ⑥,5	9.1 ⑧,6
❸	5.7 ③	1.5 ⑤,7	3.1 ⑦,8		
❹	9.8 ④	4.1 ②,9	2.5 ⑤,10	2.7 ⑥,11	
❺	11.5 ⑤	3.1 ①,12	9.5 ②,13	10.4 ③,14	4.3 ⑦,15
❻	12.4 ⑥	6.5 ③,16	9.5 ⑦,17		
❼	23.1 ⑦	6.4 ②,18	2.5 ③,19	1.4 ⑥,20	13.1 ⑧,21
❽	51.3 ⑧	9.5 ②,22	1.3 ③,23	9.6 ④,24	3.1 ⑥,25

Diag (i) Diagonal Components (REAL, i=1~N)
Index(i) Number of Non-Zero Off-Diagonals at Each ROW (INT, i=0~N)
Item(k) Non-Zero Off-Diagonal Components (Corresponding Column ID) (INT, k=1, index(N))
AMat(k) Non-Zero Off-Diagonal Components (Value) (REAL, k=1, index(N))

```
{Y}= [A]{X}

do i= 1, N
  Y(i)= D(i)*X(i)
  do k= index(i-1)+1, index(i)
    Y(i)= Y(i) + AMAT(k)*X(item(k))
  enddo
enddo
```

- Background
  - Finite Volume Method
  - **Preconditioned Iterative Solvers**
- ICCG Solver for Poisson Equations
  - How to run
    - Data Structure
  - Program
    - Initialization
    - Coefficient Matrices
    - ICCG
- OpenMP

Large-Scale Linear Equations in Scientific Applications

- Solving large-scale linear equations **Ax=b** is the most important and ***expensive*** part of various types of scientific computing.
  - for both linear and nonlinear applications
- Various types of methods proposed & developed.
  - for dense and sparse matrices
  - classified into ***direct*** and ***iterative*** methods
- Dense Matrices:密行列: Globally Coupled Problems
  - BEM, Spectral Methods, MO/MD (gas, liquid)
- Sparse Matrices:疎行列: Locally Defined Problems
  - FEM, FVM, FDM, DEM, MD (solid), BEM w/FMM

Direct Method
直接法

- Gaussian Elimination/LU Factorization
  - compute A^{-1} directly (or equivalent operations)

Good

  - Robust for wide range of applications.
  - Good for both dense and sparse matrices

Bad

  - More expensive than iterative methods (memory, CPU)
    - not scalable

What is Iterative Method ? 反復法

Linear Equations
連立一次方程式

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\mathbf{A} \qquad \mathbf{x} \qquad \mathbf{b}$$

Initial Solution
初期解

$$\mathbf{x}^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \\ \vdots \\ x_n^{(0)} \end{pmatrix}$$

Starting from a initial vector $\mathrm{x}^{(0)}$, iterative method obtains the final converged solutions by iterations

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \cdots$$

Iterative Method
反復法

- Stationary Method
  - Only x (solution vector) changes during iterations.
  - SOR, Gauss-Seidel, Jacobi
  - Generally slow, impractical

$$\mathbf{Ax} = \mathbf{b} \Rightarrow$$
$$\mathbf{x}^{(k+1)} = \mathbf{Mx}^{(k)} + \mathbf{Nb}$$

- Non-Stationary Method
  - With restriction/optimization conditions
  - Krylov-Subspace
  - CG: Conjugate Gradient
  - BiCGSTAB: Bi-Conjugate Gradient Stabilized
  - GMRES: Generalized Minimal Residual

Iterative Method (cont.)

Good

- Less expensive than direct methods, especially in memory.
- Suitable for parallel and vector computing.

Bad

- Convergence strongly depends on problems, boundary conditions (condition number etc.)
- Preconditioning is required : Key Technology for Real-World Applications in Scientific Computing (FEM, FVM, FDM etc)

Non-Stationary/Krylov Subspace Method (1/2)

非定常法・クリロフ部分空間法

$$\mathbf{Ax} = \mathbf{b} \Rightarrow \mathbf{x} = \mathbf{b} + (\mathbf{I} - \mathbf{A})\mathbf{x}$$

Compute $\mathbf{x_0}$, $\mathbf{x_1}$, $\mathbf{x_2}$, ..., $\mathbf{x_k}$ by the following iterative procedures:

$$\begin{aligned}\mathbf{x}_k &= \mathbf{b} + (\mathbf{I} - \mathbf{A})\mathbf{x}_{k-1} \\ &= (\mathbf{b} - \mathbf{A}\mathbf{x}_{k-1}) + \mathbf{x}_{k-1} \\ &= \mathbf{r}_{k-1} + \mathbf{x}_{k-1}\end{aligned}$$

$where\ \mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$ **: residual**

$\Downarrow$

$$\mathbf{x}_k = \mathbf{x}_0 + \sum_{i=0}^{k-1} \mathbf{r}_i$$

$$\begin{aligned}\mathbf{r}_k &= \mathbf{b} - \mathbf{A}\mathbf{x}_k = \mathbf{b} - \mathbf{A}(\mathbf{r}_{k-1} + \mathbf{x}_{k-1}) \\ &= (\mathbf{b} - \mathbf{A}\mathbf{x}_{k-1}) - \mathbf{A}\mathbf{r}_{k-1} = \mathbf{r}_{k-1} - \mathbf{A}\mathbf{r}_{k-1} = (\mathbf{I} - \mathbf{A})\mathbf{r}_{k-1}\end{aligned}$$

Non-Stationary/Krylov Subspace Method (2/2)

非定常法・クリロフ部分空間法

$$\mathbf{x}_k = \mathbf{x}_0 + \sum_{i=0}^{k-1} \mathbf{r}_i = \mathbf{x}_0 + \mathbf{r}_0 + \sum_{i=0}^{k-2} (\mathbf{I} - \mathbf{A}) \mathbf{r}_i = \mathbf{x}_0 + \mathbf{r}_0 + \sum_{i=1}^{k-1} (\mathbf{I} - \mathbf{A})^i \mathbf{r}_0$$

$$\mathbf{z}_k = \mathbf{r}_0 + \sum_{i=1}^{k-1} (\mathbf{I} - \mathbf{A})^i \mathbf{r}_0 = \left[\mathbf{I} + \sum_{i=1}^{k-1} (\mathbf{I} - \mathbf{A})^i \right] \mathbf{r}_0$$

↓

$\mathbf{z_k}$ is a vector which belongs to kth Krylov Subspace（クリロフ部分空間）, approximate solution vector $\mathbf{x_k}$ is derived by the Krylov Subspace:

$$\left[\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2 \mathbf{r}_0, \ldots, \mathbf{A}^{k-1} \mathbf{r}_0 \right]$$

Conjugate Gradient Method
共役勾配法

- Conjugate Gradient: CG
  - Most popular “non-stationary” iterative method
- for Symmetric Positive Definite (SPD) Matrices
  - 対称正定
  - $\{x\}^T[A]\{x\}>0$ for arbitrary $\{x\}$
  - All of diagonal components, eigenvaules and leading principal minors > 0 (主小行列式・首座行列式)
  - Matrices of Galerkin-based FEM & FVM: heat conduction, Poisson, static linear elastic problems
- Algorithm
  - “Steepest Descent Method”
  - $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
    - $x^{(i)}$: solution, $p^{(i)}$: search direction, α_i: coefficient
  - Solution $\{x\}$ minimizes $\{x-y\}^T[A]\{x-y\}$, where $\{y\}$ is exact solution.

$$\det \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & a_{24} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdots & a_{3n} \\ a_{41} & a_{42} & a_{43} & a_{44} & \cdots & a_{4n} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & a_{n3} & a_{n4} & \cdots & a_{nn} \end{bmatrix}$$

Procedures of Conjugate Gradient

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi  = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

- Mat-Vec. Multiplication
- Dot Products
- DAXPY (Double Precision: a{X} + {Y})

$x^{(i)}$: Vector

α_i : Scalar

Procedures of Conjugate Gradient

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

- Mat-Vec. Multiplication
- Dot Products
- DAXPY

$x^{(i)}$: Vector

α_i : Scalar

Procedures of Conjugate Gradient

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

- Mat-Vec. Multiplication
- Dot Products
- DAXPY

$x^{(i)}$: Vector

α_i : Scalar

Procedures of Conjugate Gradient

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

- Mat-Vec. Multiplication
- Dot Products
- DAXPY
  - Double
  - {y}= a{x} + {y}

$x^{(i)}$: Vector

α_i : Scalar

Procedures of Conjugate Gradient

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

$x^{(i)}$: Vector

α_i : Scalar

Derivation of CG Algorithm (1/5)

Solution x minimizes the following equation if y is the exact solution ($Ay=b$)

$$(x-y)^T[A](x-y)$$

$$(x-y)^T[A](x-y)=(x,Ax)-(y,Ax)-(x,Ay)+(y,Ay)$$
$$=(x,Ax)-2(x,Ay)+(y,Ay)=(x,Ax)-2(x,b)+\underline{(y,b)}$$

Const.

Therefore, the solution x minimizes the following $f(x)$:

$$f(x)=\frac{1}{2}(x,Ax)-(x,b)$$

$$f(x+h)=f(x)+(h,Ax-b)+\frac{1}{2}(h,Ah)$$

Arbitrary vector h

$$f(x)=\frac{1}{2}(x,Ax)-(x,b)$$

$$f(x+h)=f(x)+(h,Ax-b)+\frac{1}{2}(h,Ah)$$

Arbitrary vector h

$$f(x+h)=\frac{1}{2}(x+h,A(x+h))-(x+h,b)$$

$$=\frac{1}{2}(x+h,Ax)+\frac{1}{2}(x+h,Ah)-(x,b)-(h,b)$$

$$=\frac{1}{2}(x,Ax)+\underline{\frac{1}{2}(h,Ax)}+\underline{\frac{1}{2}(x,Ah)}+\frac{1}{2}(h,Ah)-(x,b)-(h,b)$$

$$=\frac{1}{2}(x,Ax)-(x,b)+(h,Ax)-(h,b)+\frac{1}{2}(h,Ah)$$

$$=f(x)+(h,Ax-b)+\frac{1}{2}(h,Ah)$$

Derivation of CG Algorithm (2/5)

CG method minimizes $f(x)$ at each iteration.
Start from initial solution $x^{(0)}$ and assume that approximate solution: $x^{(k)}$, and search direction vector $p^{(k)}$ is defined at k-th iter.

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$$

Minimization of $f(x^{(k+1)})$ is done as follows:

$$f\left(x^{(k)} + \alpha_k p^{(k)}\right) = \frac{1}{2}\alpha_k{}^2\left(p^{(k)}, Ap^{(k)}\right) - \alpha_k\left(p^{(k)}, b - Ax^{(k)}\right) + f\left(x^{(k)}\right)$$

$$\frac{\partial f\left(x^{(k)} + \alpha_k p^{(k)}\right)}{\partial \alpha_k} = 0 \Rightarrow \alpha_k = \frac{\left(p^{(k)}, b - Ax^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)} = \frac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)} \quad \text{(1)}$$

$r^{(k)} = b - Ax^{(k)}$ residual vector

Derivation of CG Algorithm (3/5)

Residual vector at $(k+1)$-th iteration:

$$r^{(k+1)} = r^{(k)} - \alpha_k A p^{(k)} \quad \textbf{(2)}$$

$$r^{(k+1)} = b - Ax^{(k+1)},\ r^{(k)} = b - Ax^{(k)}$$

$$r^{(k+1)} - r^{(k)} = -Ax^{(k+1)} + Ax^{(k)} = -\alpha_k A p^{(k)}$$

Search direction vector p is defined by the following recurrence formula:

$$p^{(k+1)} = r^{(k+1)} + \beta_k p^{(k)},\ r^{(0)} = p^{(0)} \quad \textbf{(3)}$$

It's lucky if we can get exact solution y at $(k+1)$-th iteration:

$$y = x^{(k+1)} + \alpha_{k+1} p^{(k+1)}$$

Derivation of CG Algorithm (4/5)

BTW, we have the following (convenient) orthogonality relation:

$$\left(Ap^{(k)}, y - x^{(k+1)}\right) = 0$$

$$\left(Ap^{(k)}, y - x^{(k+1)}\right) = \left(p^{(k)}, Ay - Ax^{(k+1)}\right) = \left(p^{(k)}, b - Ax^{(k+1)}\right)$$

$$= \left(p^{(k)}, b - A\left[x^{(k)} + \alpha_k p^{(k)}\right]\right) = \left(p^{(k)}, b - Ax^{(k)} - \alpha_k Ap^{(k)}\right)$$

$$= \left(p^{(k)}, r^{(k)} - \alpha_k Ap^{(k)}\right) = \left(p^{(k)}, r^{(k)}\right) - \alpha_k \left(p^{(k)}, Ap^{(k)}\right) = 0$$

$$\because \alpha_k = \frac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$$

Thus, following relation is obtained:

$$\left(Ap^{(k)}, y - x^{(k+1)}\right) = \left(Ap^{(k)}, \alpha_{k+1} p^{(k+1)}\right) = 0 \Rightarrow \left(p^{(k+1)}, Ap^{(k)}\right) = 0$$

Derivation of CG Algorithm (5/5)

$$\left(p^{(k+1)}, Ap^{(k)}\right) = \left(r^{(k+1)} + \beta_k p^{(k)}, Ap^{(k)}\right) = \left(r^{(k+1)}, Ap^{(k)}\right) + \beta_k \left(p^{(k)}, Ap^{(k)}\right) = 0$$

$$\Rightarrow \beta_k = \frac{-\left(r^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)} \quad \textbf{(4)}$$

$$\left(p^{(k+1)}, Ap^{(k)}\right) = 0$$

$p^{(k)}$ & $p^{(k+1)}$ are **"conjugate（共役）"** for matrix A

$p^{(k)}$: search direction vector, "gradient" vector

```
Compute p(0)=r(0)= b-[A]x(0)
for i= 1, 2, …
    calc. αi-1
    x(i)= x(i-1) + αi-1p(i-1)
    r(i)= r(i-1) - αi-1[A]p(i-1)

    check convergence |r|
    (if not converged)
    calc. βi-1
    p(i)= r(i) + βi-1 p(i-1)
end
```

$$\alpha_{i-1} = \frac{\left(p^{(i-1)}, r^{(i-1)}\right)}{\left(p^{(i-1)}, Ap^{(i-1)}\right)}$$

$$\beta_{i-1} = \frac{-\left(r^{(i)}, Ap^{(i-1)}\right)}{\left(p^{(i-1)}, Ap^{(i-1)}\right)}$$

Properties of CG Algorithm

Following “conjugate（共役）” relationship is obtained for arbitrary (i,j):

$$\left(p^{(i)}, Ap^{(j)}\right) = 0 \; (i \neq j)$$

Following relationships are also obtained for $p^{(k)}$ and $r^{(k)}$:

$$\left(r^{(i)}, r^{(j)}\right) = 0 \; (i \neq j), \quad \left(p^{(k)}, r^{(k)}\right) = \left(r^{(k)}, r^{(k)}\right)$$

In N-dimensional space, only N sets of orthogonal and linearly independent residual vector $r^{(k)}$. This means CG method converges after N iterations if number of unknowns is N. Actually, round-off error sometimes affects convergence.

Proof (1/3)

Mathematical Induction
数学的帰納法

$$\left(r^{(i)}, r^{(j)}\right) = 0 \ (i \neq j)$$

$$\left(p^{(i)}, Ap^{(j)}\right) = 0 \ (i \neq j)$$

(1) $$\alpha_k = \frac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$$

(2) $$r^{(k+1)} = r^{(k)} - \alpha_k A p^{(k)}$$

(3) $$p^{(k+1)} = r^{(k+1)} + \beta_k p^{(k)}, \ r^{(0)} = p^{(0)}$$

(4) $$\beta_k = \frac{-\left(r^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$$

Proof (2/3)

Mathematical Induction
数学的帰納法

$$\left(r^{(i)}, r^{(j)}\right)=0 \; (i \neq j)$$
$$\left(p^{(i)}, Ap^{(j)}\right)=0 \; (i \neq j) \quad (*)$$

(＊) is satisfied for $i \le k,\ j \le k$ where $i \neq j$

if $i < k$

$$\left(r^{(k+1)}, r^{(i)}\right)=\left(r^{(i)}, r^{(k+1)}\right)\overset{(2)}{=}\left(r^{(i)}, r^{(k)}-\alpha_k Ap^{(k)}\right)$$
$$\overset{(*)}{=}-\alpha_k\left(r^{(i)}, Ap^{(k)}\right)\overset{(3)}{=}-\alpha_k\left(p^{(i)}-\beta_{i-1}p^{(i-1)}, Ap^{(k)}\right)$$
$$=-\alpha_k\left(p^{(i)}, Ap^{(k)}\right)+\alpha_k\beta_{i-1}\left(p^{(i-1)}, Ap^{(k)}\right)\overset{(*)}{=}0$$

if $i = k$

$$\left(r^{(k+1)}, r^{(k)}\right)\overset{(2)}{=}\left(r^{(k)}, r^{(k)}\right)-\left(r^{(k)}, \alpha_k Ap^{(k)}\right)$$
$$\overset{(3)}{=}\left(r^{(k)}, r^{(k)}\right)-\left(p^{(k)}-\beta_{k-1}p^{(k-1)}, \alpha_k Ap^{(k)}\right)$$
$$\overset{(*)}{=}\left(r^{(k)}, r^{(k)}\right)-\alpha_k\left(p^{(k)}, Ap^{(k)}\right)\overset{(1)}{=}\left(r^{(k)}, r^{(k)}\right)-\left(p^{(k)}, r^{(k)}\right)$$
$$\overset{(3)}{=}\left(r^{(k)}, r^{(k)}\right)-\left(\beta_{k-1}p^{(k-1)}+r^{(k)}, r^{(k)}\right)$$
$$=-\beta_{k-1}\left(p^{(k-1)}, r^{(k)}\right)\overset{(2)}{=}-\beta_{k-1}\left(p^{(k-1)}, r^{(k-1)}-\alpha_{k-1}Ap^{(k-1)}\right)$$
$$=-\beta_{k-1}\left\{\left(p^{(k-1)}, r^{(k-1)}\right)-\alpha_{k-1}\left(p^{(k-1)}, Ap^{(k-1)}\right)\right\}\overset{(1)}{=}0$$

(1) $\alpha_k=\dfrac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$

(2) $r^{(k+1)}=r^{(k)}-\alpha_k Ap^{(k)}$

(3) $p^{(k+1)}=r^{(k+1)}+\beta_k p^{(k)}$

(4) $\beta_k=\dfrac{-\left(r^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$

Proof (3/3)

Mathematical Induction

数学的帰納法

$$\left(r^{(i)}, r^{(j)}\right) = 0 \ (i \neq j)$$
$$\left(p^{(i)}, Ap^{(j)}\right) = 0 \ (i \neq j) \quad (*)$$

(1) $\alpha_k = \dfrac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$

(2) $r^{(k+1)} = r^{(k)} - \alpha_k A p^{(k)}$

(3) $p^{(k+1)} = r^{(k+1)} + \beta_k p^{(k)}$

(4) $\beta_k = \dfrac{-\left(r^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$

(*) is satisfied for $i \leq k,\ j \leq k$ where $i \neq j$

if $i < k$

$$\left(p^{(k+1)}, Ap^{(i)}\right) \overset{(3)}{=} \left(r^{(k+1)} + \beta_k p^{(k)}, Ap^{(i)}\right)$$
$$\overset{(*)}{=} \left(r^{(k+1)}, Ap^{(i)}\right)$$
$$\overset{(2)}{=} \frac{1}{\alpha_i}\left(r^{(k+1)}, r^{(i)} - r^{(i-1)}\right) = 0$$

if $i = k$

$$\left(p^{(k+1)}, Ap^{(k)}\right) \overset{(3)}{=} \left(r^{(k+1)}, Ap^{(k)}\right) + \beta_k \left(p^{(k)}, Ap^{(k)}\right)$$
$$\overset{(4)}{=} 0$$

$$\left(r^{(k+1)}, r^{(k)}\right) = 0$$

$$\left(r^{(k+1)}, r^{(k)}\right) \overset{(2)}{=} \left(r^{(k)}, r^{(k)}\right) - \left(r^{(k)}, \alpha_k A p^{(k)}\right)$$

$$\overset{(3)}{=} \left(r^{(k)}, r^{(k)}\right) - \left(p^{(k)} - \beta_{k-1} p^{(k-1)}, \alpha_k A p^{(k)}\right)$$

$$\overset{(*)}{=} \left(r^{(k)}, r^{(k)}\right) - \alpha_k \left(p^{(k)}, A p^{(k)}\right) \overset{(1)}{=} \left(r^{(k)}, r^{(k)}\right) - \left(p^{(k)}, r^{(k)}\right) = 0$$

$$\therefore \left(r^{(k)}, r^{(k)}\right) = \left(p^{(k)}, r^{(k)}\right)$$

(1) $\alpha_k = \dfrac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$

(2) $r^{(k+1)} = r^{(k)} - \alpha_k A p^{(k)}$

(3) $p^{(k+1)} = r^{(k+1)} + \beta_k p^{(k)}$

(4) $\beta_k = \dfrac{-\left(r^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$

$\alpha_k,\ \beta_k$

Usually, we use simpler definitions of $\alpha_k,\ \beta_k$ as follows:

$$\alpha_k = \frac{\left(p^{(k)}, b - Ax^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)} = \frac{\left(p^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)} = \frac{\left(r^{(k)}, r^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$$

$$\because \left(p^{(k)}, r^{(k)}\right) = \left(r^{(k)}, r^{(k)}\right)$$

$$\beta_k = \frac{-\left(r^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)} = \frac{\left(r^{(k+1)}, r^{(k+1)}\right)}{\left(r^{(k)}, r^{(k)}\right)}$$

$$\because \left(r^{(k+1)}, Ap^{(k)}\right) = \frac{\left(r^{(k+1)}, r^{(k)} - r^{(k+1)}\right)}{\alpha_k} = -\frac{\left(r^{(k+1)}, r^{(k+1)}\right)}{\alpha_k}$$

Procedures of Conjugate Gradient

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi  = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

$x^{(i)}$: Vector

α_i : Scalar

$$\beta_{i-1} = \frac{\left(r^{(i-1)}, r^{(i-1)}\right)}{\left(r^{(i-2)}, r^{(i-2)}\right)} \quad \begin{matrix}(= \rho_{i-1}) \\ (= \rho_{i-2})\end{matrix}$$

$$\alpha_i = \frac{\left(r^{(i-1)}, r^{(i-1)}\right)}{\left(p^{(i)}, Ap^{(i)}\right)} \quad (= \rho_{i-1})$$

Preconditioning for Iterative Solvers

- Convergence rate of iterative solvers strongly depends on the spectral properties (eigenvalue distribution) of the coefficient matrix A.
  - Eigenvalue distribution is small, eigenvalues are close to 1
  - In "ill-conditioned" problems, "condition number" (ratio of max/min eigenvalue if A is symmetric) is large（条件数）.
- A preconditioner M (whose properties are similar to those of A) transforms the linear system into one with more favorable spectral properties （前処理）
  - M transforms Ax=b into A'x=b' where $A'=M^{-1}A$, $b'=M^{-1}b$
  - If M~A, $M^{-1}A$ is close to identity matrix.
  - If $M^{-1}=A^{-1}$, this is the best preconditioner (Gaussian Elim.)
  - Generally, A'x'=b' where $A'=M_L^{-1}AM_R^{-1}$, $b'=M_L^{-1}b$, $x'=M_Rx$
  - M_L/M_R: Left/Right Preconditioning（左／右前処理）

Preconditioned CG Solver

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    solve [M]z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi  = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

$[M] = [M_1][M_2]$

$[A']x' = b'$

$[A'] = [M_1]^{-1}[A][M_2]^{-1}$

$x' = [M_2]x, \quad b' = [M_1]^{-1}b$

$p' \Rightarrow [M_2]p, \quad r' \Rightarrow [M_1]^{-1}r$

$p'^{(i)} = r'^{(i-1)} + \beta'_{i-1}\, p'^{(i-1)}$

$[M_2]p^{(i)} = [M_1]^{-1}r^{(i-1)} + \beta'_{i-1}\, [M_2]p^{(i-1)}$

$p^{(i)} = [M_2]^{-1}[M_1]^{-1}r^{(i-1)} + \beta'_{i-1}\, p^{(i-1)}$

$p^{(i)} = [M]^{-1}r^{(i-1)} + \beta'_{i-1}\, p^{(i-1)}$

$\beta'_{i-1} = ([M]^{-1}r^{(i-1)}, r^{(i-1)}) / ([M]^{-1}r^{(i-2)}, r^{(i-2)})$

$\alpha'_{i-1} = ([M]^{-1}r^{(i-1)}, r^{(i-1)}) / (p^{(i-1)}, [A]p^{(i-1)})$

In CG method, preconditioner usually satisfies $[M_2]=[M_1]^T$, such as Incomplete Cholesky/Incomplete Modified Cholesky Factorizations. In this problem, let us define $[M_1]$ and $[M_2]$ as follows:

$$[M_1]=[X]^T, [M_2]=[X], [M]=[M_1][M_2]$$

$$[A']x'=b'$$

$$[A']=[M_1]^{-1}[A][M_2]^{-1}=[[X]^T]^{-1}[A][X]^{-1}=[X]^{-T}[A][X]^{-1}$$

$$x'=[X]x, \quad b'=[X]^{-T}b, \quad r'=[X]^{-T}r$$

$$\alpha'_{i-1}=\frac{\left(r'^{(i-1)},r'^{(i-1)}\right)}{\left(p'^{(i-1)},A'p'^{(i-1)}\right)}=\frac{\left([X]^{-T}r^{(i-1)},[X]^{-T}r^{(i-1)}\right)}{\left([X]p^{(i-1)},[X]^{-T}[A][X]^{-1}[X]p^{(i-1)}\right)}$$

$$=\frac{\left(\left([X]^{-T}r^{(i-1)}\right)^T,[X]^{-T}r^{(i-1)}\right)}{\left(\left([X]p^{(i-1)}\right)^T,[X]^{-T}[A]p^{(i-1)}\right)}=\frac{\left(\left(r^{(i-1)}\right)^T[X]^{-1},\left[X^T\right]^{-1}r^{(i-1)}\right)}{\left(\left(p^{(i-1)}\right)^T[X]^T,[X]^{-T}[A]p^{(i-1)}\right)}$$

$$=\frac{\left(r^{(i-1)},\left[\left[X^T\right][X]\right]^{-1}r^{(i-1)}\right)}{\left(p^{(i-1)},[A]p^{(i-1)}\right)}=\frac{\left(r^{(i-1)},[M]^{-1}r^{(i-1)}\right)}{\left(p^{(i-1)},[A]p^{(i-1)}\right)}=\frac{\left(r^{(i-1)},z^{(i-1)}\right)}{\left(p^{(i-1)},[A]p^{(i-1)}\right)}$$

$$\beta'_{i-1} = \frac{\left(r'^{(i-1)}, r'^{(i-1)}\right)}{\left(r'^{(i-2)}, r'^{(i-2)}\right)} == \frac{\left([X]^{-T} r^{(i-1)}, [X]^{-T} r^{(i-1)}\right)}{\left([X]^{-T} r^{(i-2)}, [X]^{-T} r^{(i-2)}\right)}$$

$$= \frac{\left(\left([X]^{-T} r^{(i-1)}\right)^{T}, [X]^{-T} r^{(i-1)}\right)}{\left(\left([X]^{-T} r^{(i-2)}\right)^{T}, [X]^{-T} r^{(i-2)}\right)} = \frac{\left(\left(r^{(i-1)}\right)^{T} [X]^{-1}, \left[X^{T}\right]^{-1} r^{(i-1)}\right)}{\left(\left(r^{(i-2)}\right)^{T} [X]^{-1}, \left[X^{T}\right]^{-1} r^{(i-2)}\right)}$$

$$= \frac{\left(r^{(i-1)}, \left[\left[X^{T}\right][X]\right]^{-1} r^{(i-1)}\right)}{\left(r^{(i-2)}, \left[\left[X^{T}\right][X]\right]^{-1} r^{(i-2)}\right)} = \frac{\left(r^{(i-1)}, [M]^{-1} r^{(i-1)}\right)}{\left(r^{(i-2)}, [M]^{-1} r^{(i-2)}\right)} = \frac{\left(r^{(i-1)}, z^{(i-1)}\right)}{\left(r^{(i-2)}, z^{(i-2)}\right)}$$

Preconditioned Conjugate Gradient Method（PCG）

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    solve [M]z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi  = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

Solving the following equation:

$$\{z\}=[M]^{-1}\{r\}$$

"Approximate Inverse Matrix"

$$[M]^{-1}\approx[A]^{-1},\quad [M]\approx[A]$$

Ultimate Preconditioning:
Inverse Matrix

$$[M]^{-1}=[A]^{-1},\quad [M]=[A]$$

Diagonal Scaling: Simple but weak

$$[M]^{-1}=[D]^{-1},\quad [M]=[D]$$

Diagonal Scaling, Point-Jacobi

$$[M]=\begin{bmatrix} D_1 & 0 & \dots & 0 & 0 \\ 0 & D_2 & & 0 & 0 \\ \dots & & \dots & & \dots \\ 0 & 0 & & D_{N-1} & 0 \\ 0 & 0 & \dots & 0 & D_N \end{bmatrix}$$

- **`solve [M]z`**$^{(i-1)}$**`= r`**$^{(i-1)}$ is very easy.
- Provides fast convergence for simple problems.

ILU(0), IC(0)

- Widely used Preconditioners for Sparse Matrices
  - Incomplete LU Factorization
  - Incomplete Cholesky Factorization (for Symmetric Matrices)

- Incomplete Direct Method
  - Even if original matrix is sparse, inverse matrix is not necessarily sparse.
  - **fill-in**
  - ILU(0)/IC(0) without fill-in have same non-zero pattern with the original (sparse) matrices

Full LU Factorization (or LU Decomposition)

- Direct Method
  - A^{-1} is calculated directly
  - A^{-1} can be saved
  - Fill-in's

- LU factorization

Incomplete LU Factorization (ILU)

- ILU factorization
  - Incomplete LU factorization

- Generation of fill-in's is controlled
  - Preconditioning method
  - Incomplete Inverse Matrix, "Weaker" Direct Method
  - ILU(0): NO fill-in's

Solving Linear Equations by LU Factorization

[A] is decomposed to the following form of [L][U]:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{pmatrix}$$

$$\mathbf{A} = \mathbf{LU}$$

L : Lower triangular part of matrix A

U : Upper triangular part of matrix A

Linear Equations in Matrix Form

General linear equations with "n" unknowns:

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$
$$\vdots$$
$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n$$

Matrix form:

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \Leftrightarrow \mathbf{Ax} = \mathbf{b}$$

$\mathbf{A}$ $\mathbf{x}$ $\mathbf{b}$

Solving Ax=b by LU Factorization

1 $\mathbf{A} = \mathbf{LU}$ Compute [L] and [U]

2 $\mathbf{Ly} = \mathbf{b}$ Solve $\mathbf{Ly=b}$

3 $\mathbf{Ux} = \mathbf{y}$ Solve $\mathbf{Ux=y}$

This $\mathbf{x}$ is solution of $\mathbf{Ax} = \mathbf{b}$

$$\because \mathbf{Ax} = \mathbf{LUx} = \mathbf{Ly} = \mathbf{b}$$

Solving Ly=b: Forward Substitution

$$\mathbf{Ly} = \mathbf{b} \iff \begin{pmatrix} 1 & 0 & \cdots & 0 \\ l_{21} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\iff$$

$$\begin{aligned} y_1 &= b_1 \\ l_{21} y_1 + y_2 &= b_2 \\ &\vdots \\ l_{n1} y_1 + l_{n2} y_2 + \cdots + y_n &= b_n \end{aligned} \iff \begin{aligned} y_1 &= b_1 \\ y_2 &= b_2 - l_{21} y_1 \\ &\vdots \\ y_n &= b_n - l_{n1} y_1 - l_{n2} y_2 \cdots - l_{n,n-1} y_{n-1} \\ &= b_n - \sum_{i=1}^{n-1} l_{ni} y_i \end{aligned}$$

Solving Ux=y: Backward Substitution

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

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

How to calculate LU Factorization/Decomposition

①

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{pmatrix}$$

③ ② ④

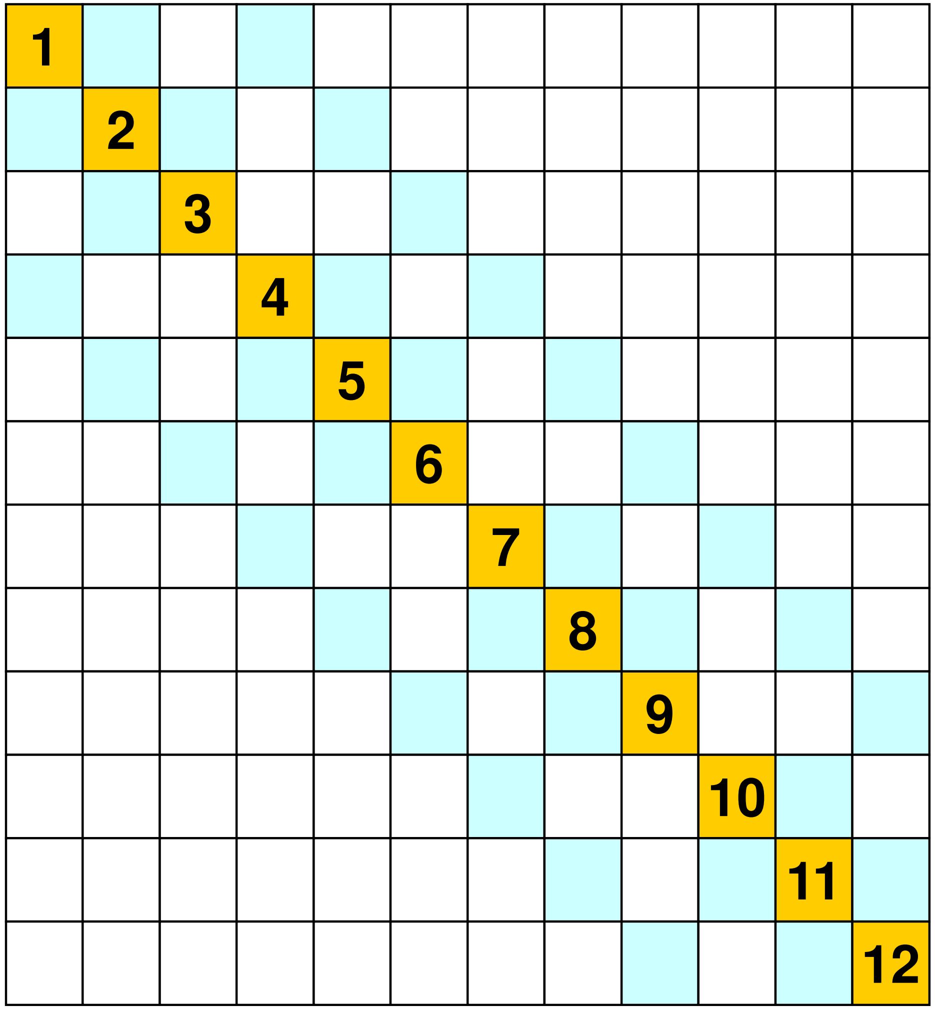
① ➡ $a_{11} = u_{11}, a_{12} = u_{12}, \cdots, a_{1n} = u_{1n} \Rightarrow u_{11}, u_{12}, \cdots, u_{1n}$

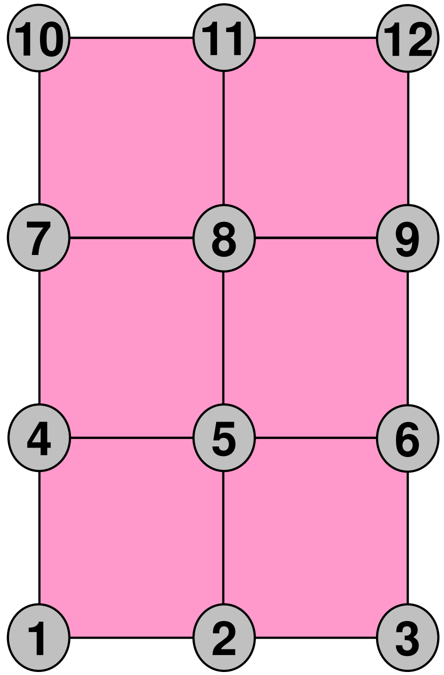
② ➡ $a_{21} = l_{21}u_{11}, a_{31} = l_{31}u_{11}, \cdots, a_{n1} = l_{n1}u_{11} \Rightarrow l_{21}, l_{31}, \cdots, l_{n1}$

③ ➡ $a_{22} = l_{21}u_{12} + u_{22}, \cdots, a_{2n} = l_{21}u_{1n} + u_{2n} \Rightarrow u_{22}, u_{23}, \cdots, u_{2n}$

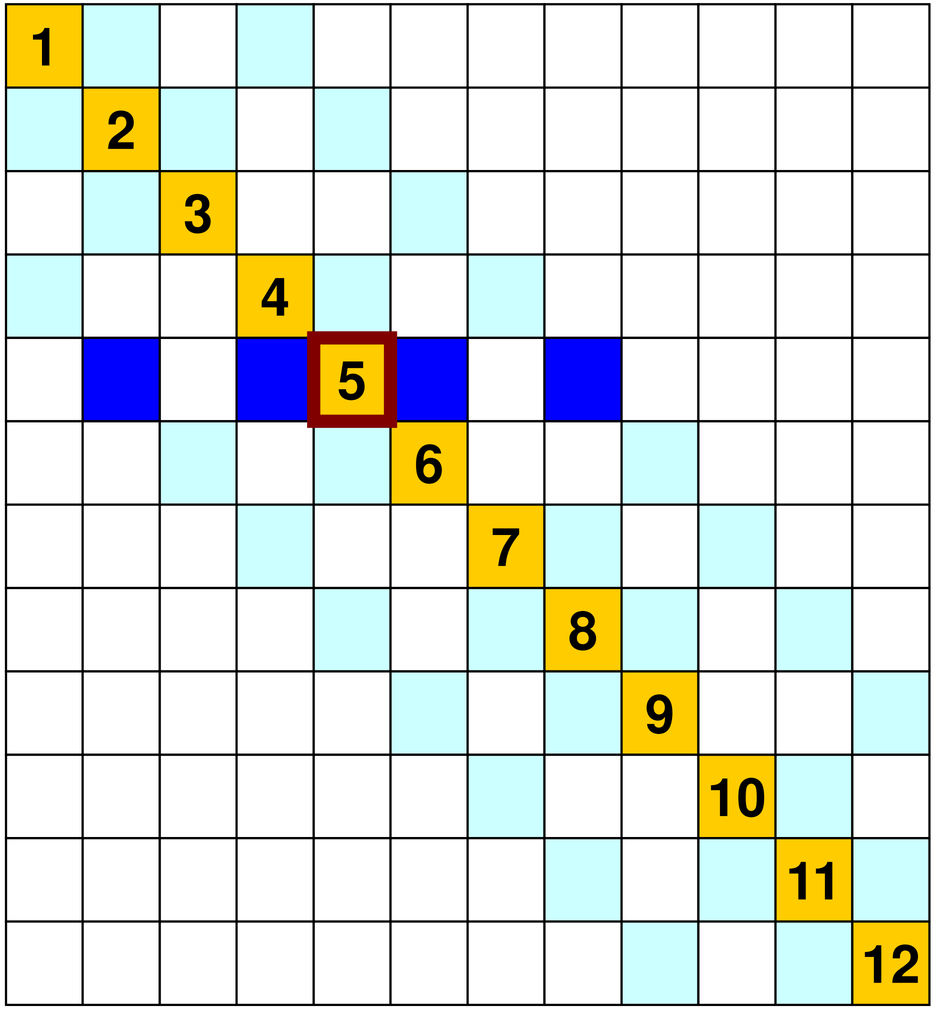
④ ➡ $a_{32} = l_{31}u_{12} + l_{32}u_{22}, \cdots \Rightarrow l_{32}, l_{42}, \cdots, l_{n2}$

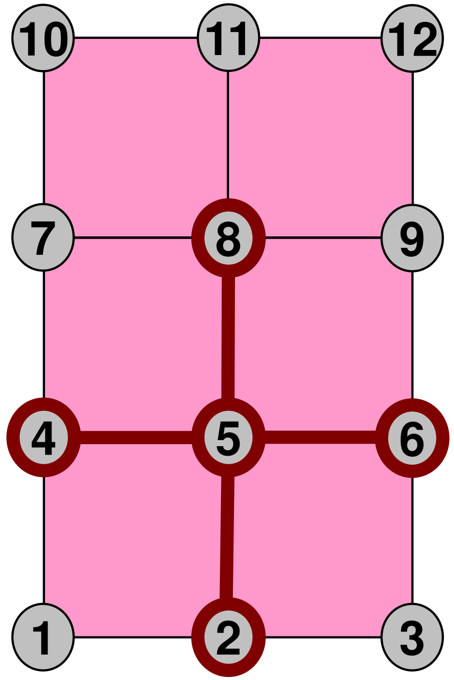
Example: 5-Point Stencil





Example: 5-Point Stencil



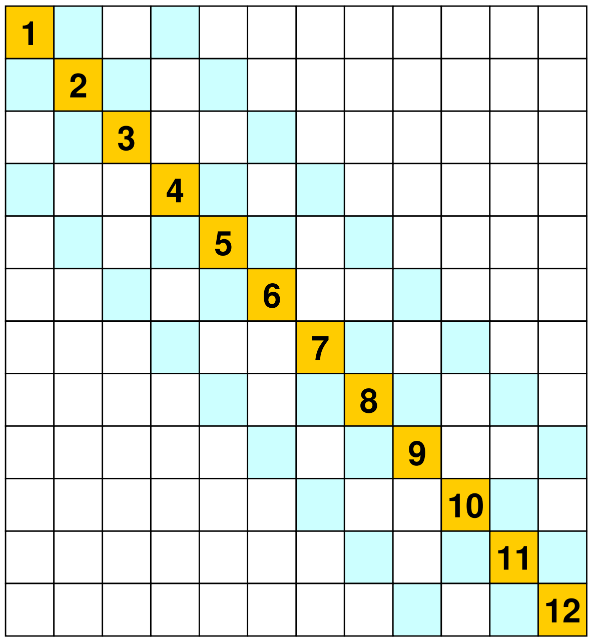


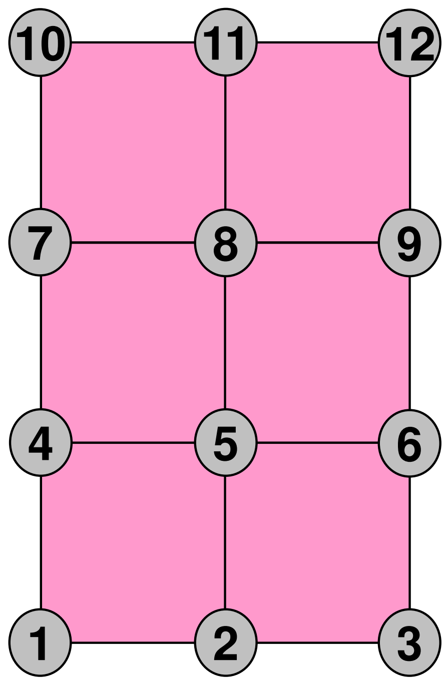
Coef. Matrix

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00

X =

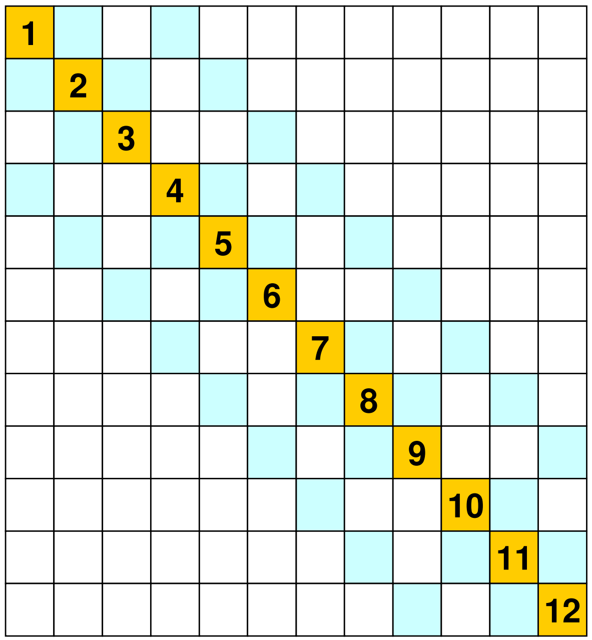
0.00
3.00
10.00
11.00
10.00
19.00
20.00
16.00
28.00
42.00
36.00
52.00

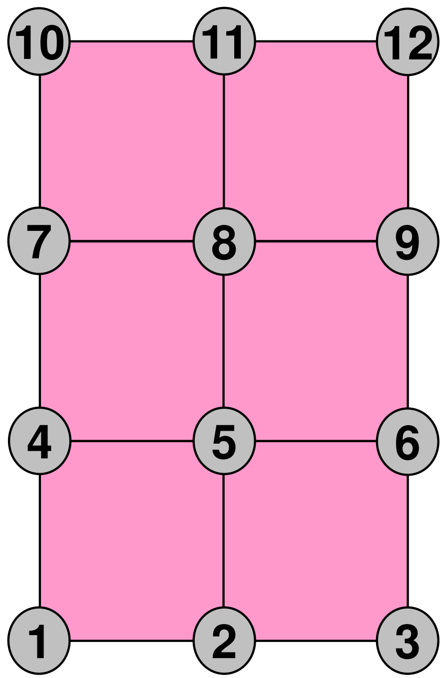




Solution

$$
\begin{pmatrix}
6.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & 6.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & -1.00 & 6.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
-1.00 & 0.00 & 0.00 & 6.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & -1.00 & 0.00 & -1.00 & 6.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & -1.00 & 0.00 & -1.00 & 6.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 6.00 & -1.00 & 0.00 & -1.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & -1.00 & 6.00 & -1.00 & 0.00 & -1.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & -1.00 & 6.00 & 0.00 & 0.00 & -1.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 & 6.00 & -1.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & -1.00 & 6.00 & -1.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & -1.00 & 6.00
\end{pmatrix}
\begin{pmatrix}
1.00 \\ 2.00 \\ 3.00 \\ 4.00 \\ 5.00 \\ 6.00 \\ 7.00 \\ 8.00 \\ 9.00 \\ 10.00 \\ 11.00 \\ 12.00
\end{pmatrix}
=
\begin{pmatrix}
0.00 \\ 3.00 \\ 10.00 \\ 11.00 \\ 10.00 \\ 19.00 \\ 20.00 \\ 16.00 \\ 28.00 \\ 42.00 \\ 36.00 \\ 52.00
\end{pmatrix}
$$





Full LU Factorization

Original Matrix

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00

LU Factorization

[L][U]

Diagonal Components of [L] (=1) are not displayed

fill-in occurred

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	−0.03	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	−0.03	0.00	5.83	−1.03	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	−0.03	−0.18	5.64	−1.03	−0.18	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.64	−0.03	−0.18	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03	−0.18	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63	−0.03	−0.18	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63

ILU Factorization (without Fill-in)

ILU Factorization
[L][U]
Diagonal Components of [L] (=1) are not displayed

NO fill-in's

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65

LU Factorization
[L][U]
Diagonal Components of [L] (=1) are not displayed

fill-in occurred

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	−0.03	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	−0.03	0.00	5.83	−1.03	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	−0.03	−0.18	5.64	−1.03	−0.18	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.64	−0.03	−0.18	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03	−0.18	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63	−0.03	−0.18	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63

Solution: A little bit inaccurate ...

ILU

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65

0.92
1.75
2.76
3.79
4.46
5.57
6.66
7.25
8.46
9.66
10.54
11.83

Full LU

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	−0.03	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	−0.03	0.00	5.83	−1.03	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	−0.03	−0.18	5.64	−1.03	−0.18	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.64	−0.03	−0.18	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03	−0.18	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63	−0.03	−0.18	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63

1.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00

Solution: A little bit inaccurate ...

ILU

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65

→

0.92
1.75
2.76
3.79
4.46
5.57
6.66
7.25
8.46
9.66
10.54
11.83

Diagonal Scaling (Point Jacobi)

6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.00

→

0.00
0.50
1.67
1.83
1.67
3.17
3.33
2.67
4.67
7.00
6.00
8.67

ILU(0), IC(0)

- Incomplete Factorization without Fill-in's
  - Saving Memory, Smaller Computations

- **If we solve equations by this incomplete factorization, we can get "incomplete" solutions.**
  - **But those are not far from accurate ones.**
  - **"Accuracy"/"Inaccuracy" depends on property of matrices**

Classification of Preconditioning Methods: Trade-off

Weak ⟷ **Strong**

Point Jacobi

Diagonal Blocking

ILU(0)

ILU(1)

ILU(2)

Gaussian Elimination

- Simple
- Easy to be Parallelized
- Cheap

- Complicated
- Global Dependency
- Expensive

- Background
  - Finite Volume Method
  - Preconditioned Iterative Solvers
- **ICCG Solver for Poisson Equations**
  - **How to run**
    - **Data Structure**
  - Program
    - Initialization
    - Coefficient Matrices
    - ICCG

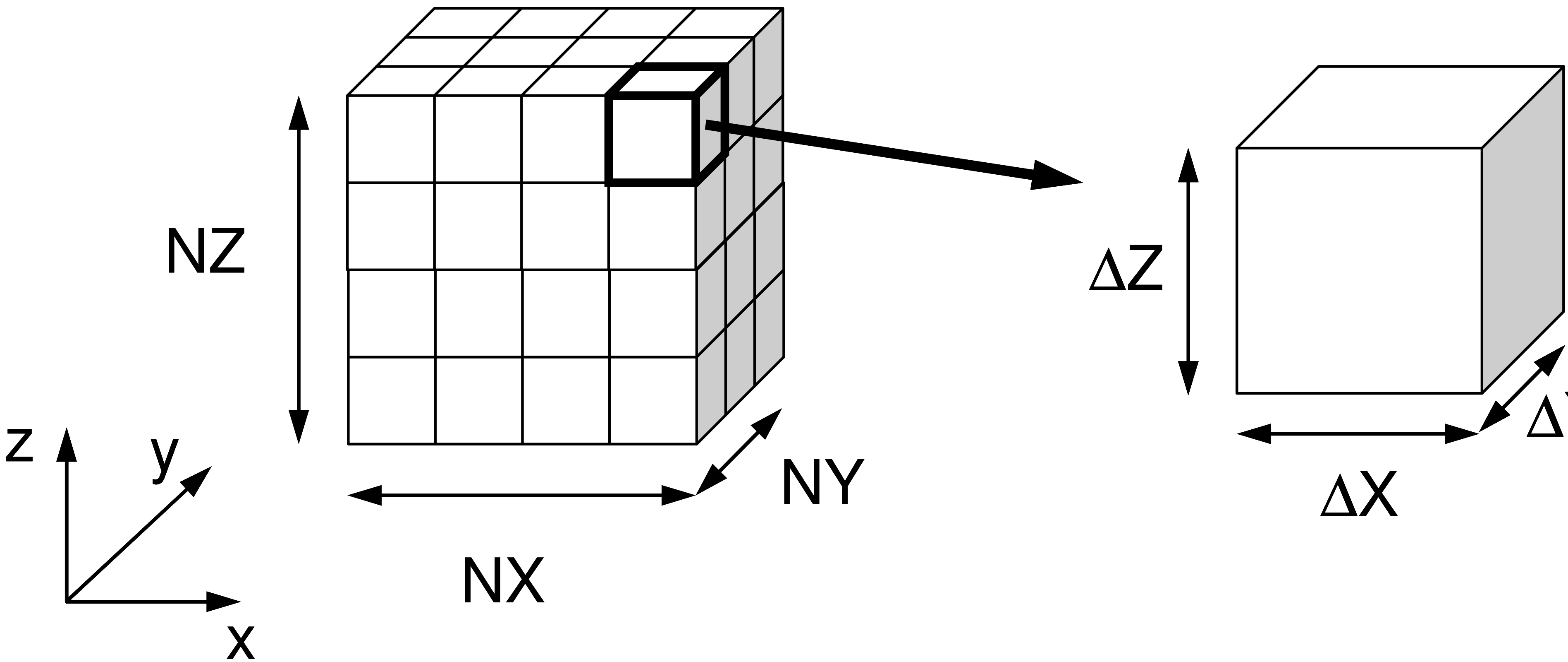
Target Application

- 3D Poisson Equation/Poisson's Equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

- Finite Volume Method (FVM)
  - Arbitrary Shape Meshes, Cell-Centered
  - "Direct" Finite Difference Method
- Boundary Conditions (B.C.) etc.
  - Dirichlet B.C., Volume Flux
- Preconditioned Iterative Solvers
  - Conjugate Gradient + Preconditioner

3D Structured Mesh
Internal data structure is "unstructured"



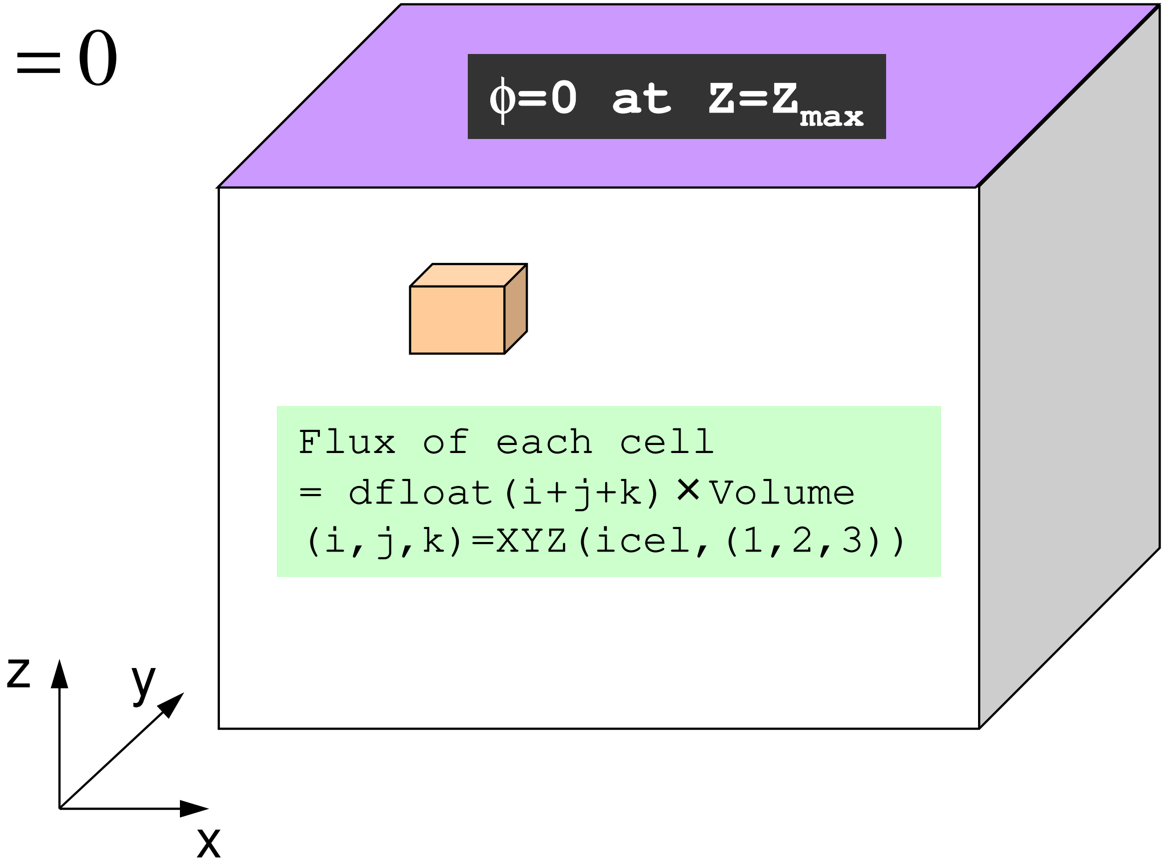
Target Problem: Variables are defined at cell-center's

Poisson Equation/ Poisson's Equation

$$\frac{\partial^2 \phi}{\partial x^2}+\frac{\partial^2 \phi}{\partial y^2}+\frac{\partial^2 \phi}{\partial z^2}+f=0$$

Boundary Conditions (B.C.) etc.

- Volume Flux
- ϕ=0@Z=Z_{max}



Poisson Equation by Finite Volume Method (FVM)

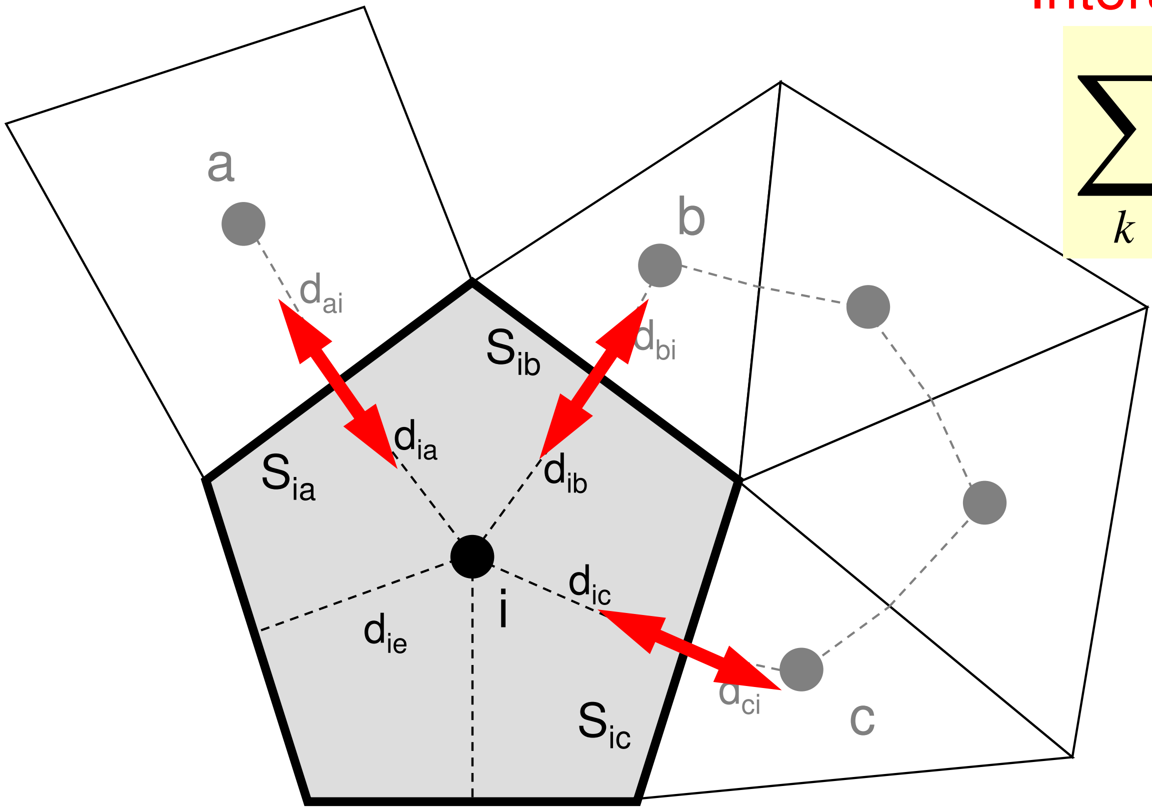
$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

Conservation of Fluxes through Surfaces

Diffusion:
Interaction with Neighbors

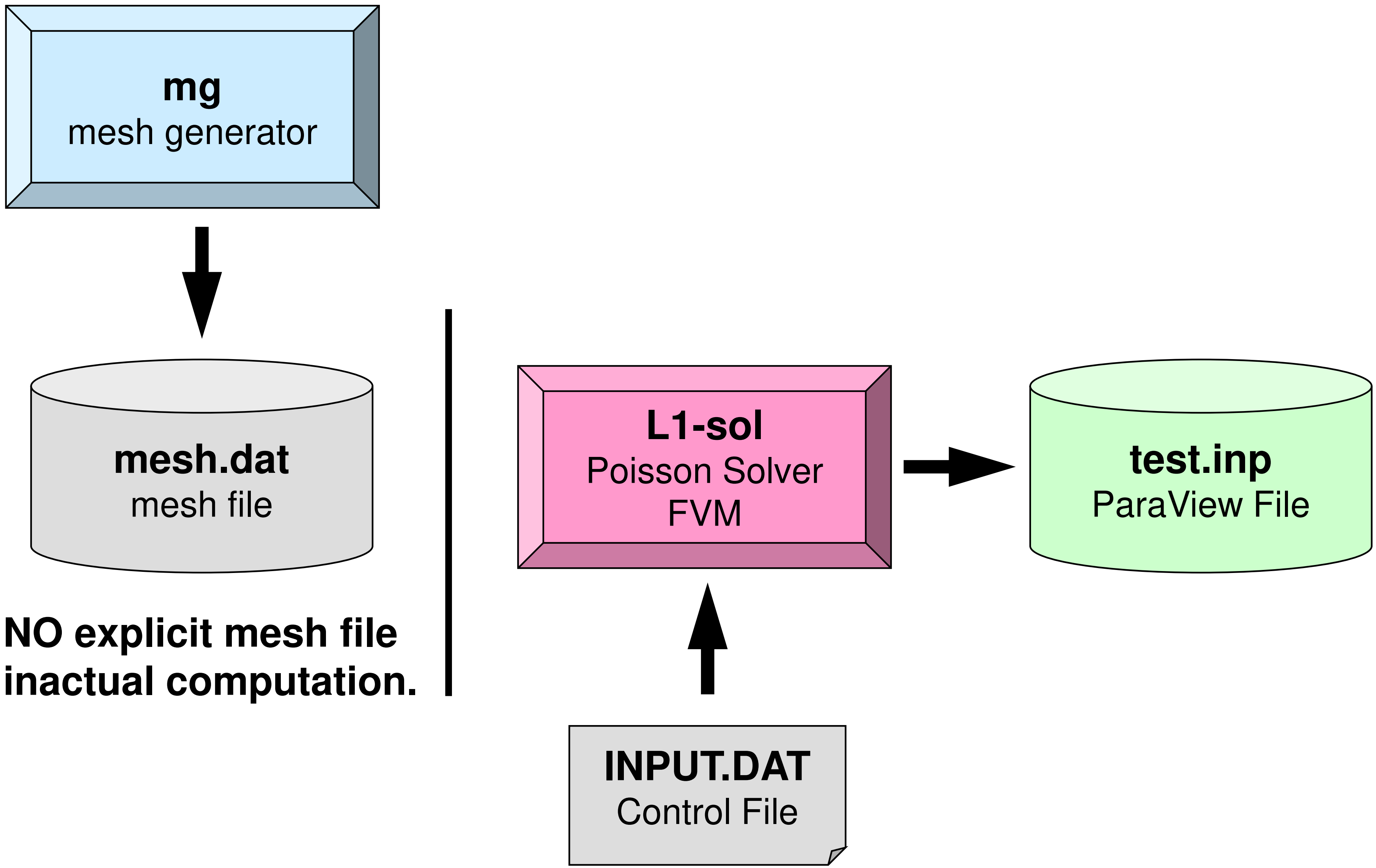
$$\sum_k \frac{S_{ik}}{d_{ik} + d_{ki}} (\phi_k - \phi_i) + V_i \dot{Q}_i = 0$$

Volume Flux




```
Vi   : Volume
S    : Surface Area
dij  : Distance between
       Cell-Center &
       Surface
Q    : Volume Flux
```

Running the Program: <$E-L1>/run



Running the Program

Compiling

```
$> cd multicore-f/L1/run

$> gfortran -O mg.f -o mg (or cc -O mg.c -o mg)
$> ls mg
      mg

$> cd ../src
$> make
$> ls ../run/L1-sol
      L1-sol
```

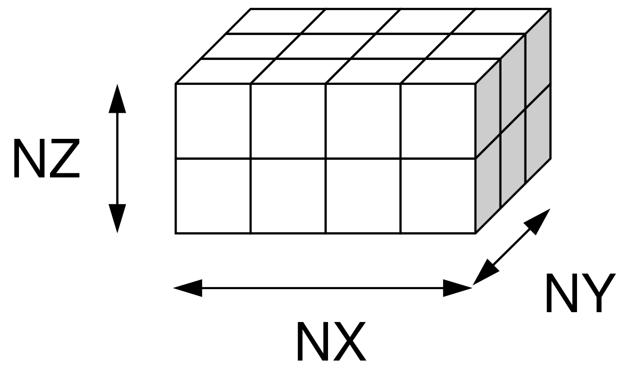
Mesh Generator: **mg**

Poisson Solver (FVM): **L1-sol**

Running the Program
Mesh Generation

```
$> cd ../run
$> ./mg
   4 3 2
$> ls mesh.dat
     mesh.dat
```

NX, NY, NZ



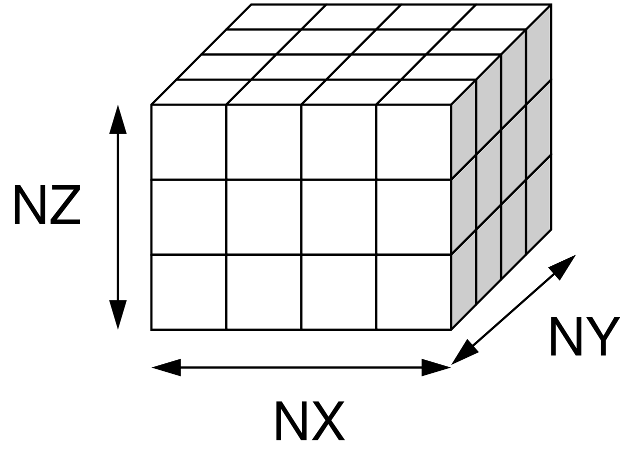
mesh.dat (1/5)

```
   4    3    2
  24
   1    0    2    0    5    0   13    1    1    1
   2    1    3    0    6    0   14    2    1    1
   3    2    4    0    7    0   15    3    1    1
   4    3    0    0    8    0   16    4    1    1
   5    0    6    1    9    0   17    1    2    1
   6    5    7    2   10    0   18    2    2    1
   7    6    8    3   11    0   19    3    2    1
   8    7    0    4   12    0   20    4    2    1
   9    0   10    5    0    0   21    1    3    1
  10    9   11    6    0    0   22    2    3    1
  11   10   12    7    0    0   23    3    3    1
  12   11    0    8    0    0   24    4    3    1
  13    0   14    0   17    1    0    1    1    2
  14   13   15    0   18    2    0    2    1    2
  15   14   16    0   19    3    0    3    1    2
  16   15    0    0   20    4    0    4    1    2
  17    0   18   13   21    5    0    1    2    2
  18   17   19   14   22    6    0    2    2    2
  19   18   20   15   23    7    0    3    2    2
  20   19    0   16   24    8    0    4    2    2
  21    0   22   17    0    9    0    1    3    2
  22   21   23   18    0   10    0    2    3    2
  23   22   24   19    0   11    0    3    3    2
  24   23    0   20    0   12    0    4    3    2
```

```
read (21,'(10i10)') NX , NY , NZ
read (21,'(10i10)') ICELTOT

do i= 1, ICELTOT
  read (21, '(10i10)' ) ii, (NEIBcell(i,k), k= 1, 6), (XYZ(i,j), j= 1, 3)
enddo
```

mesh.dat (2/5)

```
   4    3    2
  24
   1    0    2    0    5    0   13    1    1    1
   2    1    3    0    6    0   14    2    1    1
   3    2    4    0    7    0   15    3    1    1
   4    3    0    0    8    0   16    4    1    1
   5    0    6    1    9    0   17    1    2    1
   6    5    7    2   10    0   18    2    2    1
   7    6    8    3   11    0   19    3    2    1
   8    7    0    4   12    0   20    4    2    1
   9    0   10    5    0    0   21    1    3    1
  10    9   11    6    0    0   22    2    3    1
  11   10   12    7    0    0   23    3    3    1
  12   11    0    8    0    0   24    4    3    1
  13    0   14    0   17    1    0    1    1    2
  14   13   15    0   18    2    0    2    1    2
  15   14   16    0   19    3    0    3    1    2
  16   15    0    0   20    4    0    4    1    2
  17    0   18   13   21    5    0    1    2    2
  18   17   19   14   22    6    0    2    2    2
  19   18   20   15   23    7    0    3    2    2
  20   19    0   16   24    8    0    4    2    2
  21    0   22   17    0    9    0    1    3    2
  22   21   23   18    0   10    0    2    3    2
  23   22   24   19    0   11    0    3    3    2
  24   23    0   20    0   12    0    4    3    2
```



Number of meshes in X/Y/Z directions

```
read (21,'(10i10)') NX , NY , NZ
read (21,'(10i10)') ICELTOT

do i= 1, ICELTOT
  read (21, '(10i10)' ) ii, (NEIBcell(i,k), k= 1, 6), (XYZ(i,j), j= 1, 3)
enddo
```

mesh.dat (3/5)

```
   4   3   2
  24
   1   0   2   0   5   0  13   1   1   1
   2   1   3   0   6   0  14   2   1   1
   3   2   4   0   7   0  15   3   1   1
   4   3   0   0   8   0  16   4   1   1
   5   0   6   1   9   0  17   1   2   1
   6   5   7   2  10   0  18   2   2   1
   7   6   8   3  11   0  19   3   2   1
   8   7   0   4  12   0  20   4   2   1
   9   0  10   5   0   0  21   1   3   1
  10   9  11   6   0   0  22   2   3   1
  11  10  12   7   0   0  23   3   3   1
  12  11   0   8   0   0  24   4   3   1
  13   0  14   0  17   1   0   1   1   2
  14  13  15   0  18   2   0   2   1   2
  15  14  16   0  19   3   0   3   1   2
  16  15   0   0  20   4   0   4   1   2
  17   0  18  13  21   5   0   1   2   2
  18  17  19  14  22   6   0   2   2   2
  19  18  20  15  23   7   0   3   2   2
  20  19   0  16  24   8   0   4   2   2
  21   0  22  17   0   9   0   1   3   2
  22  21  23  18   0  10   0   2   3   2
  23  22  24  19   0  11   0   3   3   2
  24  23   0  20   0  12   0   4   3   2
```

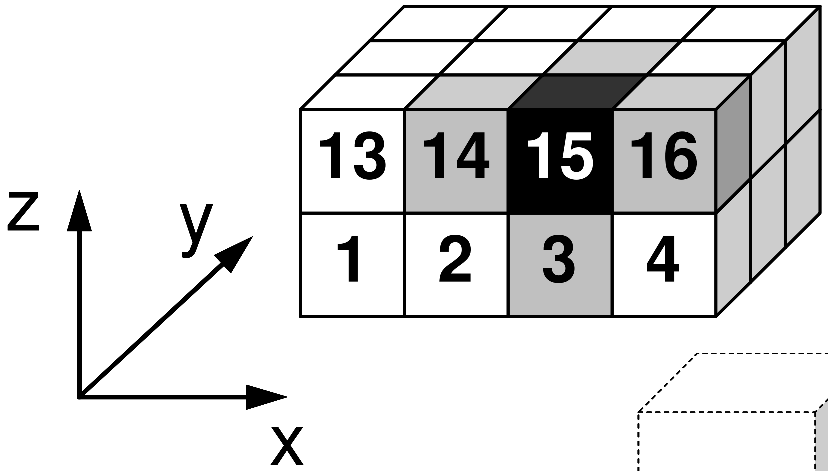
Number of Meshes (Cells) = NX x NY x NZ

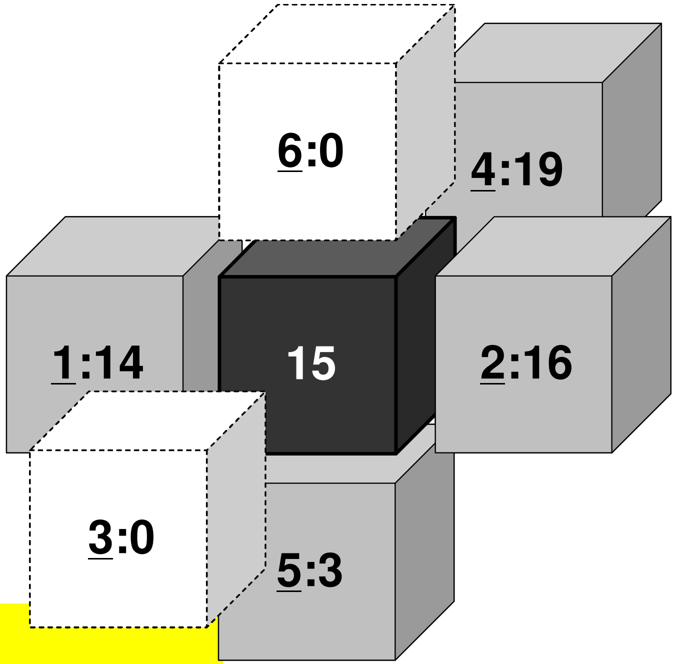
```
read (21,'(10i10)') NX , NY , NZ
read (21,'(10i10)') ICELTOT

do i= 1, ICELTOT
  read (21, '(10i10)' ) ii, (NEIBcell(i,k), k= 1, 6), (XYZ(i,j), j= 1, 3)
enddo
```

mesh.dat (4/5)

```
   4    3    2
  24
   1    0    2    0    5    0   13    1    1    1
   2    1    3    0    6    0   14    2    1    1
   3    2    4    0    7    0   15    3    1    1
   4    3    0    0    8    0   16    4    1    1
   5    0    6    1    9    0   17    1    2    1
   6    5    7    2   10    0   18    2    2    1
   7    6    8    3   11    0   19    3    2    1
   8    7    0    4   12    0   20    4    2    1
   9    0   10    5    0    0   21    1    3    1
  10    9   11    6    0    0   22    2    3    1
  11   10   12    7    0    0   23    3    3    1
  12   11    0    8    0    0   24    4    3    1
  13    0   14    0   17    1    0    1    1    2
  14   13   15    0   18    2    0    2    1    2
  15   14   16    0   19    3    0    3    1    2
  16   15    0    0   20    4    0    4    1    2
  17    0   18   13   21    5    0    1    2    2
  18   17   19   14   22    6    0    2    2    2
  19   18   20   15   23    7    0    3    2    2
  20   19    0   16   24    8    0    4    2    2
  21    0   22   17    0    9    0    1    3    2
  22   21   23   18    0   10    0    2    3    2
  23   22   24   19    0   11    0    3    3    2
  24   23    0   20    0   12    0    4    3    2
```

Neighboring Cells: NEIBcell(i,k)

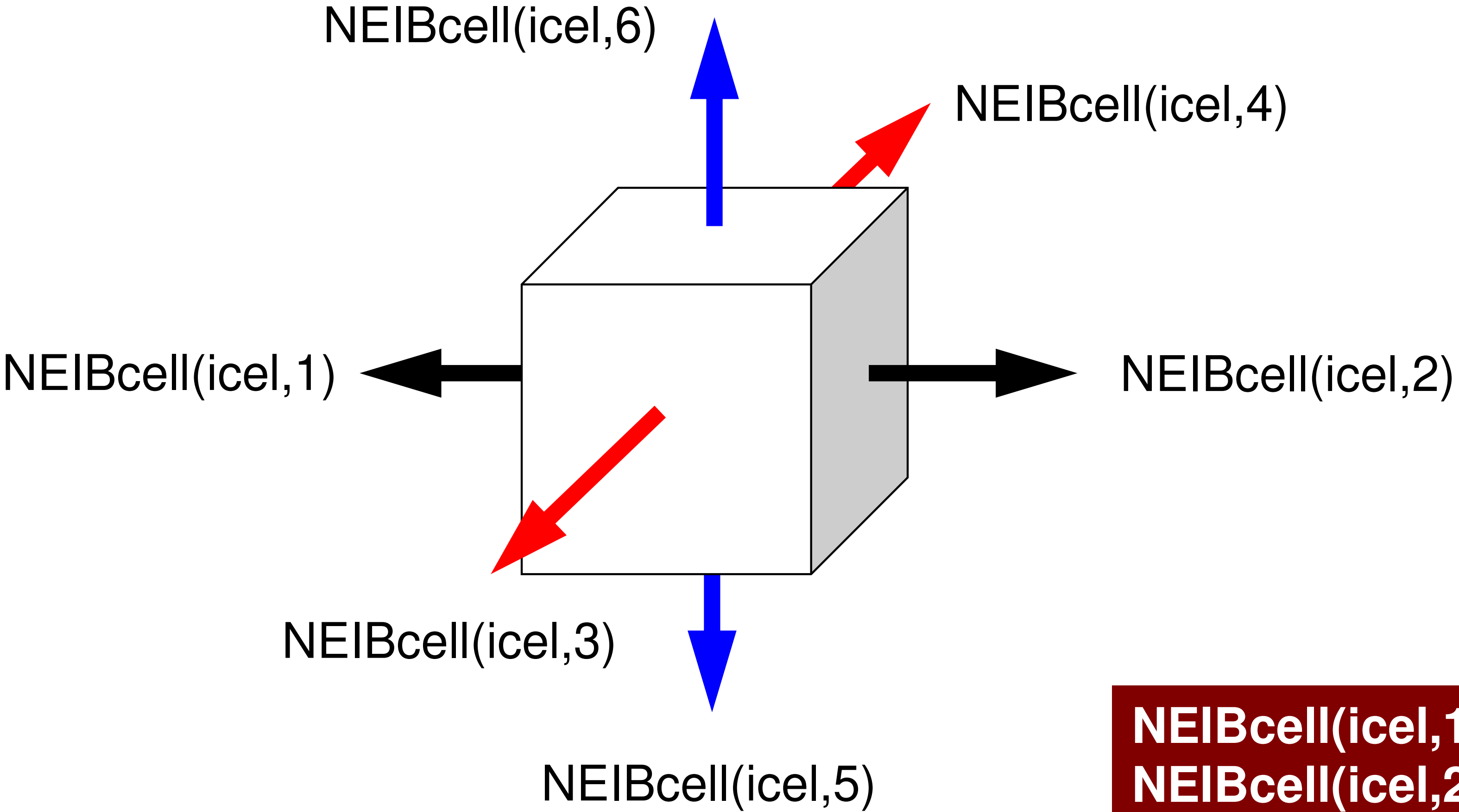





```
read (21,'(10i10)') NX , NY , NZ
read (21,'(10i10)') ICELTOT

do i= 1, ICELTOT
  read (21, '(10i10)' ) ii, (NEIBcell(i,k), k= 1, 6), (XYZ(i,j), j= 1, 3)
enddo
```

1st Col.: Global ID of the Cell

NEIBcell: ID of Neighboring Mesh/Cell =0: for Boundary Surface

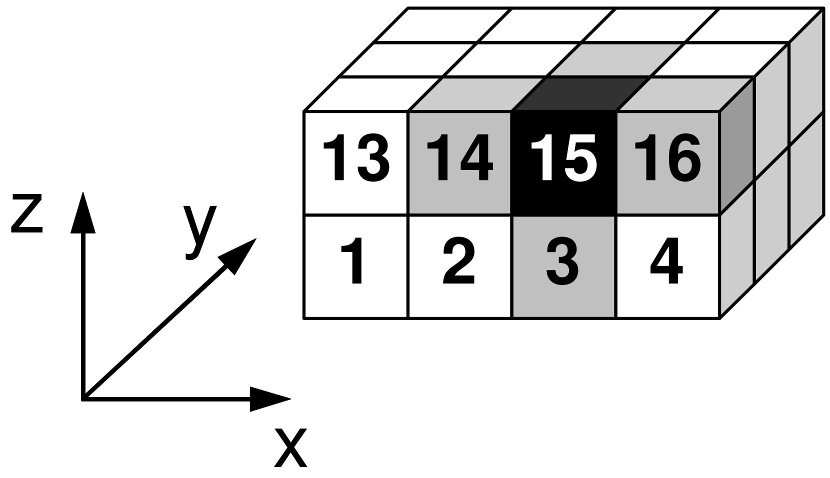


NEIBcell(icel,1)= icel – 1
NEIBcell(icel,2)= icel + 1
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,6)= icel + NX*NY

mesh.dat (5/5)

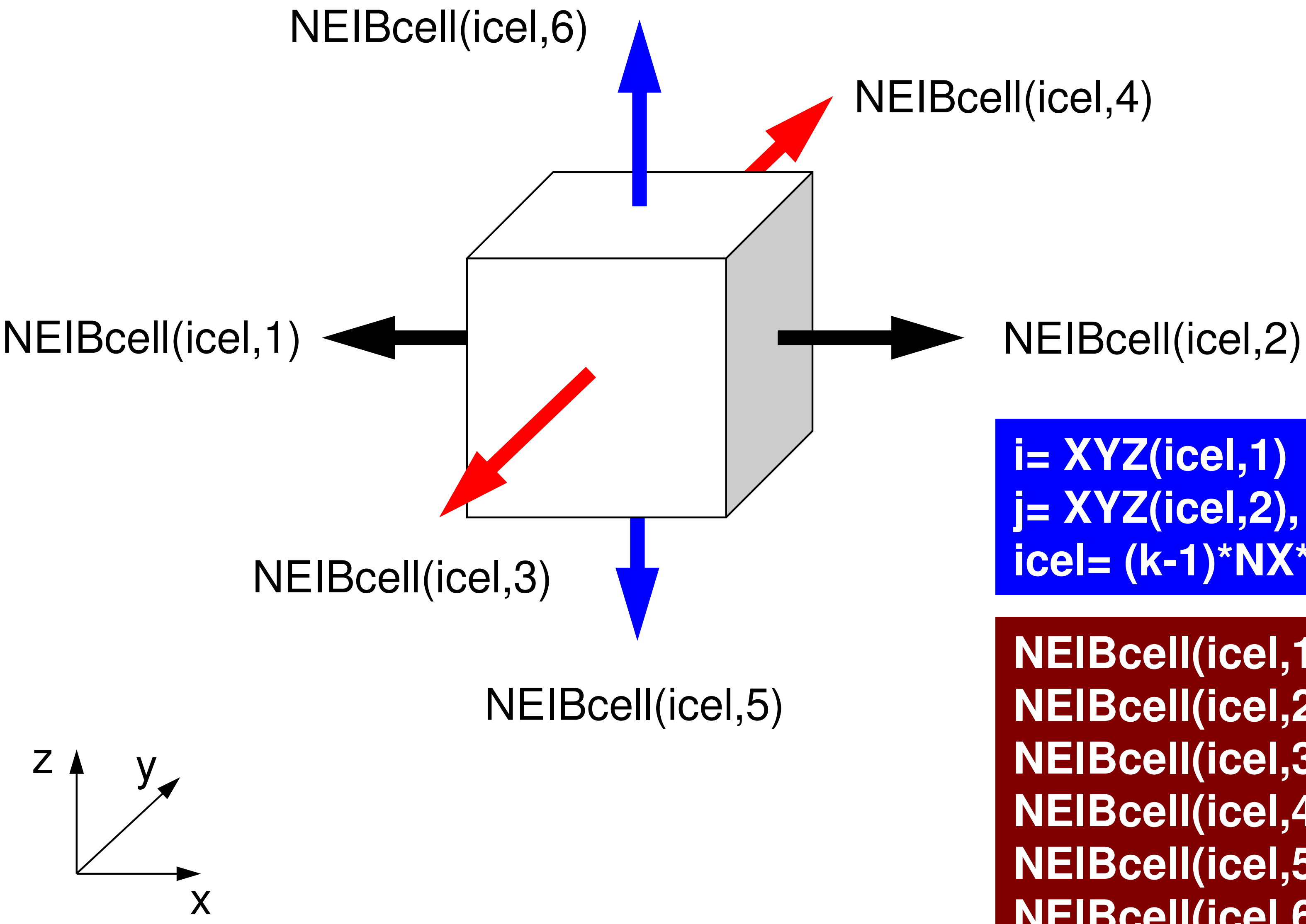
Location in X,Y,Z-directions: XYZ(i,j)

```
   4    3    2
  24
   1    0    2    0    5    0   13    1    1    1
   2    1    3    0    6    0   14    2    1    1
   3    2    4    0    7    0   15    3    1    1
   4    3    0    0    8    0   16    4    1    1
   5    0    6    1    9    0   17    1    2    1
   6    5    7    2   10    0   18    2    2    1
   7    6    8    3   11    0   19    3    2    1
   8    7    0    4   12    0   20    4    2    1
   9    0   10    5    0    0   21    1    3    1
  10    9   11    6    0    0   22    2    3    1
  11   10   12    7    0    0   23    3    3    1
  12   11    0    8    0    0   24    4    3    1
  13    0   14    0   17    1    0    1    1    2
  14   13   15    0   18    2    0    2    1    2
  15   14   16    0   19    3    0    3    1    2
  16   15    0    0   20    4    0    4    1    2
  17    0   18   13   21    5    0    1    2    2
  18   17   19   14   22    6    0    2    2    2
  19   18   20   15   23    7    0    3    2    2
  20   19    0   16   24    8    0    4    2    2
  21    0   22   17    0    9    0    1    3    2
  22   21   23   18    0   10    0    2    3    2
  23   22   24   19    0   11    0    3    3    2
  24   23    0   20    0   12    0    4    3    2
```




```
read (21,'(10i10)') NX , NY , NZ
read (21,'(10i10)') ICELTOT

do i= 1, ICELTOT
  read (21, '(10i10)' ) ii, (NEIBcell(i,k), k= 1, 6), (XYZ(i,j), j= 1, 3)
enddo
```

NEIBcell: ID of Neighboring Mesh/Cell =0: for Boundary Surface



i= XYZ(icel,1)
j= XYZ(icel,2), k= XYZ(icel,3)
icel= (k-1)*NX*NY + (j-1)*NX + i

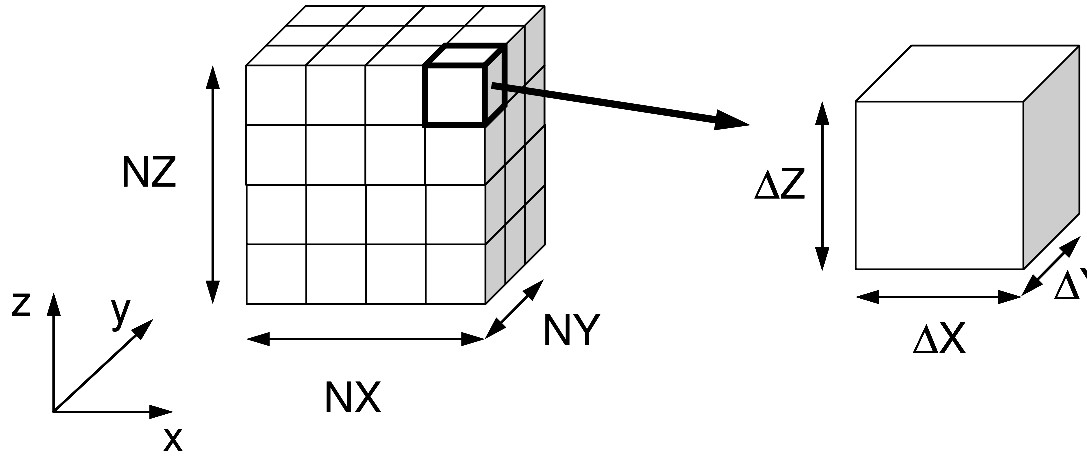
NEIBcell(icel,1)= icel – 1
NEIBcell(icel,2)= icel + 1
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,6)= icel + NX*NY

Running the Program

Control Data: <$E-L1>/run/INPUT.DAT

```
32 32 32                                 NX/NY/NZ
1                                        MEHOD 1:2:3
1.00e-00 1.00e-00 1.00e-00               DX/DY/DZ
1.0e-08                                  EPSICCG
```

- NX, NY, NZ
  - Number of meshes in X/Y/Z dir.
- METHOD
  - Preconditioner
- DX, DY, DZ
  - Size of meshes
- EPSICCG
  - Convergence Criteria for ICCG



Preconditioning Method

```
32 32 32                                     NX/NY/NZ
1                                            MEHOD 1:2:3
1.00e-00 1.00e-00 1.00e-00                   DX/DY/DZ
1.0e-08                                      EPSICCG
```

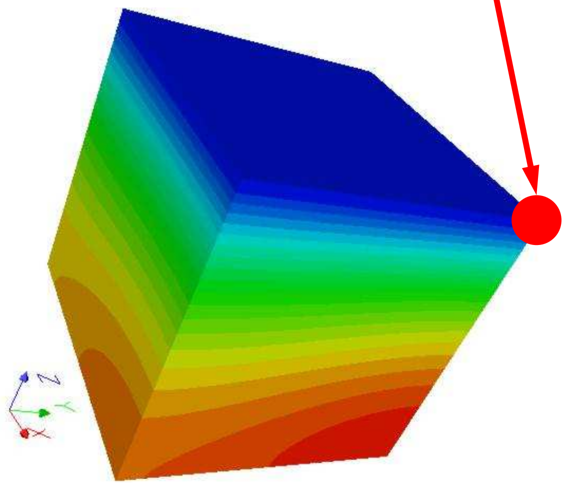
- METHOD=1 Incomplete Modified Cholesky Fact. (Off-Diagonal Components unchanged)
- METHOD=2 Incomplete Modified Cholesky Fact. (Fortran ONLY)
- METHOD=3 Diagonal Scaling/Point Jacobi

Running the Program

Running, Post Processing by ParaView

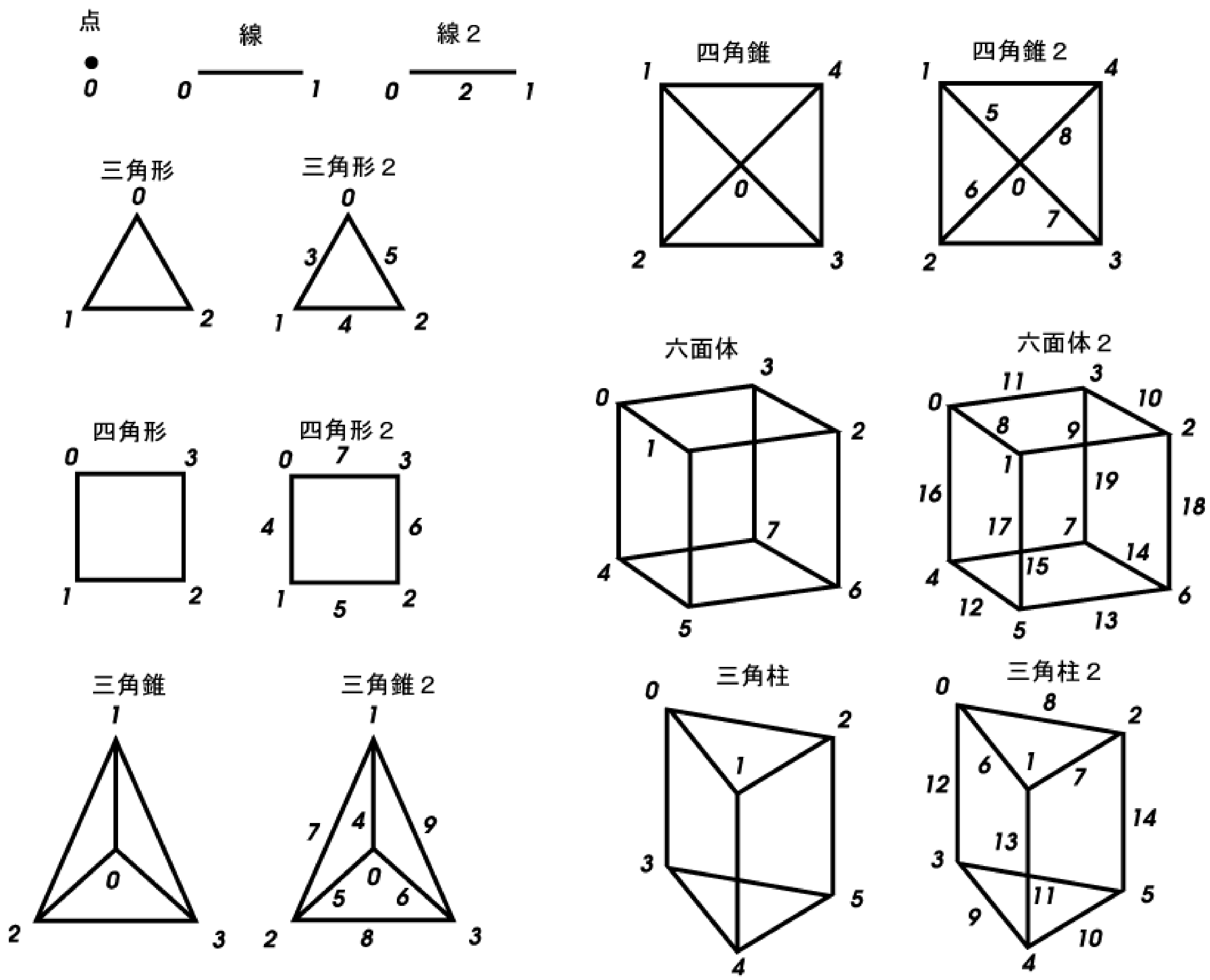
http://nkl.cc.u-tokyo.ac.jp/21s/ParaView.pdf

```
$> cd
$> cd multicore-f/L1/run
$> ./L1-sol
    1     4.504513E+00   Residual at the 1st Iteration
   75     8.377861E-09   Residual at convergence (<10-8)

##ANSWER      32768     9.297409E+02   Result at ●-point

$> ls test.inp
   test.inp
```



UCD Format (1/2)
Unstructured Cell Data

要素の種類	キーワード
点	pt
線	line
三角形	tri
四角形	quad
四面体	tet
角錐	pyr
三角柱	prism
六面体	hex
二次要素	
線2	line2
三角形2	tri2
四角形2	quad2
四面体2	tet2
角錐2	pyr2
三角柱2	prism2
六面体2	hex2



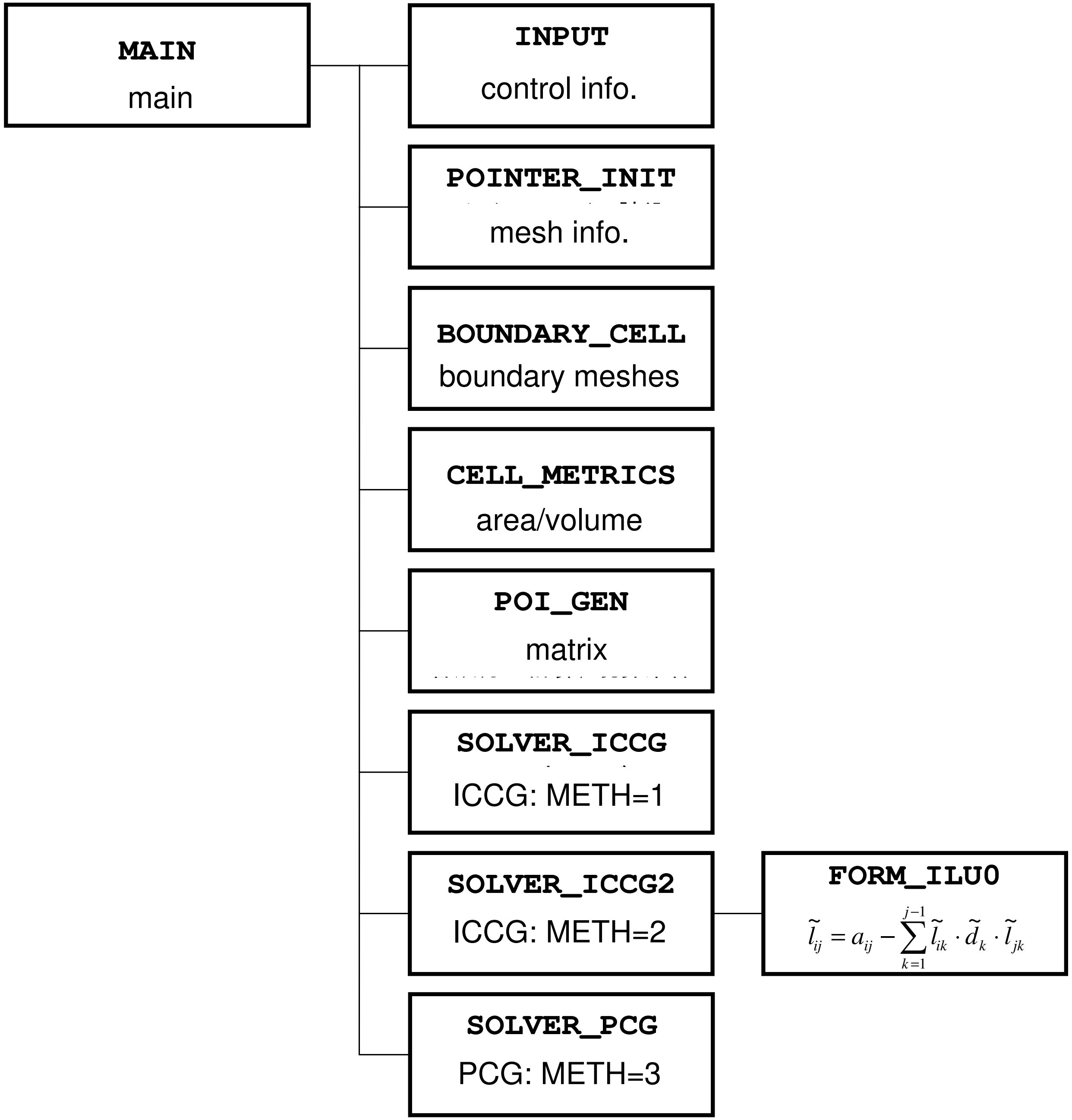
UCD Format (2/2)

- Originally for AVS, microAVS
- Extension of the UCD file is “inp”
- There are two types of formats. Only old type can be read by ParaView.

- Background
  - Finite Volume Method
  - Preconditioned Iterative Solvers
- **ICCG Solver for Poisson Equations**
  - How to run
    - Data Structure
  - **Program**
    - **Initialization**
    - **Coefficient Matrices**
    - ICCG

Structure of the Program

```
program MAIN

use STRUCT
use PCG
use solver_ICCG
use solver_ICCG2
use solver_PCG

implicit REAL*8 (A-H,O-Z)

call INPUT
call POINTER_INIT
call BOUNDARY_CELL
call CELL_METRICS
call POI_GEN

PHI=  0.d0

if (METHOD.eq.1) call solve_ICCG  (…)
if (METHOD.eq.2) call solve_ICCG2(…)
if (METHOD.eq.3) call solve_PCG   (…)

call OUTUCD

stop
end
```



module STRUCT

```
      module STRUCT

      include 'precision.inc'

!C
!C-- METRICs & FLUX
      integer (kind=kint) :: ICELTOT, ICELTOTp, N
      integer (kind=kint) :: NX, NY, NZ, NXP1, NYP1, NZP1, IBNODTOT
      integer (kind=kint) :: NXc, NYc, NZc

      real (kind=kreal) ::                                          &
     &       DX, DY, DZ, XAREA, YAREA, ZAREA, RDX, RDY, RDZ,        &
     &       RDX2, RDY2, RDZ2, R2DX, R2DY, R2DZ

      real (kind=kreal), dimension(:), allocatable ::               &
     &      VOLCEL, VOLNOD, RVC, RVN

      integer (kind=kint), dimension(:,:), allocatable ::           &
     &          XYZ, NEIBcell

!C
!C-- BOUNDARYs
      integer (kind=kint) :: ZmaxCELtot
      integer (kind=kint), dimension(:), allocatable :: BC_INDEX, BC_NOD
      integer (kind=kint), dimension(:), allocatable :: ZmaxCEL

!C
!C-- WORK
      integer (kind=kint), dimension(:,:), allocatable :: IWKX
      real(kind=kreal),    dimension(:,:), allocatable :: FCV

      end module STRUCT
```

ICELTOT:

Number of meshes (NX x NY x NZ)

N:

Number of nodes

NX,NY,NZ:

Number of meshes in x/y/z directions

NXP1,NYP1,NZP1:

Number of nodes in x/y/z directions

IBNODTOT:

= NXP1 x NYP1

XYZ(ICELTOT,3):

Location of meshes

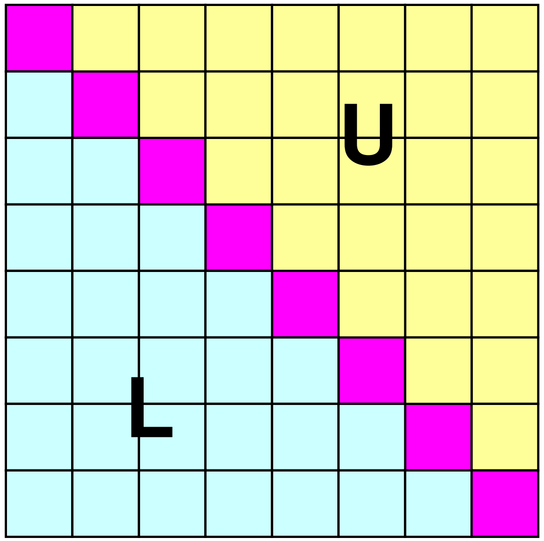
NEIBcell(ICELTOT,6):

Neighboring meshes

module PCG (1/5)

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL, METHOD
integer :: NPL, NPU

real(kind=8) :: EPSICCG

real(kind=8), dimension(:), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

integer, dimension(:), allocatable :: indexL, itemL
integer, dimension(:), allocatable :: indexU, itemU

end module PCG
```

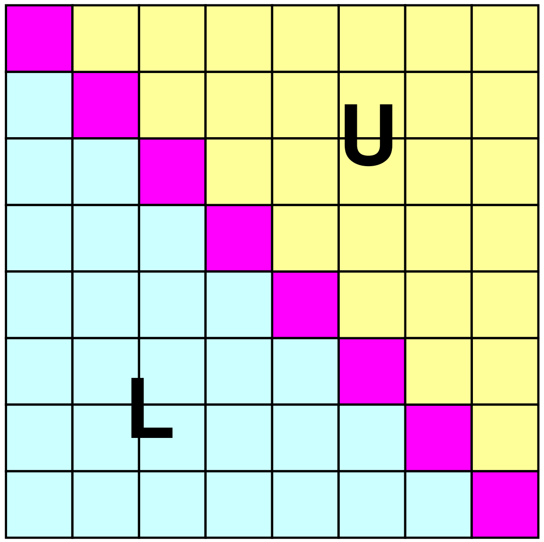
- Sparse Matrix
- Only non-zero off-diagonal components (CRS)
- Diagonal/Lower/Upper components are stored separately
- Although the matrix is symmetric, all the components are stored for efficient computing.



module PCG (2/5)

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL, METHOD
integer :: NPL, NPU

real(kind=8) :: EPSICCG

real(kind=8), dimension(:), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

integer, dimension(:), allocatable :: indexL, itemL
integer, dimension(:), allocatable :: indexU, itemU

end module PCG
```

`INL(ICELTOT)`	# Non-zero off-diag. components (lower)
`IAL(NL,ICELTOT)`	Col. ID: non-zero off-diag. comp. (lower)
`INU(ICELTOT)`	# Non-zero off-diag. components (upper)
`IAU(NU,ICELTOT)`	Col. ID: non-zero off-diag. comp. (upper)
`NU,NL`	Max # of L/U non-zero off-diag. comp. (=6)
`indexL(0:ICELTOT)`	**# Non-zero off-diag. comp. (lower, CRS)**
`indexU(0:ICELTOT)`	**# Non-zero off-diag. comp. (upper, CRS)**
`NPL, NPU`	**Total # of L/U non-zero off-diag. comp.**
`itemL(NPL),itemU(NPU)`	**Col. ID: non-zero off-diag. comp. (L/U, CRS)**



module PCG (3/5)

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL, METHOD
integer :: NPL, NPU

real(kind=8) :: EPSICCG

real(kind=8), dimension(:), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

integer, dimension(:), allocatable :: indexL, itemL
integer, dimension(:), allocatable :: indexU, itemU

end module PCG
```

`METHOD`	Preconditioning method (=1, =2, =3)
`EPSICCG`	Convergence criteria for ICCG
`D      (ICELTOT)`	Diagonal components of the matrix
`PHI    (ICLETOT)`	Unknown vector
`BFORCE(ICELTOT)`	RHS vector
`AL(NPL), AU(NPU)`	Non-zero off-diagonal L/U components of the matrix (CRS)

module PCG (4/5)

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL, METHOD
integer :: NPL, NPU

real(kind=8) :: EPSICCG

real(kind=8), dimension(:), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

integer, dimension(:), allocatable :: indexL, itemL
integer, dimension(:), allocatable :: indexU, itemU

end module PCG
```

Auxiliary Arrays

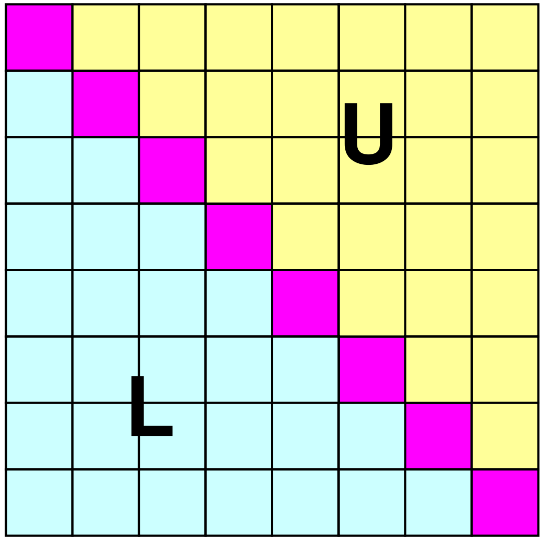
Lower Part (Column ID)

`IAL(icou,i) < i`

Upper Part (Column ID)

`IAU(icou,i) > i`

`INL(ICELTOT)`	# Non-zero off-diag. components (lower)
`IAL(NL,ICELTOT)`	**Col. ID: non-zero off-diag. comp. (lower)**
`INU(ICELTOT)`	# Non-zero off-diag. components (upper)
`IAU(NU,ICELTOT)`	**Col. ID: non-zero off-diag. comp. (upper)**
`NU,NL`	Max # of L/U non-zero off-diag. comp.s (=6)
`indexL(0:ICELTOT)`	# Non-zero off-diag. comp. (lower, CRS)
`indexU(0:ICELTOT)`	# Non-zero off-diag. comp. (upper, CRS)
`NPL, NPU`	Total # of L/U non-zero off-diag. comp.
`itemL(NPL),itemU(NPU)`	Col. ID: non-zero off-diag. comp. (L/U, CRS)



module PCG (5/5)

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL, METHOD
integer :: NPL, NPU

real(kind=8) :: EPSICCG

real(kind=8), dimension(:), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

integer, dimension(:), allocatable :: indexL, itemL
integer, dimension(:), allocatable :: indexU, itemU

end module PCG
```

Auxiliary Arrays

Lower Part (Column ID)

`IAL(icou,i) < i`

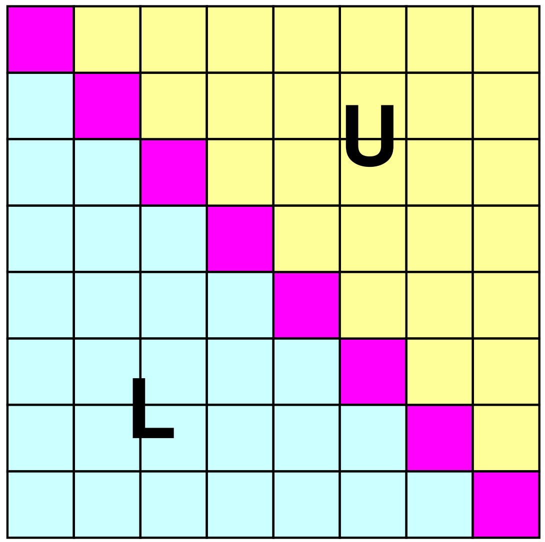
`INL(i)` : Number@each row

Upper Part (Column ID)

`IAU(icou,i) > i`

`INU(i)` : Number@each row

INL(ICELTOT)	**# Non-zero off-diag. components (lower)**
IAL(NL,ICELTOT)	Col. ID: non-zero off-diag. comp. (lower)
INU(ICELTOT)	**# Non-zero off-diag. components (upper)**
IAU(NU,ICELTOT)	Col. ID: non-zero off-diag. comp. (upper)
NU,NL	Max # of L/U non-zero off-diag. comp.s (=6)
indexL(0:ICELTOT)	# Non-zero off-diag. comp. (lower, CRS)
indexU(0:ICELTOT)	# Non-zero off-diag. comp. (upper, CRS)
NPL, NPU	Total # of L/U non-zero off-diag. comp.
itemL(NPL),itemU(NPU)	Col. ID: non-zero off-diag. comp. (L/U, CRS)



Variables/Arrays for Matrix

Name	Type	Content
D(N)	**R**	Diagonal components of the matrix (N= ICELTOT)
BFORCE(N)	**R**	RHS vector
PHI(N)	**R**	Unknown vector
indexL(0:N)	**I**	Number of Lower non-zero off-diag. comp. (CRS)
indexU(0:N)	**I**	Number of Upper non-zero off-diag. comp. (CRS)
NPL	**I**	Total number of Lower non-zero off-diag. comp. (CRS)
NPU	**I**	Total number of Upper non-zero off-diag. comp. (CRS)
itemL(NPL)	**I**	Column ID of Lower non-zero off-diag. comp. (CRS)
itemU(NPU)	**I**	Column ID of Upper non-zero off-diag. comp. (CRS)
AL(NPL)	**R**	Lower non-zero off-diag. comp. (CRS)
AU(NPU)	**R**	Upper non-zero off-diag. comp. (CRS)

Variables/Arrays for Matrix Auxiliary Arrays

Name	Type	Content
NL,NU	**I**	MAX. number of Lower/Upper non-zero off-diag. comp. for each mesh (=6 in this case)
INL(N)	**I**	Number of Lower non-zero off-diag. comp.
INU(N)	**I**	Number of Upper non-zero off-diag. comp.
IAL(NL,N)	**I**	Column ID of Lower non-zero off-diag. comp.
IAU(NU,N)	**I**	Column ID of Uppwer non-zero off-diag. comp.

- INL, INU ⇒ indexL, indexU
- IAL, IAU ⇒ itemL, itemU

Why Auxiliary Arrays ?

① NPL and NPU are unknown before computation.

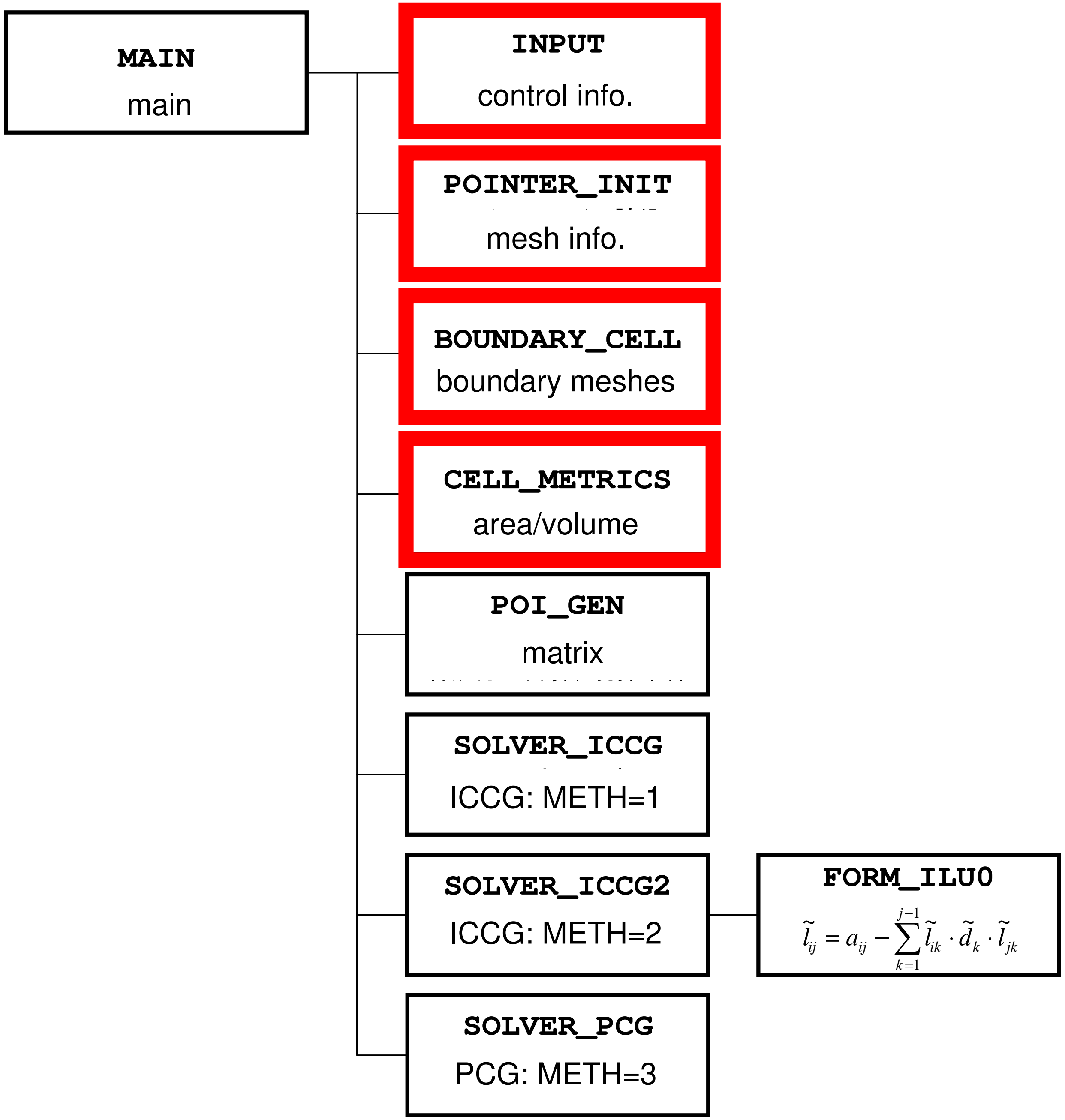
② CRS is not suitable for reordering.

Mat-Vec Multiplication: {q}=[A]{p}

```
do i= 1, N

  VAL= D(i)*p(i)

  do k= indexL(i-1)+1, indexL(i)
    VAL= VAL + AL(k)*p(itemL(k))
  enddo

  do k= indexU(i-1)+1, indexU(i)
    VAL= VAL + AU(k)*p(itemU(k))
  enddo

  q(i)= VAL

enddo
```

Structure of the Program

```
program MAIN

use STRUCT
use PCG
use solver_ICCG
use solver_ICCG2
use solver_PCG

 implicit REAL*8 (A-H,O-Z)

call INPUT
call POINTER_INIT
call BOUNDARY_CELL
call CELL_METRICS
call POI_GEN

PHI= 0.d0

 if (METHOD.eq.1) call solve_ICCG (…)
 if (METHOD.eq.2) call solve_ICCG2(…)
 if (METHOD.eq.3) call solve_PCG  (…)

call OUTUCD

stop
end
```



input: reading “INPUT.DAT”

```
!C
!C***
!C*** INPUT
!C***
!C
!C    INPUT CONTROL DATA
!C
      subroutine INPUT
      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

      character*80 CNTFIL

!C
!C-- CNTL. file
      open  (11, file='INPUT.DAT', status='unknown')
        read (11,*) NX, NY, NZ
        read (11,*) METHOD
        read (11,*) DX, DY, DZ
        read (11,*) EPSICCG
      close (11)
!C===

      return
      end
```

```
32 32 32                                     NX/NY/NZ
1                                            MEHOD 1-3
1.00e-00 1.00e-00 1.00e-00                   DX/DY/DZ
1.0e-08                                      EPSICCG
```

pointer_init (1/3): "mesh.dat"

```
!C
!C***
!C*** POINTER_INIT
!C***
!C
      subroutine POINTER_INIT

      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)

!C
!C +-----------------------+
!C | Generating MESH info. |
!C +-----------------------+
!C===
      ICELTOT= NX  * NY  * NZ

      NXP1= NX + 1
      NYP1= NY + 1
      NZP1= NZ + 1

      allocate (NEIBcell(ICELTOT,6), XYZ(ICELTOT,3))
      NEIBcell= 0
```

NX,NY,NZ:
Number of meshes in x/y/z directions

NXP1,NYP1,NZP1:
Number of nodes in x/y/z directions (for visualization)

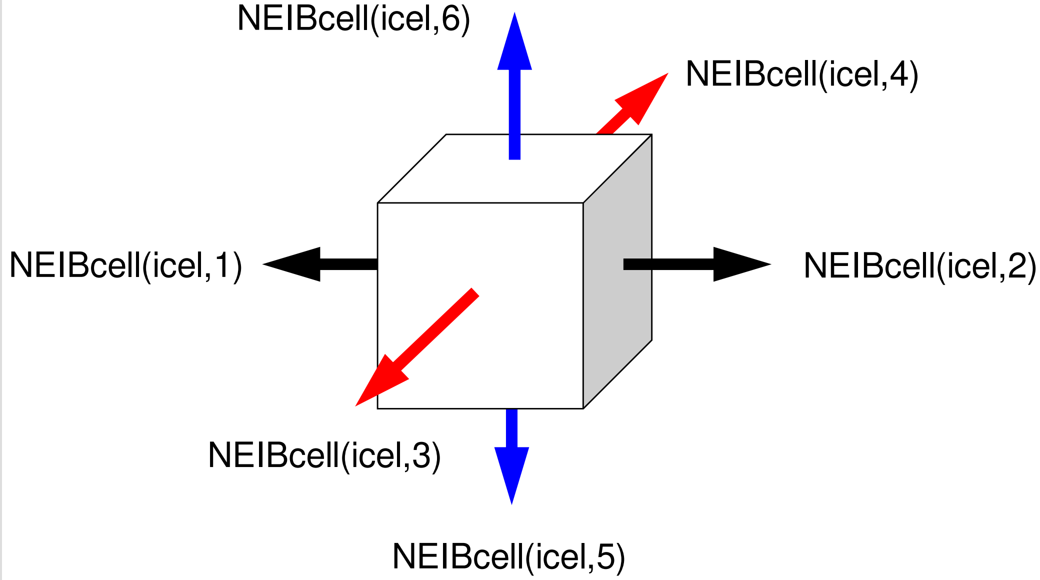
ICELTOT:
Number of meshes (NX x NY x NZ)

XYZ(ICELTOT,3):
Location of meshes

NEIBcell(ICELTOT,6):
Neighboring meshesc

pointer_init (2/3): “mesh.dat”

```
      do k= 1, NZ
        do j= 1, NY
          do i= 1, NX
            icel= (k-1)*NX*NY + (j-1)*NX + i
            NEIBcell(icel,1)= icel - 1
            NEIBcell(icel,2)= icel + 1
            NEIBcell(icel,3)= icel - NX
            NEIBcell(icel,4)= icel + NX
            NEIBcell(icel,5)= icel - NX*NY
            NEIBcell(icel,6)= icel + NX*NY
            if (i.eq. 1) NEIBcell(icel,1)= 0
            if (i.eq.NX) NEIBcell(icel,2)= 0
            if (j.eq. 1) NEIBcell(icel,3)= 0
            if (j.eq.NY) NEIBcell(icel,4)= 0
            if (k.eq. 1) NEIBcell(icel,5)= 0
            if (k.eq.NZ) NEIBcell(icel,6)= 0

            XYZ(icel,1)= i
            XYZ(icel,2)= j
            XYZ(icel,3)= k

          enddo
        enddo
      enddo
!C===
```



i= XYZ(icel,1)
j= XYZ(icel,2), k= XYZ(icel,3)
icel= (k-1)*NX*NY + (j-1)*NX + i

NEIBcell(icel,1)= icel – 1
NEIBcell(icel,2)= icel + 1
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,6)= icel + NX*NY

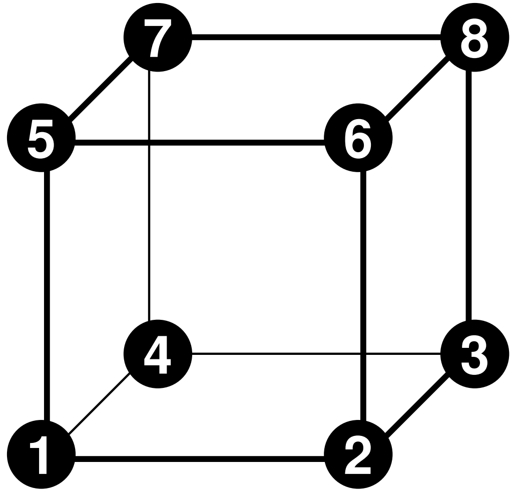
pointer_init (3/3): “mesh.dat”

```
!C
!C +-------------+
!C | Parameters |
!C +-------------+
!C===
      if (DX.le.0.0e0) then
        DX= 1.d0 / dfloat(NX)
        DY= 1.d0 / dfloat(NY)
        DZ= 1.d0 / dfloat(NZ)
      endif

      NXP1= NX + 1
      NYP1= NY + 1
      NZP1= NZ + 1

      IBNODTOT= NXP1 * NYP1
      N       = NXP1 * NYP1 * NZP1
!C===
      return
      end
```

if DX is no larger than 0.0

pointer_init (3/3): “mesh.dat”

```
!C
!C +-------------+
!C | Parameters |
!C +-------------+
!C===
      if (DX.le.0.0e0) then
        DX= 1.d0 / dfloat(NX)
        DY= 1.d0 / dfloat(NY)
        DZ= 1.d0 / dfloat(NZ)
      endif

      NXP1= NX + 1
      NYP1= NY + 1
      NZP1= NZ + 1

      IBNODTOT= NXP1 * NYP1
      N       = NXP1 * NYP1 * NZP1
!C===
      return
      end
```



NXP1,NYP1,NZP1:
Number of nodes in x/y/z directions

IBNODTOT:
= NXP1 x NYP1

N:
Number of modes meshes (for visualization)

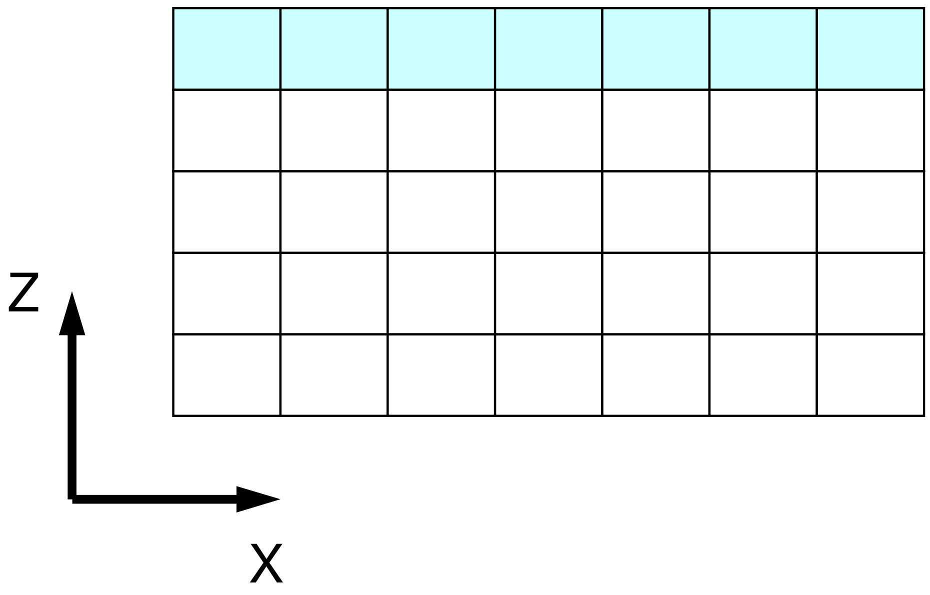
boundary_cell

```
!C
!C***
!C*** BOUNDARY_CELL
!C***
!C
      subroutine BOUNDARY_CELL
      use STRUCT

      implicit REAL*8 (A-H,O-Z)

!C
!C +-------+
!C | Zmax |
!C +-------+
!C===
      IFACTOT= NX * NY
      ZmaxCELtot= IFACTOT

      allocate (ZmaxCEL(ZmaxCELtot))

      icou= 0
      k   = NZ
      do j= 1, NY
      do i= 1, NX
        icel= (k-1)*IFACTOT + (j-1)*NX + i
        icou= icou + 1
        ZmaxCEL(icou)= icel
      enddo
      enddo
!C===
      return
      end
```

Meshes @ $Z = Z_{max}$

Number: ZmaxCELtot

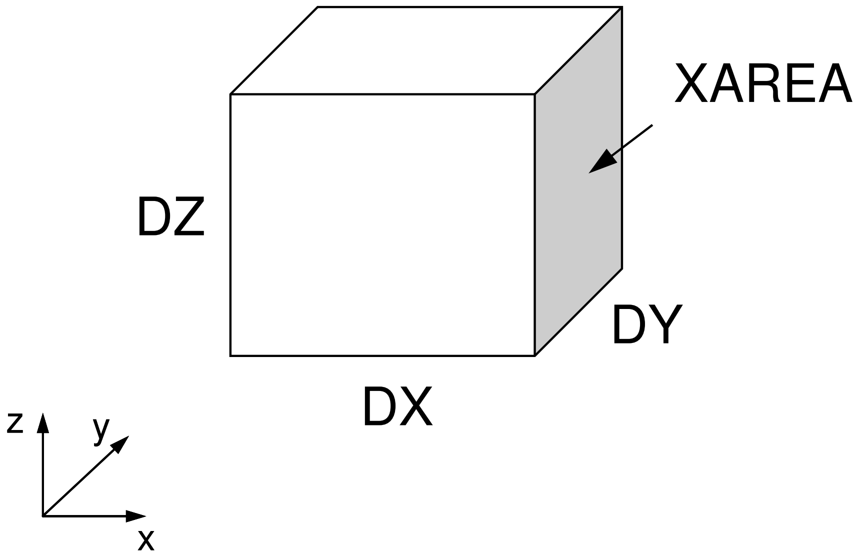
Mesh ID: ZmaxCEL(:)



cell_metrics

```
!C
!C***
!C*** CELL_METRICS
!C***
!C
      subroutine CELL_METRICS
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)
!C
!C-- ALLOCATE
      allocate (VOLCEL(ICELTOT))
      allocate (   RVC(ICELTOT))
!C
!C-- VOLUME, AREA, PROJECTION etc.
      XAREA= DY * DZ
      YAREA= DX * DZ
      ZAREA= DX * DY

      RDX= 1.d0 / DX
      RDY= 1.d0 / DY
      RDZ= 1.d0 / DZ

      RDX2= 1.d0 / (DX**2)
      RDY2= 1.d0 / (DY**2)
      RDZ2= 1.d0 / (DZ**2)
      R2DX= 1.d0 / (0.50d0*DX)
      R2DY= 1.d0 / (0.50d0*DY)
      R2DZ= 1.d0 / (0.50d0*DZ)

       V0= DX * DY * DZ
      RV0= 1.d0/V0
      VOLCEL=  V0
      RVC   = RV0

      return
      end
```

Parameters for Computations



$$XAREA = \Delta Y \times \Delta Z, \quad YAREA = \Delta Z \times \Delta X,$$

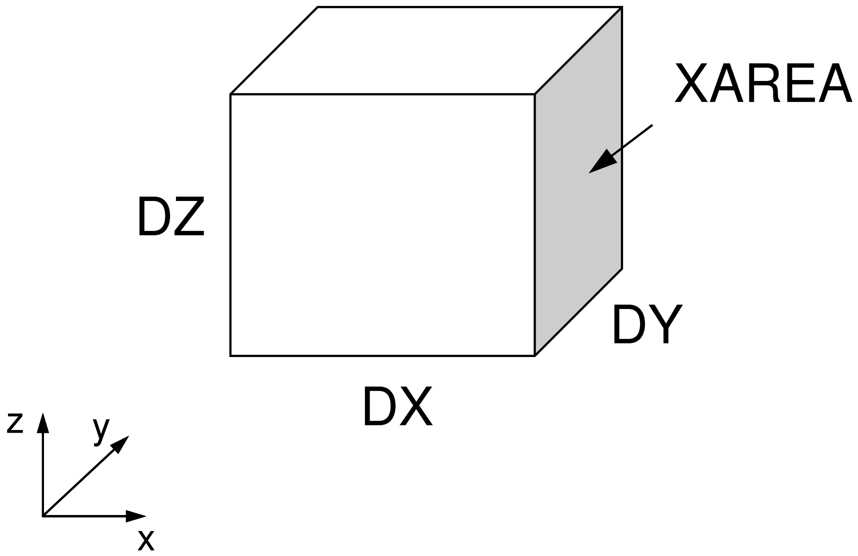
$$ZAREA = \Delta X \times \Delta Y$$

$$RDX = \frac{1}{\Delta X}, \quad RDY = \frac{1}{\Delta Y}, \quad RDZ = \frac{1}{\Delta Z}$$

cell_metrics

```
!C
!C***
!C*** CELL_METRICS
!C***
!C
      subroutine CELL_METRICS
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)
!C
!C-- ALLOCATE
      allocate (VOLCEL(ICELTOT))
      allocate (   RVC(ICELTOT))
!C
!C-- VOLUME, AREA, PROJECTION etc.
      XAREA= DY * DZ
      YAREA= DX * DZ
      ZAREA= DX * DY

      RDX= 1.d0 / DX
      RDY= 1.d0 / DY
      RDZ= 1.d0 / DZ

      RDX2= 1.d0 / (DX**2)
      RDY2= 1.d0 / (DY**2)
      RDZ2= 1.d0 / (DZ**2)
      R2DX= 1.d0 / (0.50d0*DX)
      R2DY= 1.d0 / (0.50d0*DY)
      R2DZ= 1.d0 / (0.50d0*DZ)

       V0= DX * DY * DZ
      RV0= 1.d0/V0
      VOLCEL=  V0
      RVC   = RV0

      return
      end
```

Parameters for Computations



$$RDX2=\frac{1}{\Delta X^2},\quad RDY2=\frac{1}{\Delta Y^2},\quad RDZ2=\frac{1}{\Delta Z^2}$$

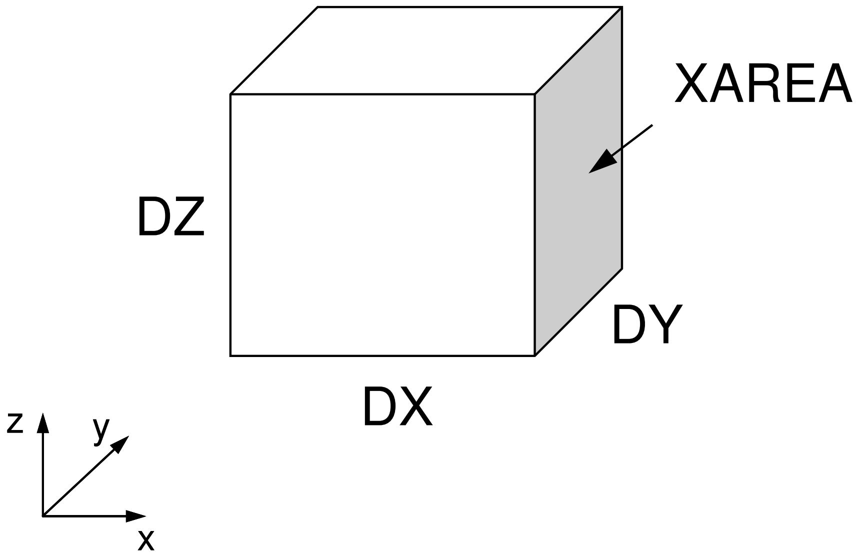
$$R2DX=\frac{1}{0.5\times\Delta X},\quad R2DY=\frac{1}{0.5\times\Delta Y},$$

$$R2DZ=\frac{1}{0.5\times\Delta Z}$$

cell_metrics

```
!C
!C***
!C*** CELL_METRICS
!C***
!C
      subroutine CELL_METRICS
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)
!C
!C-- ALLOCATE
      allocate (VOLCEL(ICELTOT))
      allocate (   RVC(ICELTOT))
!C
!C-- VOLUME, AREA, PROJECTION etc.
      XAREA= DY * DZ
      YAREA= DX * DZ
      ZAREA= DX * DY

      RDX= 1.d0 / DX
      RDY= 1.d0 / DY
      RDZ= 1.d0 / DZ

      RDX2= 1.d0 / (DX**2)
      RDY2= 1.d0 / (DY**2)
      RDZ2= 1.d0 / (DZ**2)
      R2DX= 1.d0 / (0.50d0*DX)
      R2DY= 1.d0 / (0.50d0*DY)
      R2DZ= 1.d0 / (0.50d0*DZ)

       V0= DX * DY * DZ
      RV0= 1.d0/V0
      VOLCEL=  V0
      RVC   = RV0

      return
      end
```

Parameters for Computations

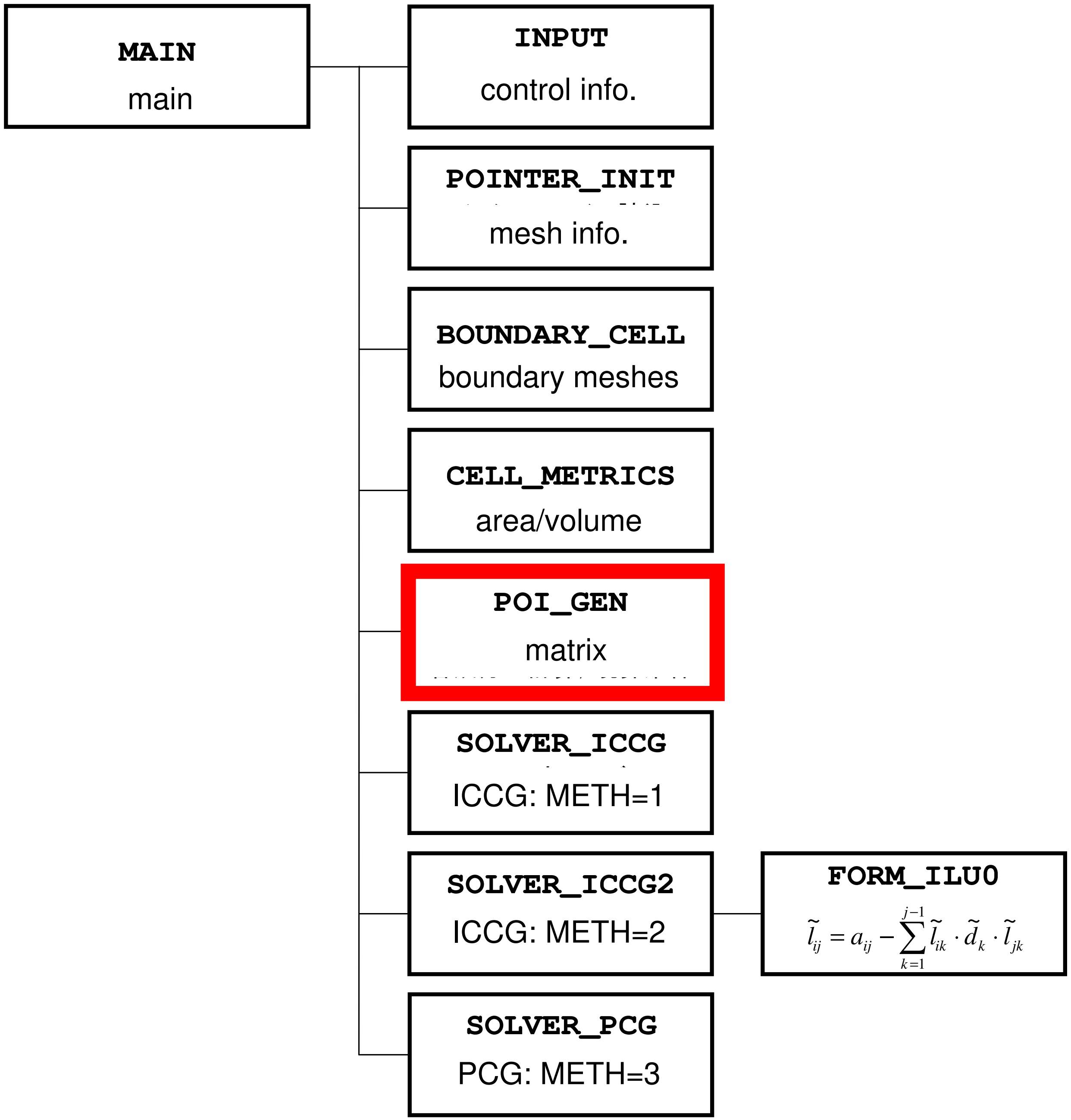


$$VOLCEL = V0 = \Delta X \times \Delta Y \times \Delta Z$$

$$RV0 = RVC = \frac{1}{VOLCEL}$$

Structure of the Program

```
program MAIN

use STRUCT
use PCG
use solver_ICCG
use solver_ICCG2
use solver_PCG

 implicit REAL*8 (A-H,O-Z)

call INPUT
call POINTER_INIT
call BOUNDARY_CELL
call CELL_METRICS
call POI_GEN

PHI= 0.d0

 if (METHOD.eq.1) call solve_ICCG (…)
 if (METHOD.eq.2) call solve_ICCG2(…)
 if (METHOD.eq.3) call solve_PCG  (…)

call OUTUCD

stop
end
```



poi_gen (1/7)

```
      subroutine POI_GEN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

!C
!C-- INIT.
      nn = ICELTOT

      NU= 6
      NL= 6

      allocate (BFORCE(nn), D(nn), PHI(nn))
      allocate (INL(nn), INU(nn), IAL(NL,nn), IAU(NU,nn))

      PHI= 0.d0
        D= 0.d0

      INL= 0
      INU= 0
      IAL= 0
      IAU= 0
```

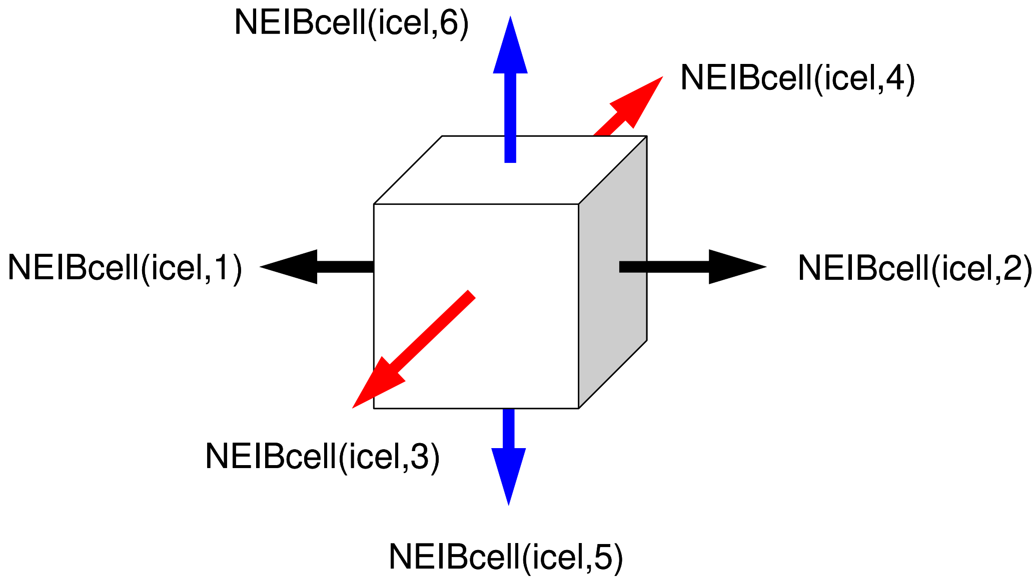
Variables/Arrays for Matrix

Name	Type	Content
D(N)	**R**	Diagonal components of the matrix `(N= ICELTOT)`
BFORCE(N)	**R**	RHS vector
PHI(N)	**R**	Unknown vector
indexL(0:N), indexU(0:N)	**I**	# of L/U non-zero off-diag. comp. (CRS)
NPL, NPU	**I**	Total # of L/U non-zero off-diag. comp. (CRS)
itemL(NPL), itemU(NPU)	**I**	Column ID of L/U non-zero off-diag. comp. (CRS)
AL(NPL), AU(NPU)	**R**	L/U non-zero off-diag. comp. (CRS)

Name	Type	Content
NL,NU	**I**	MAX. # of L/U non-zero off-diag. comp. for each mesh (=6)
INL(N), INU(N)	**I**	# of L/U non-zero off-diag. comp.
IAL(NL,N), IAU(NU,N)	**I**	Column ID of L/U non-zero off-diag. comp.

poi_gen (2/7)

```
!C
!C +--------------+
!C | CONNECTIVITY |
!C +--------------+
!C===
      do icel= 1, ICELTOT
        icN1= NEIBcell(icel,1)
        icN2= NEIBcell(icel,2)
        icN3= NEIBcell(icel,3)
        icN4= NEIBcell(icel,4)
        icN5= NEIBcell(icel,5)
        icN6= NEIBcell(icel,6)

        icouG= 0
        if (icN5.ne.0) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN5
          INL(     icel)= icou
        endif

        if (icN3.ne.0) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN3
          INL(     icel)= icou
        endif

        if (icN1.ne.0) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN1
          INL(     icel)= icou
        endif
```

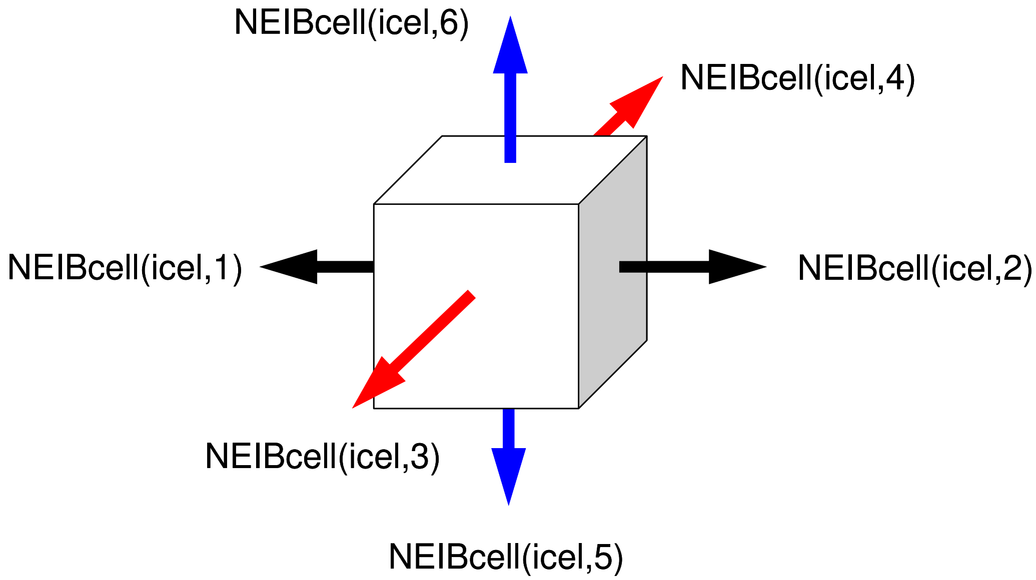


Lower Triangular Part

NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,1)= icel – 1

poi_gen (3/7)

```
         if (icN2.ne.0) then
           icou= INU(icel) + 1
           IAU(icou,icel)= icN2
           INU(     icel)= icou
         endif

         if (icN4.ne.0) then
           icou= INU(icel) + 1
           IAU(icou,icel)= icN4
           INU(     icel)= icou
         endif

         if (icN6.ne.0) then
           icou= INU(icel) + 1
           IAU(icou,icel)= icN6
           INU(     icel)= icou
         endif
       enddo
!C===
```



Upper Triangular Part

NEIBcell(icel,2)= icel + 1
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,6)= icel + NX*NY

poi_gen (4/7)

```
!C
!C-- 1D array

      allocate (indexL(0:nn), indexU(0:nn))
      indexL= 0
      indexU= 0

      do icel= 1, ICELTOT
        indexL(icel)= INL(icel)
        indexU(icel)= INU(icel)
      enddo

      do icel= 1, ICELTOT
        indexL(icel)= indexL(icel) + indexL(icel-1)
        indexU(icel)= indexU(icel) + indexU(icel-1)
      enddo

      NPL= indexL(ICELTOT)
      NPU= indexU(ICELTOT)

      allocate (itemL(NPL), AL(NPL))
      allocate (itemU(NPU), AU(NPU))

      itemL= 0
      itemU= 0

         AL= 0.d0
         AU= 0.d0
!C===
```

Name	Type	Content
D(N)	R	Diagonal components of the matrix (N= ICELTOT)
BFORCE(N)	R	RHS vector
PHI(N)	R	Unknown vector
indexL(0:N), indexU(0:N)	I	# of L/U non-zero off-diag. comp. (CRS)
NPL, NPU	I	Total # of L/U non-zero off-diag. comp. (CRS)
itemL(NPL), itemU(NPU)	I	Column ID of L/U non-zero off-diag. comp. (CRS)
AL(NPL), AU(NPU)	R	L/U non-zero off-diag. comp. (CRS)

```
do i= 1, N

  VAL= D(i)*p(i)

  do k= indexL(i-1)+1, indexL(i)
    VAL= VAL + AL(k)*p(itemL(k))
  enddo

  do k= indexU(i-1)+1, indexU(i)
    VAL= VAL + AU(k)*p(itemU(k))
  enddo

  q(i)= VAL

enddo
```

Poisson Equation by Finite Volume Method (FVM)

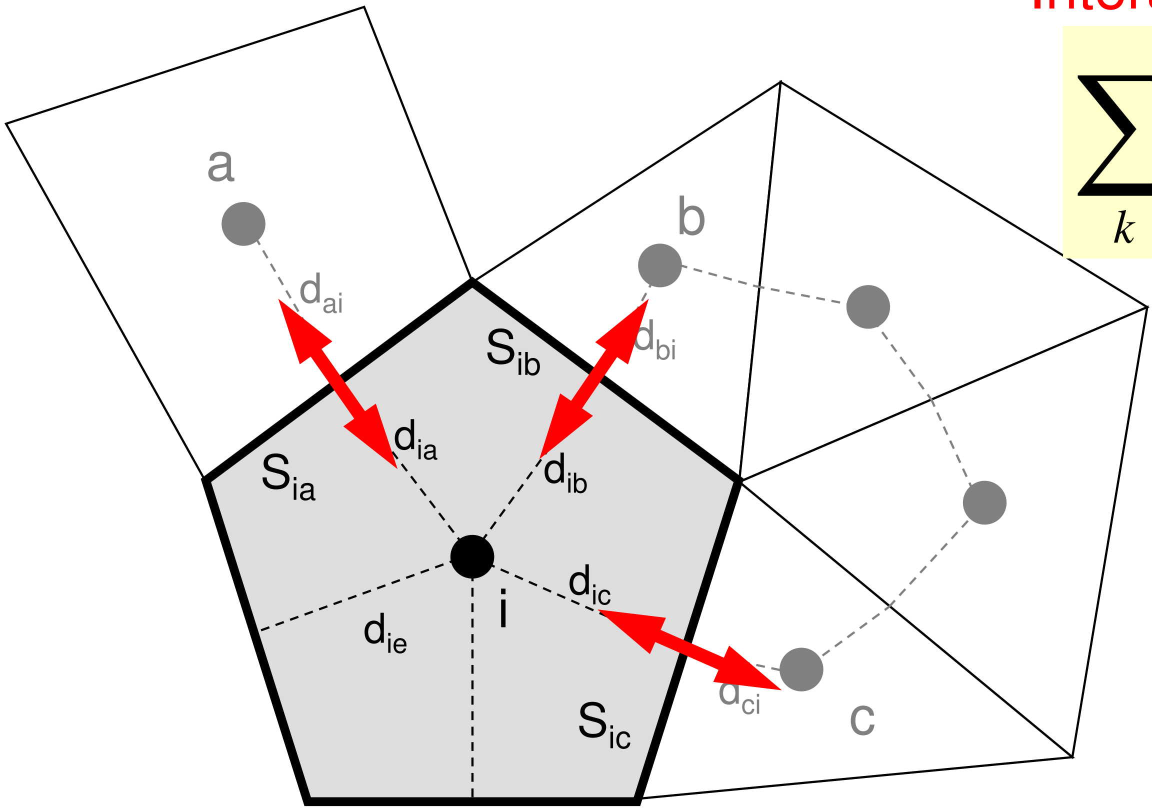
$$\frac{\partial^2 \phi}{\partial x^2}+\frac{\partial^2 \phi}{\partial y^2}+\frac{\partial^2 \phi}{\partial z^2}+f=0$$

Conservation of Fluxes through Surfaces

Diffusion:
Interaction with Neighbors

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

Volume Flux




```
Vi   : Volume
S    : Surface Area
dij  : Distance between
       Cell-Center &
       Surface
Q    : Volume Flux
```

Constructing Coefficient Matrix

Conservation for i-th mesh

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

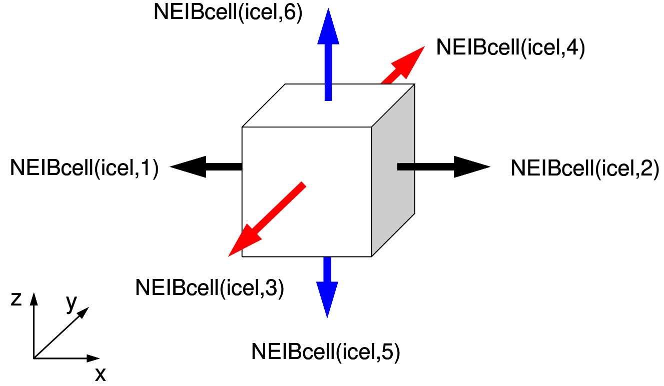
$$+\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k-\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_i=-V_i\dot{Q}_i$$

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

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

poi_gen (5/7)

```
!C
!C +-----------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-----------------------------------+
!C===
      icouG= 0
      do icel= 1, ICELTOT
        icN1= NEIBcell(icel,1)
        icN2= NEIBcell(icel,2)
        icN3= NEIBcell(icel,3)
        icN4= NEIBcell(icel,4)
        icN5= NEIBcell(icel,5)
        icN6= NEIBcell(icel,6)
        VOL0= VOLCEL(icel)
        icou= 0
        if (icN5.ne.0) then
          coef    =RDZ * ZAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                   k    = icou + indexL(icel-1)
          itemL(k)= icN5
             AL(k)= coef
        endif

        if (icN3.ne.0) then
          coef    =RDY * YAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                   k    = icou + indexL(icel-1)
          itemL(k)= icN3
             AL(k)= coef
        endif

        if (icN1.ne.0) then
          coef    =RDX * XAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                   k    = icou + indexL(icel-1)
          itemL(k)= icN1
             AL(k)= coef
         endif
```

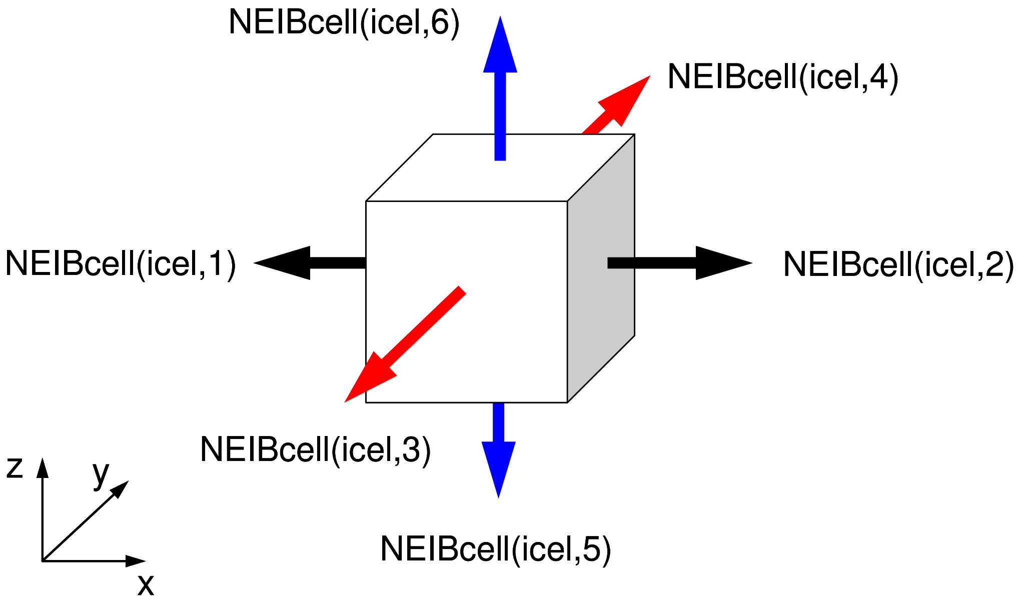


$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

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

Calculations of Coefficients



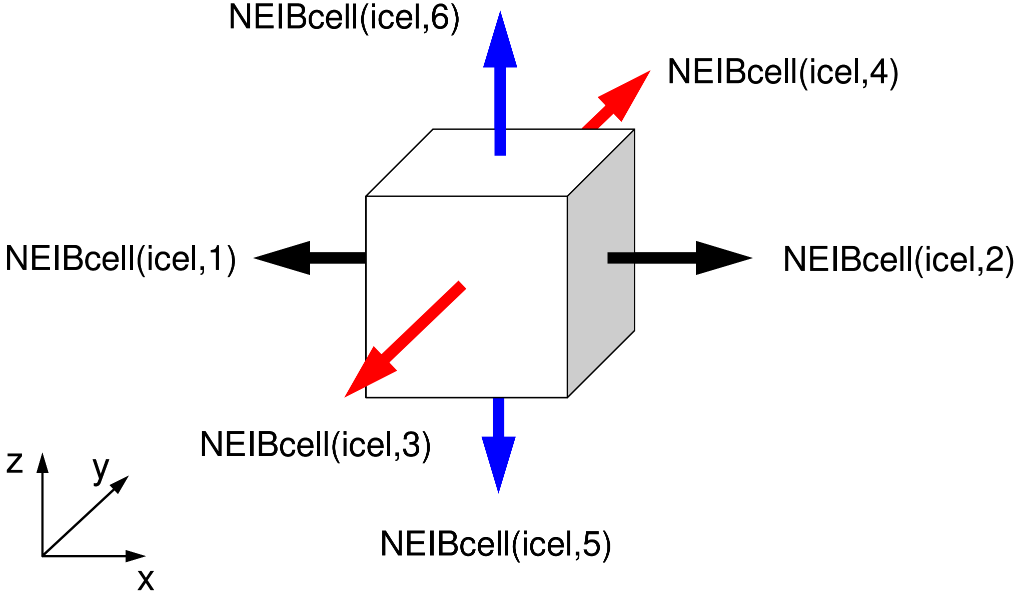

```
if (icN5.ne.0) then
  coef    = RDZ * ZAREA
  D(icel)= D(icel) - coef

  icou= icou + 1
     k= icou + indexL(icel-1)

  itemL(k)= icN5
     AL(k)= coef
endif
```

$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

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

Calculations of Coefficients




```
if (icN5.ne.0) then
  coef   = RDZ * ZAREA
  D(icel)= D(icel) - coef

  icou= icou + 1
     k= icou + indexL(icel-1)

  itemL(k)= icN5
     AL(k)= coef
endif
```

$$\frac{\Delta y \Delta z}{\Delta x}\left(\phi_{neib(icel,1)} - \phi_{icel}\right) + \frac{\Delta y \Delta z}{\Delta x}\left(\phi_{neib(icel,2)} - \phi_{icel}\right) +$$

$$\frac{\Delta z \Delta x}{\Delta y}\left(\phi_{neib(icel,3)} - \phi_{icel}\right) + \frac{\Delta z \Delta x}{\Delta y}\left(\phi_{neib(icel,4)} - \phi_{icel}\right) +$$

ZAREA

RDZ

$$\frac{\Delta x \Delta y}{\Delta z}\left(\phi_{neib(icel,5)} - \phi_{icel}\right) + \frac{\Delta x \Delta y}{\Delta z}\left(\phi_{neib(icel,6)} - \phi_{icel}\right) + f_{icel}\Delta x \Delta y \Delta z = 0$$

poi_gen (6/7)

```
        icou= 0
        if (icN2.ne.0) then
          coef    = RDX * XAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                    k   = icou + indexU(icel-1)
          itemU(k)= icN2
             AU(k)= coef
        endif

        if (icN4.ne.0) then
          coef    = RDY * YAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                   k   = icou + indexU(icel-1)
          itemU(k)= icN4
             AU(k)= coef
        endif

        if (icN6.ne.0) then
          coef    = RDZ * ZAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                   k   = icou + indexU(icel-1)
          itemU(k)= icN6
             AU(k)= coef
        endif

        ii= XYZ(icel,1)
        jj= XYZ(icel,2)
        kk= XYZ(icel,3)

        BFORCE(icel)= -dfloat(ii+jj+kk) * VOL0
      enddo
!C===
```

poi_gen (6/7)

```
      icou= 0
      if (icN2.ne.0) then
        coef    = RDX * XAREA
        D(icel)= D(icel) - coef
                 icou= icou + 1
                  k   = icou + indexU(icel-1)
        itemU(k)= icN2
           AU(k)= coef
      endif

      if (icN4.ne.0) then
        coef    = RDY * YAREA
        D(icel)= D(icel) - coef
                 icou= icou + 1
                 k   = icou + indexU(icel-1)
        itemU(k)= icN4
           AU(k)= coef
      endif

      if (icN6.ne.0) then
        coef    = RDZ * ZAREA
        D(icel)= D(icel) - coef
                 icou= icou + 1
                 k   = icou + indexU(icel-1)
        itemU(k)= icN6
           AU(k)= coef
      endif

      ii= XYZ(icel,1)
      jj= XYZ(icel,2)
      kk= XYZ(icel,3)

      BFORCE(icel)= -dfloat(ii+jj+kk) * VOL0
    enddo
!C===
```

Volume Flux

$$f = dfloat(i_0 + j_0 + k_0)$$

$$i_0 = XYZ(icel,1),$$

$$j_0 = XYZ(icel,2),$$

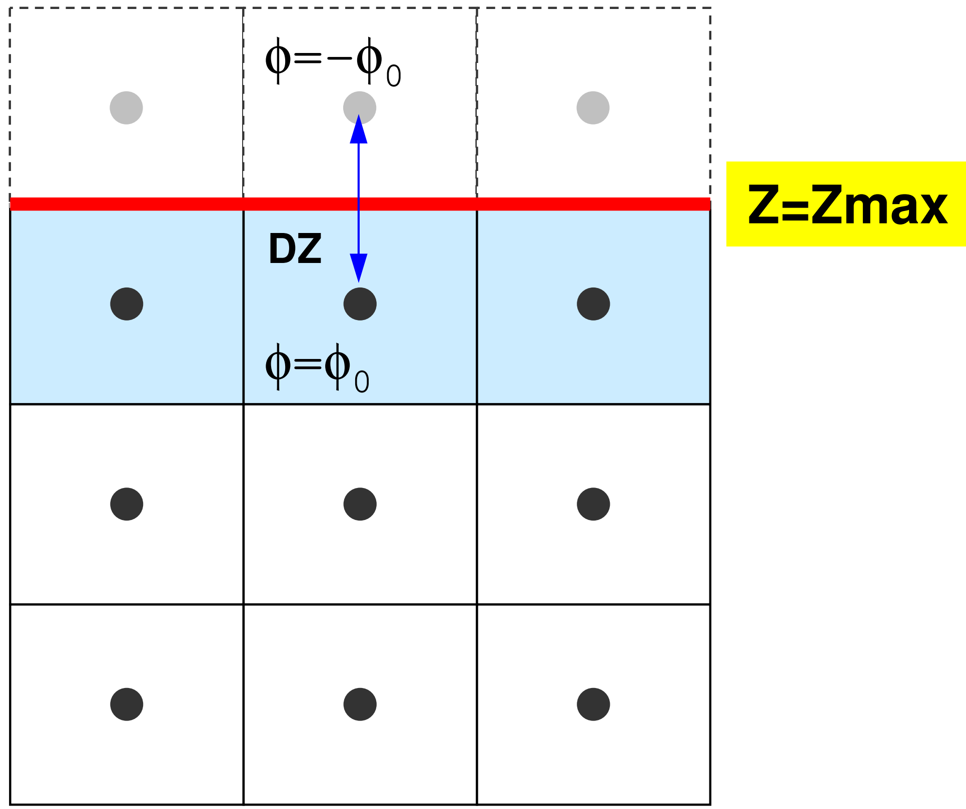
$$k_0 = XYZ(icel,3)$$

XYZ(icel, k)（k=1,2,3）
Index for location of finite-difference mesh in X-/Y-/Z-axis.

poi_gen (7/7)

```
!C
!C +--------------------------+
!C | DIRICHLET BOUNDARY CELLs |
!C +--------------------------+
!C   TOP SURFACE
!C===
      do ib= 1, ZmaxCELtot
        icel= ZmaxCEL(ib)
        coef= 2.d0 * RDZ * ZAREA
        D(icel)= D(icel) - coef
      enddo
!C===
      return
      end
```

Calculation of Coefficients on Boundary Surface @ $Z=Z_{max}$



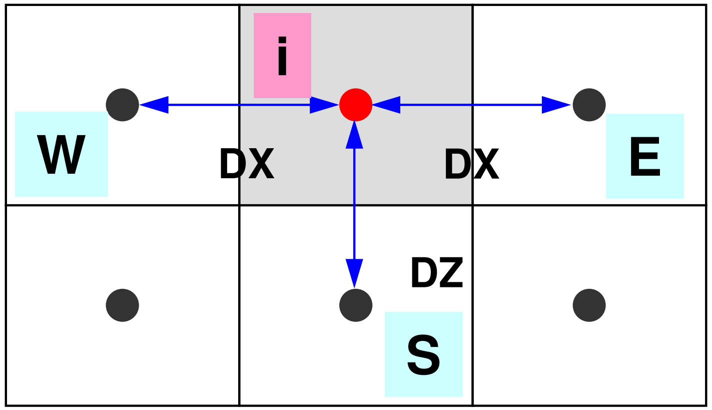
1st Order Approximation:

Mirror Image according to $Z=Z_{max}$ surface.

$\phi=-\phi_0$ at the center of the (virtual) mesh

$\phi=0$ @ $Z=Z_{max}$ surface

Dirichlet B.C.



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

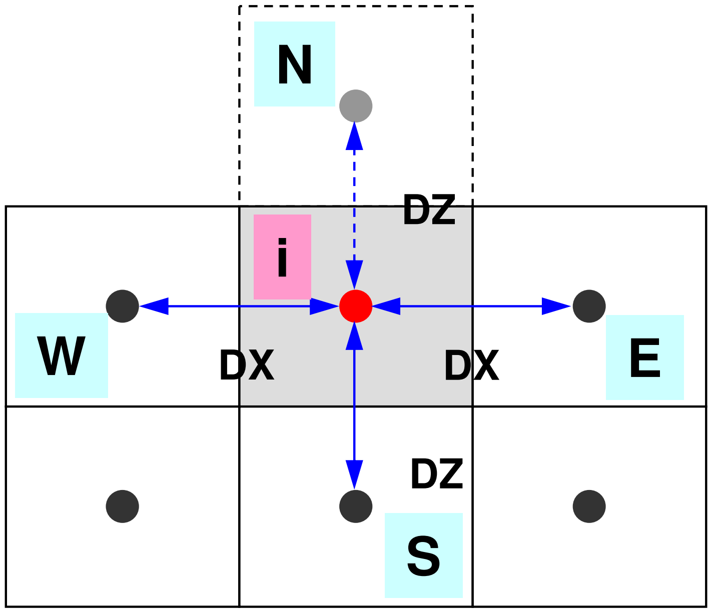
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal)

AL, AU (off-diag.)

BFORCE (RHS)

Dirichlet B.C.



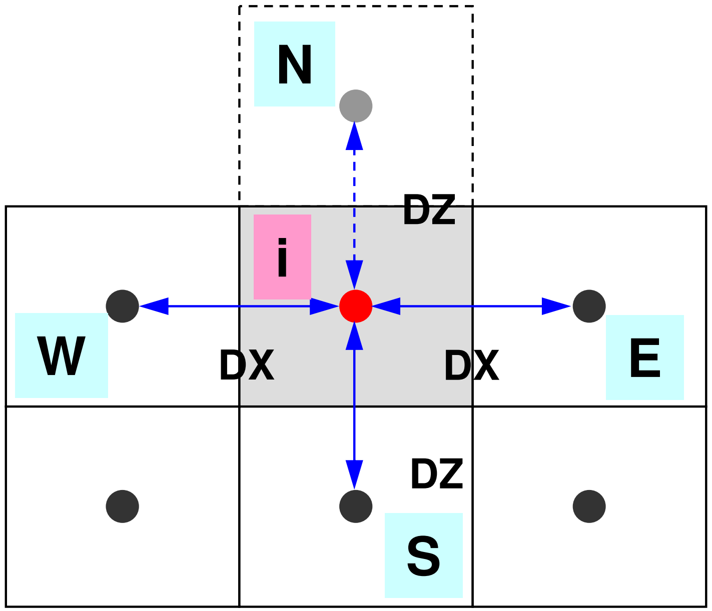
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

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

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.



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

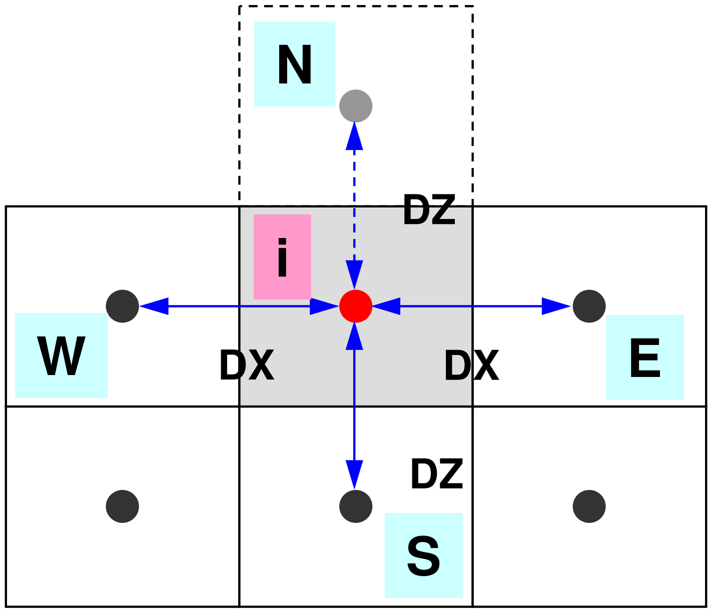
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i + \left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right] = -V_i \dot{Q}_i$$

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

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

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

Dirichlet B.C.



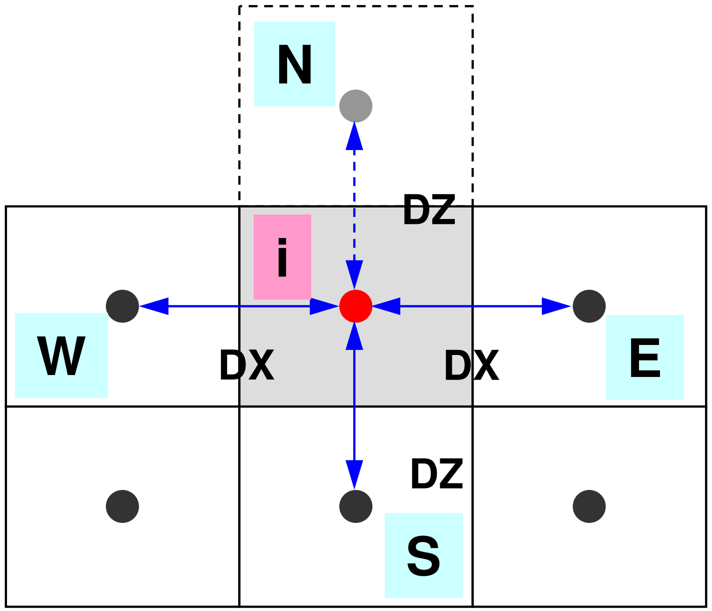
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

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

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.



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

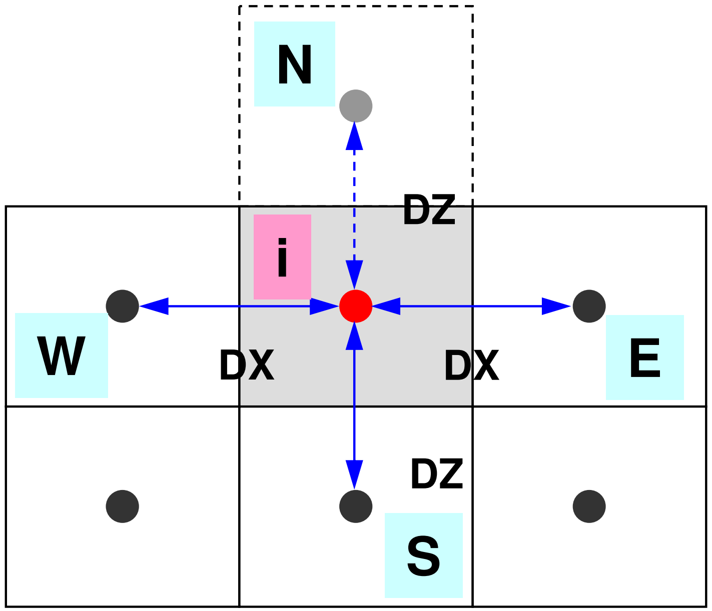
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

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

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

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

Dirichlet B.C.



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

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

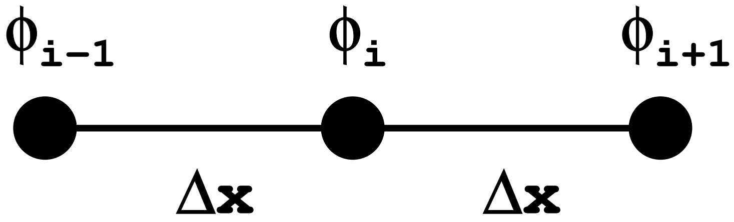
D (diagonal) **AL, AU (off-diag.)** **BFORCE (RHS)**

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

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

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

Taylor Series Expansion



$$\phi_{i+1} = \phi_i + \Delta x \left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(\Delta x)^2}{2!}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + \frac{(\Delta x)^3}{3!}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i \cdots$$

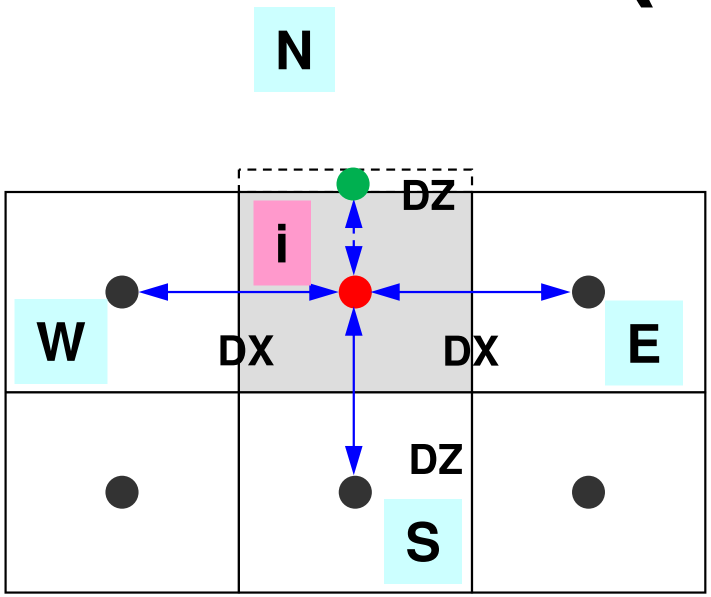
$$\phi_{i-1} = \phi_i - \Delta x \left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(\Delta x)^2}{2!}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i - \frac{(\Delta x)^3}{3!}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i \cdots$$

$$\phi_{i-1} + \phi_{i+1} = 2\phi_i + 2\times\frac{(\Delta x)^2}{2!}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + 2\times\frac{(\Delta x)^4}{4!}\left(\frac{\partial^4 \phi}{\partial x^4}\right)_i \cdots$$

$$\frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{(\Delta x)^2} = \left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + \boxed{\frac{(\Delta x)^2}{12}\left(\frac{\partial^4 \phi}{\partial x^4}\right)_i} \cdots$$

Truncation Err.: 2nd Order
2nd Order Accuracy
If Δx is not uniform: 1st or Lower Order Accuracy

Dirichlet B.C. "N" is very thin (=ε) 1st order (or lower) Accuracy



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

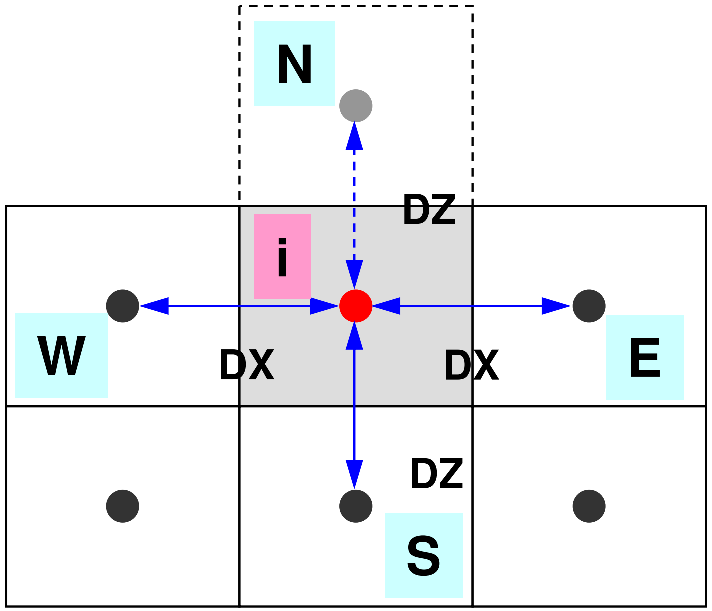
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

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

$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]+\frac{\phi_N-\phi_i}{\left(\frac{\Delta z}{2}+\frac{\varepsilon}{2}\right)}\Delta x\Delta y=-V_i\dot{Q}_i,\quad \phi_N=0,\quad \varepsilon\sim 0$$

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

Dirichlet B.C. using Mirror Image



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

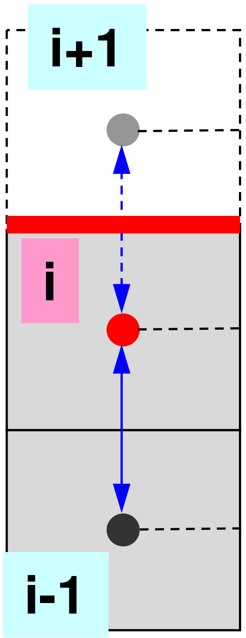
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

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

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

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

Higher Order Approximation for Dirichlet B.C. in 1D Problem



$$z=+\frac{\Delta z}{2}=+l$$

$$\phi=0\ @\ z=0$$

$$z=-\frac{\Delta z}{2}=-l$$

$$z=-\frac{3}{2}\Delta z=-3l$$

more complicated in 2D/3D cases

$$\phi=az^2+bz+c$$

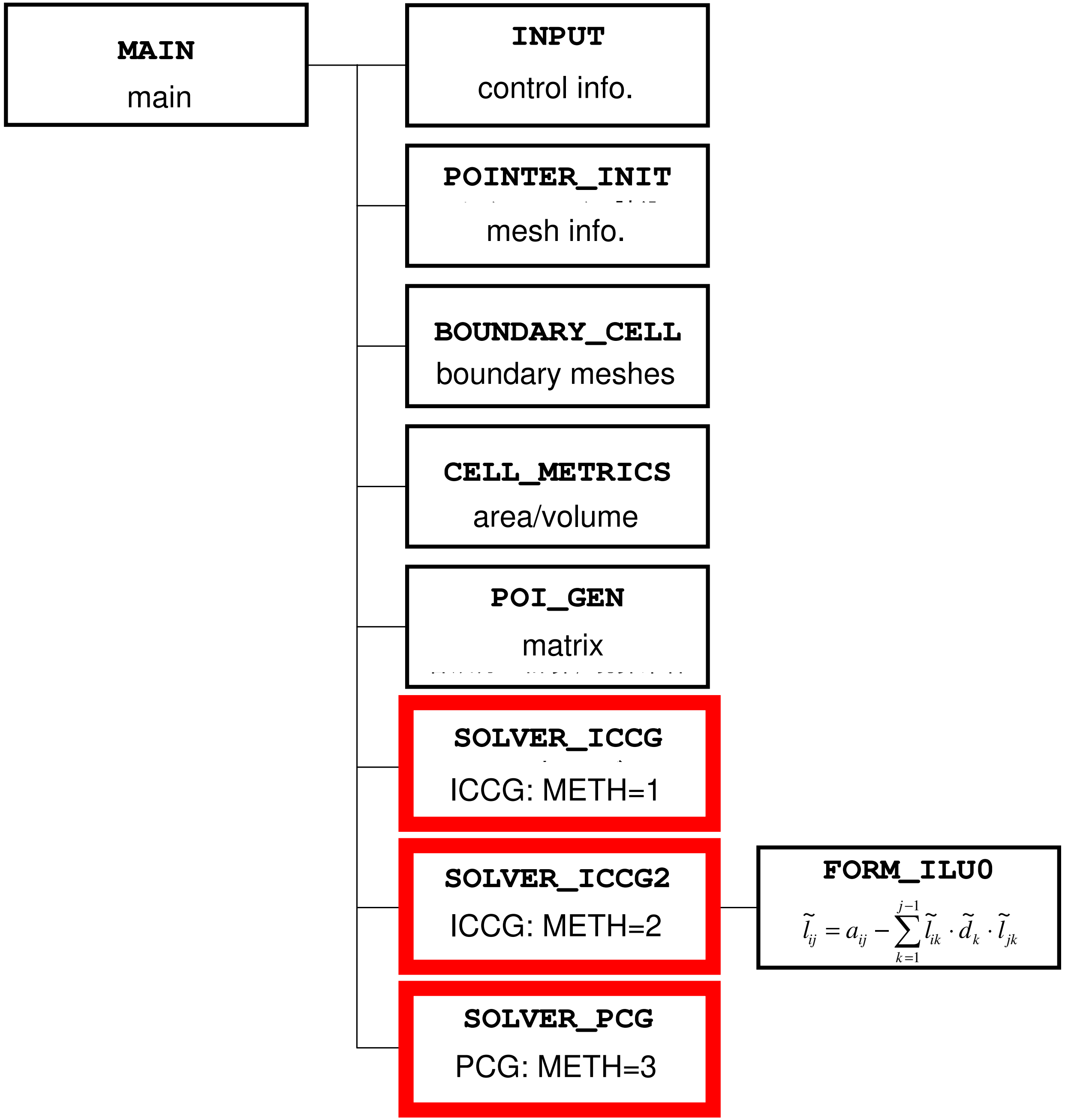
$$\phi(z=0)=c=0$$

$$\phi_i=al^2-bl+c=al^2-bl,\quad \phi_{i-1}=9al^2-3bl+c=9al^2-3bl$$

$$a=\frac{\phi_{i-1}-3\phi_i}{6l^2},\quad b=\frac{\phi_{i-1}-9\phi_i}{6l}\Rightarrow \phi_{i+1}=al^2+bl=\frac{1}{3}\phi_{i-1}-2\phi_i$$

Structure of the Program

```
program MAIN

use STRUCT
use PCG
use solver_ICCG
use solver_ICCG2
use solver_PCG

 implicit REAL*8 (A-H,O-Z)

call INPUT
call POINTER_INIT
call BOUNDARY_CELL
call CELL_METRICS
call POI_GEN

PHI=  0.d0

 if (METHOD.eq.1) call solve_ICCG (…)
 if (METHOD.eq.2) call solve_ICCG2(…)
 if (METHOD.eq.3) call solve_PCG  (…)

call OUTUCD

stop
end
```



- Background
  - Finite Volume Method
  - Preconditioned Iterative Solvers
- **ICCG Solver for Poisson Equations**
  - How to run
    - Data Structure
  - **Program**
    - Initialization
    - Coefficient Matrices
    - **ICCG**

Solving Linear Equations

- Conjugate Gradient, CG
- Preconditioner: Incomplete Cholesky Factorization, IC
  - Incomplete “Modified” Cholesky Factorization, more precisely

- ICCG

“Modified” Cholesky Factorization

- LU factorization of symmetric matrices
- Symmetric matrix [A] can be factorized into the form of [A]= [L][D][L]^T
  - LDL^T Factorization, Modified Cholesky Factorization
  - [A]= [L][L]^T => Cholesky Factorization

N=5

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} & 0 \\ l_{51} & l_{52} & l_{53} & l_{54} & l_{55} \end{bmatrix} \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 \\ 0 & 0 & 0 & d_4 & 0 \\ 0 & 0 & 0 & 0 & d_5 \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} & l_{41} & l_{51} \\ 0 & l_{22} & l_{32} & l_{42} & l_{52} \\ 0 & 0 & l_{33} & l_{43} & l_{53} \\ 0 & 0 & 0 & l_{44} & l_{54} \\ 0 & 0 & 0 & 0 & l_{55} \end{bmatrix}$$

Incomplete "Modified" Cholesky Factorization (NO Fill-in)

$$\sum_{k=1}^{j} l_{ik} \cdot d_k \cdot l_{jk} = a_{ij} \quad (j = 1,2,\cdots,i-1)$$

$$\sum_{k=1}^{i} l_{ik} \cdot d_k \cdot l_{ik} = a_{ii}$$

if $l_{ii} \cdot d_i = 1$, following relationship is obtained:

$$l_{ii} \cdot d_i = 1$$

$$l_{ij} \cdot d_j \cdot l_{jj} + \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk} = l_{ij} + \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk} = a_{ij}$$

$i = 1,2,\cdots,n$

- $j = 1,2,\cdots,i-1$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{-1}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} & 0 \\ l_{51} & l_{52} & l_{53} & l_{54} & l_{55} \end{bmatrix} \begin{bmatrix} d_1 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 \\ 0 & 0 & 0 & d_4 & 0 \\ 0 & 0 & 0 & 0 & d_5 \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} & l_{41} & l_{51} \\ 0 & l_{22} & l_{32} & l_{42} & l_{52} \\ 0 & 0 & l_{33} & l_{43} & l_{53} \\ 0 & 0 & 0 & l_{44} & l_{54} \\ 0 & 0 & 0 & 0 & l_{55} \end{bmatrix}$$

$$= \begin{bmatrix} l_{11} & 0 & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} & 0 \\ l_{51} & l_{52} & l_{53} & l_{54} & l_{55} \end{bmatrix} \begin{bmatrix} d_1 \cdot l_{11} & d_1 \cdot l_{21} & d_1 \cdot l_{31} & d_1 \cdot l_{41} & d_1 \cdot l_{51} \\ 0 & d_2 \cdot l_{22} & d_2 \cdot l_{32} & d_2 \cdot l_{42} & d_2 \cdot l_{52} \\ 0 & 0 & d_3 \cdot l_{33} & d_3 \cdot l_{43} & d_3 \cdot l_{53} \\ 0 & 0 & 0 & d_4 \cdot l_{44} & d_4 \cdot l_{54} \\ 0 & 0 & 0 & 0 & d_5 \cdot l_{55} \end{bmatrix}$$

$$= \begin{bmatrix} l_{11} \cdot d_1 \cdot l_{11} & l_{11} \cdot d_1 \cdot l_{21} & l_{11} \cdot d_1 \cdot l_{31} & l_{11} \cdot d_1 \cdot l_{41} & l_{11} \cdot d_1 \cdot l_{51} \\ l_{21} \cdot d_1 \cdot l_{11} & l_{21} \cdot d_1 \cdot l_{21} + l_{22} \cdot d_2 \cdot l_{22} & l_{21} \cdot d_1 \cdot l_{31} + l_{22} \cdot d_2 \cdot l_{32} & l_{21} \cdot d_1 \cdot l_{41} + l_{22} \cdot d_2 \cdot l_{42} & l_{21} \cdot d_1 \cdot l_{51} + l_{22} \cdot d_2 \cdot l_{52} \\ l_{31} \cdot d_1 \cdot l_{11} & l_{31} \cdot d_1 \cdot l_{21} + l_{32} \cdot d_2 \cdot l_{22} & l_{31} \cdot d_1 \cdot l_{31} + l_{32} \cdot d_2 \cdot l_{32} + l_{33} \cdot d_3 \cdot l_{33} & l_{31} \cdot d_1 \cdot l_{41} + l_{32} \cdot d_2 \cdot l_{42} + l_{33} \cdot d_3 \cdot l_{43} & l_{31} \cdot d_1 \cdot l_{51} + l_{32} \cdot d_2 \cdot l_{52} + l_{33} \cdot d_3 \cdot l_{53} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix}$$

$$\sum_{k=1}^{j} l_{ik} \cdot d_k \cdot l_{jk} = a_{ij} \quad (j = 1, 2, \cdots, i-1)$$

$$\sum_{k=1}^{i} l_{ik} \cdot d_k \cdot l_{ik} = a_{ii}$$

$$a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$= l_{ij} \cdot \underline{d_j \cdot l_{jj}} = l_{ij}$$

Incomplete "Modified" Cholesky Factorization (NO Fill-in)

$$\sum_{k=1}^{j} l_{ik} \cdot d_k \cdot l_{jk} = a_{ij} \quad (j = 1, 2, \cdots, i-1)$$

$$\sum_{k=1}^{i} l_{ik} \cdot d_k \cdot l_{ik} = a_{ii}$$

if $l_{ii} \cdot d_i = 1$, following relationship is obtained:

$$i = 1, 2, \cdots, n$$

$$j = 1, 2, \cdots, i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk} \;\rightarrow\; \boxed{l_{ij} = a_{ij}}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\;2} \cdot d_k \right)^{-1} = l_{ii}^{\;-1}$$

Actually, more "incomplete" factorization is applied in practical use.

Running the Program

<$E-L1>/run/INPUT.DAT

```
32 32 32                                NX/NY/NZ
1                                       MEHOD 1:2:3
1.00e-00 1.00e-00 1.00e-00              DX/DY/DZ
0.10      1.0e-08                       OMEGA, EPSICCG
```

- METHOD: Preconditioning Method
  1. Incomplete Modified Cholesky Fact. (Off-Diagonal Components unchanged)
  2. Incomplete Modified Cholesky Fact.(Fortran ONLY)
  3. Diagonal Scaling/Point Jacobi

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}{}^2 \cdot d_k \right)^{-1} = l_{ii}{}^{-1}$$

Incomplete "Modified" Cholesky Factorization (NO Fill-in)

$$\sum_{k=1}^{j} l_{ik} \cdot d_k \cdot l_{jk} = a_{ij} \quad (j = 1,2,\cdots,i-1)$$

$$\sum_{k=1}^{i} l_{ik} \cdot d_k \cdot l_{ik} = a_{ii}$$

if $l_{ii} \cdot d_i = 1$, following relationship is obtained:

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk} \rightarrow l_{ij} = a_{ij}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\;2} \cdot d_k \right)^{-1} = l_{ii}^{\;-1}$$

Only diagonal components are changed

Forward/Backward Substitution for Incomplete Modified Cholesky Fact.

$$(M)\{z\}=\left(LDL^T\right)\{z\}=\{r\}$$

$$\{z\}=\left(LDL^T\right)^{-1}\{r\} \longrightarrow \begin{matrix}(L)\{y\}=\{r\}\\ \left(DL^T\right)\{z\}=\{y\}\end{matrix}$$

$$\begin{bmatrix} d_1 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 \\ 0 & 0 & 0 & d_4 & 0 \\ 0 & 0 & 0 & 0 & d_5 \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} & l_{41} & l_{51} \\ 0 & l_{22} & l_{32} & l_{42} & l_{52} \\ 0 & 0 & l_{33} & l_{43} & l_{53} \\ 0 & 0 & 0 & l_{44} & l_{54} \\ 0 & 0 & 0 & 0 & l_{55} \end{bmatrix} = \begin{bmatrix} 1 & l_{21}/l_{11} & l_{31}/l_{11} & l_{41}/l_{11} & l_{51}/l_{11} \\ 0 & 1 & l_{32}/l_{22} & l_{42}/l_{22} & l_{52}/l_{22} \\ 0 & 0 & 1 & l_{43}/l_{33} & l_{53}/l_{33} \\ 0 & 0 & 0 & 1 & l_{54}/l_{44} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Forward/Backward Substitution for Incomplete Modified Cholesky Fact.

```
!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===
```

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

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

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

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

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

Forward Substitution for Incomplete Modified Cholesky Fact.

```
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
```

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

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

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

$$l_{11}y_1 = r_1$$

$$l_{21}y_1 + l_{22}y_2 = r_2$$

$$\vdots$$

$$l_{n1}y_1 + l_{n2}y_2 + \cdots + l_{nn}y_n = r_n$$

$\Leftrightarrow$

$$y_1 = r_1 / l_{11}$$

$$y_2 = \left(r_2 - l_{21}y_1\right) / l_{22}$$

$$\vdots$$

$$y_n = \left(r_n - l_{n1}y_1 - l_{n2}y_2 \ldots = r_n - \sum_{j=1}^{n-1} l_{nj}y_j \right) / l_{nn}$$

Forward Substitution for Incomplete Modified Cholesky Fact.

```
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
```

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

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

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

$$y_i = \left(r_i - \sum_{j=1}^{i-1} l_{ij} y_j \right) / l_{ii}$$

WVAL

Backward Substitution for Incomplete Modified Cholesky Fact.

```
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
```

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

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

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

$$\begin{aligned} z_n &= y_n \\ z_{n-1} + \left(l_{n-1,n}/l_{n-1,n-1}\right) z_n &= y_{n-1} \\ &\vdots \\ z_1 + \left(l_{21}/l_{11}\right) z_2 + \cdots + \left(l_{n1}/l_{11}\right) z_n &= y_1 \end{aligned}$$

$$\Longleftrightarrow$$

$$\begin{aligned} z_n &= y_n \\ z_{n-1} &= y_{n-1} - \left(l_{n-1,n} z_n\right)/l_{n-1,n-1} \\ &\vdots \\ z_1 &= y_1 - \left(\sum_{j=2}^{n} l_{j1} z_j\right)/l_{11} \end{aligned}$$

Backward Substitution for Incomplete Modified Cholesky Fact.

```
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
```

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

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

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

$$z_i = y_i - \left(\sum_{j=i+1}^{n} l_{ij} z_j \right) / l_{ii}$$

SW

Forward/Backward Substitution for Incomplete Modified Cholesky Fact.

```
!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===
```

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

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

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

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

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

solve_ICCG (1/7): METHOD= 1

```
!C***
!C*** module solver_ICCG
!C***
!
      module solver_ICCG
      contains
!C
!C*** solve_ICCG
!C
      subroutine solve_ICCG                                          &
     &         ( N, NPL, NPU, indexL, itemL, indexU, itemU, D, B, X,    &
     &           AL, AU, EPS, ITR, IER)

      implicit REAL*8 (A-H,O-Z)

      real(kind=8), dimension(N)   :: D
      real(kind=8), dimension(N)   :: B
      real(kind=8), dimension(N)   :: X
      real(kind=8), dimension(NPL) :: AL
      real(kind=8), dimension(NPU) :: AU

      integer, dimension(0:N):: indexL, indexU
      integer, dimension(NPL):: itemL
      integer, dimension(NPU):: itemU
      real(kind=8), dimension(:,:), allocatable :: W

      integer, parameter ::  R= 1
      integer, parameter ::  Z= 2
      integer, parameter ::  Q= 2
      integer, parameter ::  P= 3
      integer, parameter :: DD= 4
```

ICELTOT → N
BFORCE → B
PHI → X
EPSICCG → EPS

W(i,1)= W(i,R) ⇒ {r}
W(i,2)= W(i,Z) ⇒ {z}
W(i,2)= W(i,Q) ⇒ {q}
W(i,3)= W(i,P) ⇒ {p}

W(i,4)= W(i,DD) ⇒ {d}

solve_ICCG (2/7): METHOD= 1

```
!C
!C +-------+
!C | INIT |
!C +-------+
!C===
      allocate (W(N,4))

      do i= 1, N
        X(i)   = 0.d0
        W(i,1)= 0.0D0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,4)= 0.0D0
      enddo

      do i= 1, N
        VAL= D(i)
        do k= indexL(i-1)+1, indexL(i)
          VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
        enddo
        W(i,DD)= 1.d0/VAL
      enddo
!C===
```

W(i,DD)= d_i
in incomplete modified Cholesky factorization

W(i,DD):	d_i
D(i):	a_{ii}
itemL(j):	k
AL(j):	a_{ik}

$i = 1,2,\cdots,n$

$j = 1,2,\cdots,i-1$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk} \rightarrow l_{ij} = a_{ij}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{\ -1}$$

Only diagonal components are changed

solve_ICCG (3/7): METHOD= 1

```
!C
!C +-----------------------+
!C | {r0}= {b} - [A]{xini} |
!C +-----------------------+
!C===
      do i= 1, N
        VAL= D(i)*X(i)
        do k= indexL(i-1)+1, indexL(i)
          VAL= VAL + AL(k)*X(itemL(k))
        enddo
        do k= indexU(i-1)+1, indexU(i)
          VAL= VAL + AU(k)*X(itemU(k))
        enddo
        W(i,R)= B(i) - VAL
      enddo

      BNRM2= 0.0D0
      do i= 1, N
        BNRM2 = BNRM2 + B(i)  **2
      enddo
!C===
```

BNRM2=|b|²
Convergence criteria

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    solve [M]z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

solve_ICCG (4/7): METHOD= 1

```
!C
!C************************************************   ITERATION
      ITR= N

      do L= 1, ITR
!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===
```

Compute $r^{(0)}= b-[A]x^{(0)}$
<u>for</u> i= 1, 2, …
  solve $[M]z^{(i-1)}= r^{(i-1)}$
  $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
  <u>if</u> i=1
    $p^{(1)}= z^{(0)}$
  <u>else</u>
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  <u>endif</u>
  $q^{(i)}= [A]p^{(i)}$
  $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
  $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
  $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
  check convergence $|r|$
<u>end</u>

solve_ICCG (4/7): METHOD= 1

```
!C
!C***************************************************  ITERATION
      ITR= N

      do L= 1, ITR
!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, ind
          SW= SW + AU(k) * W(itemU(k),Z)
        enddo
        W(i,Z)= W(i,Z) - W(i,DD)*SW
      enddo
!C===
```

$$(M)\{z\}=(LDL^T)\{z\}=\{r\}$$

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

前進代入
Forward Substitution

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

後退代入
Backward Substitution

solve_ICCG (5/7): METHOD= 1

```
!C
!C +--------------+
!C | RHO= {r}{z}  |
!C +--------------+
!C===
      RHO= 0.d0
      do i= 1, N
        RHO= RHO + W(i,R)*W(i,Z)
      enddo
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$
<u>for</u> i= 1, 2, …
    solve $[M]z^{(i-1)}= r^{(i-1)}$
    $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
    <u>if</u> i=1
      $p^{(1)}= z^{(0)}$
     <u>else</u>
      $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
      $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
    <u>endif</u>
    $q^{(i)}= [A]p^{(i)}$
    $\alpha_i\ = \rho_{i-1}/p^{(i)}q^{(i)}$
    $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
    $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
    check convergence $|r|$
<u>end</u>

solve_ICCG (6/7): METHOD= 1

```
!C
!C +-----------------------------+
!C | {p} = {z} if      ITER=1    |
!C | BETA= RHO / RHO1  otherwise |
!C +-----------------------------+
!C===
      if ( L.eq.1 ) then

        do i= 1, N
          W(i,P)= W(i,Z)
        enddo
       else
         BETA= RHO / RHO1
         do i= 1, N
           W(i,P)= W(i,Z) + BETA*W(i,P)
         enddo
      endif
!C===

!C
!C +-------------+
!C | {q}= [A]{p} |
!C +-------------+
!C===
      do i= 1, N
        VAL= D(i)*W(i,P)
        do k= indexL(i-1)+1, indexL(i)
          VAL= VAL + AL(k)*W(itemL(k),P)
        enddo
        do k= indexU(i-1)+1, indexU(i)
          VAL= VAL + AU(k)*W(itemU(k),P)
        enddo
        W(i,Q)= VAL
      enddo
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$

<u>for</u> i= 1, 2, …

    solve $[M]z^{(i-1)}= r^{(i-1)}$

    $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$

    <u>if</u> i=1

        $p^{(1)}= z^{(0)}$

    <u>else</u>

        $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$

        $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$

    <u>endif</u>

    $q^{(i)}= [A]p^{(i)}$

    $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$

    $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$

    $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$

    check convergence $|r|$

<u>end</u>

solve_ICCG (7/7): METHOD= 1

```
!C
!C +---------------------+
!C | ALPHA= RHO / {p}{q} |
!C +---------------------+
!C===
      C1= 0.d0
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      ALPHA= RHO / C1
!C===
!C
!C +----------------------+
!C | {x}= {x} + ALPHA*{p} |
!C | {r}= {r} - ALPHA*{q} |
!C +----------------------+
!C===
      do i= 1, N
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
      DNRM2= 0.d0
      do i= 1, N
        DNRM2= DNRM2 + W(i,R)**2
      enddo
!C===
      ERR = dsqrt(DNRM2/BNRM2)
      if (ERR .lt. EPS) then
          IER = 0
          goto 900
         else
          RHO1 = RHO
        endif
      enddo
      IER = 1
```

Compute $r^{(0)}= b-[A]x^{(0)}$

for $i= 1, 2, \ldots$

- solve $[M]z^{(i-1)}= r^{(i-1)}$
- $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
- **if $i=1$**
  - $p^{(1)}= z^{(0)}$
- **else**
  - $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
  - $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
- **endif**
- $q^{(i)}= [A]p^{(i)}$
- $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
- $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
- $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
- check convergence $|r|$

end

solve_ICCG (7/7): METHOD= 1

```
!C
!C +----------------------+
!C | ALPHA= RHO / {p}{q}  |
!C +----------------------+
!C===
      C1= 0.d0
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      ALPHA= RHO / C1
!C===
!C
!C +----------------------+
!C | {x}= {x} + AL
!C | {r}= {r} - AL
!C +-------------
!C===
      do i= 1, N
        X(i)   = X(i)    + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
      DNRM2= 0.d0
      do i= 1, N
        DNRM2= DNRM2 + W(i,R)**2
      enddo
!C===
      ERR = dsqrt(DNRM2/BNRM2)
      if (ERR .lt. EPS) then
          IER = 0
          goto 900
        else
          RHO1 = RHO
        endif
      enddo
      IER = 1
```

$$|r|,|b|: 2/L2/Euclidean-norm \quad (\|r\|_2, \|b\|_2)$$

Compute $r^{(0)}= b-[A]x^{(0)}$
for $i= 1, 2, \ldots$
  solve $[M]z^{(i-1)}= r^{(i-1)}$
  $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
  if i=1
    $p^{(1)}= z^{(0)}$
  else
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  endif
  $q^{(i)}= [A]p^{(i)}$
  $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
  $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
  $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
  check convergence $|r|$
end

r= b-[A]x
DNRM2= $|r|^2$
BNRM2= $|b|^2$

ERR= $|r|/|b|$

$$ERR=\sqrt{\frac{\mathrm{DNorm2}}{\mathrm{BNorm2}}}=\frac{|r|}{|b|}=\frac{|b-Ax|}{|b|}\le \mathrm{Eps}$$

$$Ax=b \Rightarrow \alpha Ax=\alpha b$$
$$r=b-Ax \Rightarrow R=\alpha b-\alpha Ax=\alpha r$$

solve_ICCG2 (1/3): METHOD= 2

Fortran ONLY

```
!C
!C***
!C*** module solver_ICCG2
!C***
!
      module solver_ICCG2
      contains
!C
!C*** solve_ICCG2
!C
      subroutine solve_ICCG2                                        &
     &  ( N, NPL, NPU, indexL, itemL, indexU, itemU, D, B, X,       &
     &     AL, AU, EPS, ITR, IER)

      implicit REAL*8 (A-H,O-Z)

      real(kind=8), dimension(N)   :: D
      real(kind=8), dimension(N)   :: B
      real(kind=8), dimension(N)   :: X
      real(kind=8), dimension(NPL) :: AL
      real(kind=8), dimension(NPU) :: AU

      integer, dimension(0:N)   :: indexL, indexU
      integer, dimension(NPL):: itemL
      integer, dimension(NPU):: itemU

      real(kind=8), dimension(:,:), allocatable :: W

      integer, parameter ::  R= 1
      integer, parameter ::  Z= 2
      integer, parameter ::  Q= 2
      integer, parameter ::  P= 3
      integer, parameter :: DD= 4

      real(kind=8), dimension(:), allocatable :: ALlu0, AUlu0
      real(kind=8), dimension(:), allocatable :: Dlu0
```

Compute $r^{(0)}= b-[A]x^{(0)}$
<u>for</u> i= 1, 2, …
  solve $[M]z^{(i-1)}= r^{(i-1)}$
  $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
  <u>if</u> i=1
    $p^{(1)}= z^{(0)}$
  <u>else</u>
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  <u>endif</u>
  $q^{(i)}= [A]p^{(i)}$
  $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
  $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
  $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
  check convergence $|r|$
<u>end</u>

solve_ICCG2 (2/3): METHOD= 2

Fortran ONLY

```
!C
!C +-------+
!C | INIT |
!C +-------+
!C===
      allocate (W(N,4))

      do i= 1, N
        X(i)   = 0.d0
        W(i,1)= 0.0D0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,4)= 0.0D0
      enddo

      call FORM_ILU0
!C===
```

Dlu0, ALlu0, AUlu0:

Factorized Matrix Components

FORM_ILU0 (1/2): Fortran only

Incomplete Modified LU Factorization

in solve_ICCG2

```
 contains

!C
!C***
!C*** FORM_ILU0
!C***
!C
!C    form ILU(0) matrix
!C
      subroutine FORM_ILU0
      implicit REAL*8 (A-H,O-Z)
      integer, dimension(:), allocatable :: IW1 , IW2
      integer, dimension(:), allocatable :: IWsL, IWsU
      real (kind=8):: RHS_Aij, DkINV, Aik, Akj

!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (ALlu0(NPL), AUlu0(NPU))
      allocate (Dlu0(N))

      do i= 1, N
        Dlu0(i)= D(i)
        do k= 1, INL(i)
          ALlu0(k,i)= AL(k,i)
        enddo

        do k= 1, INU(i)
          AUlu0(k,i)= AU(k,i)
        enddo
      enddo
!C===
```

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\,2} \cdot d_k \right)^{-1} = l_{ii}^{\,-1}$$

Dlu0, ALlu0, AUlu0:

Factorized Matrix Components

Initial Conditions

Dlu0 = D

ALlu0= AL

AUlu0= AU

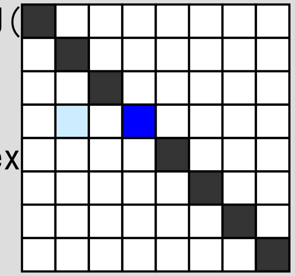
FORM_ILU0 (2/2): Fortran only

```
!C
!C +----------------------+
!C | ILU(0) factorization |
!C +----------------------+
!C===
      allocate (IW1(N) , IW2(N))
      IW1=0
      IW2= 0

      do i= 1, N
        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= k0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= k0
        enddo

        do icon= indexL(i-1)+1, indexL(i)
            k= itemL(icon)
          D11= Dlu0(k)

          DkINV= 1.d0/D11
            Aik= ALlu0(icon)

          do kcon= indexU(k-1)+1, indexU(k)
            j= itemU(kcon)

            if (j.eq.i) then
                   Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj
              Dlu0(i)= Dlu0(i) - RHS_Aij
            endif

            if (j.lt.i .and. IW1(j).ne.0) then
                   Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                       ij0 = IW1(j)
              ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
            endif

            if (j.gt.i .and. IW2(j).ne.0) then
                   Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                       ij0 = IW2(j)
              AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
            endif

          enddo
        enddo

        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= 0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= 0
        enddo
      enddo

      do i= 1, N
        Dlu0(i)= 1.d0 / Dlu0(i)
      enddo
      deallocate (IW1, IW2)
!C===
      end subroutine FORM_ILU0
```

```
do i= 1, N
  do k= 1, i-1
    if (A(i,k) is non-zero) then
      do j= k+1, N
        if (A(i,j) is non-zero) then
          A(i,j)=  A(i,j)                          &
                 -A(i,k)*(A(k,k))^-1*A(k,j)
        endif
      enddo
    endif
  enddo
enddo
```

FORM_ILU0 (2/2): Fortran only

```
!C
!C +----------------------+
!C | ILU(0) factorization |
!C +----------------------+
!C===
      allocate (IW1(N) , IW2(N))
      IW1=0
      IW2= 0

      do i= 1, N
        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= k0
        enddo

        do k0= indexU(i-1)+1, indexU(
          IW2(itemU(k0))= k0
        enddo

        do icon= indexL(i-1)+1, index
            k= itemL(icon)
          D11= Dlu0(k)

          DkINV= 1.d0/D11
            Aik= ALlu0(icon)

          do kcon= indexU(k-1)+1, indexU(k)
            j= itemU(kcon)

            if (j.eq.i) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj
              Dlu0(i)= Dlu0(i) - RHS_Aij
            endif

            if (j.lt.i .and. IW1(j).ne.0) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                      ij0 = IW1(j)
                ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
            endif
```

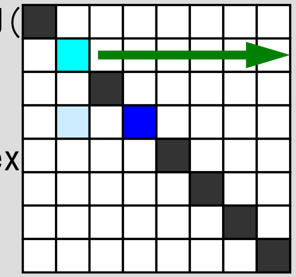


```
            if (j.gt.i .and. IW2(j).ne.0) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                      ij0 = IW2(j)
              AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
            endif

          enddo
        enddo

        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= 0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= 0
        enddo
      enddo

      do i= 1, N
        Dlu0(i)= 1.d0 / Dlu0(i)
      enddo
      deallocate (IW1, IW2)
!C===
      end subroutine FORM_ILU0
```

```
do i= 1, N
  do k= 1, i-1
    if (A(i,k) is non-zero) then
      do j= k+1, N
        if (A(i,j) is non-zero) then
          A(i,j)=  A(i,j)                              &
                   -A(i,k)*(A(k,k))^-1*A(k,j)
        endif
      enddo
    endif
  enddo
enddo
```

FORM_ILU0 (2/2): Fortran only

```
!C
!C +----------------------+
!C | ILU(0) factorization |
!C +----------------------+
!C===
      allocate (IW1(N) , IW2(N))
      IW1=0
      IW2= 0

      do i= 1, N
        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= k0
        enddo

        do k0= indexU(i-1)+1, indexU(
          IW2(itemU(k0))= k0
        enddo

        do icon= indexL(i-1)+1, index
            k= itemL(icon)
          D11= Dlu0(k)

          DkINV= 1.d0/D11
            Aik= ALlu0(icon)

          do kcon= indexU(k-1)+1, indexU(k)
            j= itemU(kcon)

            if (j.eq.i) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj
              Dlu0(i)= Dlu0(i) - RHS_Aij
            endif

            if (j.lt.i .and. IW1(j).ne.0) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                      ij0 = IW1(j)
              ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
            endif
```



```
            if (j.gt.i .and. IW2(j).ne.0) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                      ij0 = IW2(j)
              AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
            endif

          enddo
        enddo

        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= 0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= 0
        enddo
      enddo

      do i= 1, N
        Dlu0(i)= 1.d0 / Dlu0(i)
      enddo
      deallocate (IW1, IW2)
!C===
      end subroutine FORM_ILU0
```

```
do i= 1, N
  do k= 1, i-1
    if (A(i,k) is non-zero) then
      do j= k+1, N
        if (A(i,j) is non-zero) then
          A(i,j)= A(i,j)                            &
                 -A(i,k)*(A(k,k))^{-1}*A(k,j)
        endif
      enddo
    endif
  enddo
enddo
```

FORM_ILU0 (2/2): Fortran only

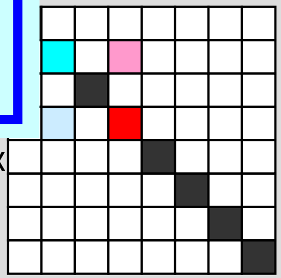
```
!C
!C +-----------------------+
!C | ILU(0) factorization |
!C +-----------------------+
!C===
```

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{\ -1}$$



```
        do icon= indexL(i-1)+1, index
          k= itemL(icon)
        D11= Dlu0(k)

        DkINV= 1.d0/D11
          Aik= ALlu0(icon)

        do kcon= indexU(k-1)+1, indexU(k)
          j= itemU(kcon)

          if (j.eq.i) then
               Akj= AUlu0(kcon)
           RHS_Aij= Aik * DkINV * Akj
           Dlu0(i)= Dlu0(i) - RHS_Aij
          endif

          if (j.lt.i .and. IW1(j).ne.0) then
               Akj= AUlu0(kcon)
           RHS_Aij= Aik * DkINV * Akj

                  ij0 = IW1(j)
             ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
          endif

          if (j.gt.i .and. IW2(j).ne.0) then
               Akj= AUlu0(kcon)
           RHS_Aij= Aik * DkINV * Akj

                  ij0 = IW2(j)
             AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
          endif

          enddo
        enddo

        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= 0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= 0
        enddo
      enddo

      do i= 1, N
        Dlu0(i)= 1.d0 / Dlu0(i)
      enddo
      deallocate (IW1, IW2)
!C===
      end subroutine FORM_ILU0
```

j=i

```
do i= 1, N
  do k= 1, i-1
    if (A(i,k) is non-zero) then
      do j= k+1, N
        if (A(i,j) is non-zero) then
          A(i,j)=  A(i,j)                          &
                -A(i,k)*(A(k,k))-1*A(k,j)
        endif
      enddo
    endif
  enddo
enddo
```

FORM_ILU0 (2/2): Fortran only

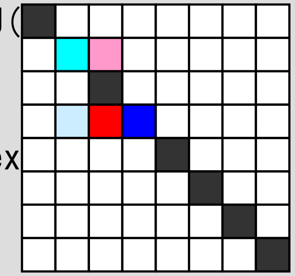
$$i = 1, 2, \cdots, n$$

$$j = 1, 2, \cdots, i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{2} \cdot d_k \right)^{-1} = l_{ii}^{-1}$$

```
      do k0= indexU(i-1)+1, indexU(
        IW2(itemU(k0))= k0
      enddo

      do icon= indexL(i-1)+1, index
          k= itemL(icon)
        D11= Dlu0(k)

        DkINV= 1.d0/D11
          Aik= ALlu0(icon)

        do kcon= indexU(k-1)+1, indexU(k)
          j= itemU(kcon)

          if (j.eq.i) then
                 Akj= AUlu0(kcon)
            RHS_Aij= Aik * DkINV * Akj
            Dlu0(i)= Dlu0(i) - RHS_Aij
          endif

          if (j.lt.i .and. IW1(j).ne.0) then
                 Akj= AUlu0(kcon)
            RHS_Aij= Aik * DkINV * Akj

                    ij0 = IW1(j)
              ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
          endif
```



j<i

```
          if (j.gt.i .and. IW2(j).ne.0) then
                 Akj= AUlu0(kcon)
            RHS_Aij= Aik * DkINV * Akj

                    ij0 = IW2(j)
            AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
          endif

          enddo
        enddo

        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= 0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= 0
        enddo
      enddo

      do i= 1, N
        Dlu0(i)= 1.d0 / Dlu0(i)
      enddo
      deallocate (IW1, IW2)
!C===
      end subroutine FORM_ILU0
```

```
do i= 1, N
  do k= 1, i-1
    if (A(i,k) is non-zero) then
      do j= k+1, N
        if (A(i,j) is non-zero) then
          A(i,j)=  A(i,j)                          &
                 -A(i,k)*(A(k,k))-1*A(k,j)
        endif
      enddo
    endif
  enddo
enddo
```

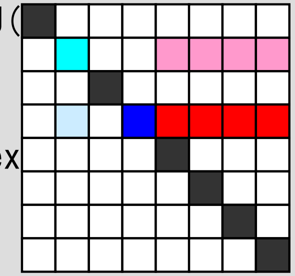
FORM_ILU0 (2/2): Fortran only

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{\ -1}$$



```
      do k0= indexU(i-1)+1, indexU(
        IW2(itemU(k0))= k0
      enddo

      do icon= indexL(i-1)+1, index
         k= itemL(icon)
        D11= Dlu0(k)

        DkINV= 1.d0/D11
          Aik= ALlu0(icon)

        do kcon= indexU(k-1)+1, indexU(k)
          j= itemU(kcon)

          if (j.eq.i) then
                Akj= AUlu0(kcon)
            RHS_Aij= Aik * DkINV * Akj
            Dlu0(i)= Dlu0(i) - RHS_Aij
          endif

          if (j.lt.i .and. IW1(j).ne.0) then
                Akj= AUlu0(kcon)
            RHS_Aij= Aik * DkINV * Akj

                    ij0 = IW1(j)
              ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
          endif

          if (j.gt.i .and. IW2(j).ne.0) then
                Akj= AUlu0(kcon)
            RHS_Aij= Aik * DkINV * Akj

                    ij0 = IW2(j)
            AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
          endif

        enddo
      enddo

      do k0= indexL(i-1)+1, indexL(i)
        IW1(itemL(k0))= 0
      enddo

      do k0= indexU(i-1)+1, indexU(i)
        IW2(itemU(k0))= 0
      enddo
    enddo

    do i= 1, N
      Dlu0(i)= 1.d0 / Dlu0(i)
    enddo
    deallocate (IW1, IW2)
!C===
    end subroutine FORM_ILU0
```

j>i

```
do i= 1, N
  do k= 1, i-1
    if (A(i,k) is non-zero) then
      do j= k+1, N
        if (A(i,j) is non-zero) then
          A(i,j)=  A(i,j)                                  &
                  -A(i,k)*(A(k,k))^-1*A(k,j)
        endif
      enddo
    endif
  enddo
enddo
```

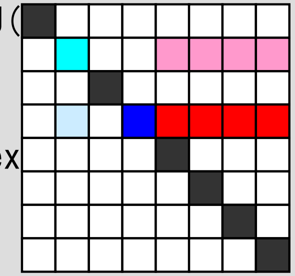
FORM_ILU0 (2/2): Fortran only

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\;2} \cdot d_k \right)^{-1} = l_{ii}^{\;-1}$$



```
        do k0= indexU(i-1)+1, indexU(
          IW2(itemU(k0))= k0
        enddo

        do icon= indexL(i-1)+1, index
            k= itemL(icon)
          D11= Dlu0(k)

          DkINV= 1.d0/D11
            Aik= ALlu0(icon)

          do kcon= indexU(k-1)+1, indexU(k)
            j= itemU(kcon)

            if (j.eq.i) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj
              Dlu0(i)= Dlu0(i) - RHS_Aij
            endif

            if (j.lt.i .and. IW1(j).ne.0) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                      ij0 = IW1(j)
                ALlu0(ij0)= ALlu0(ij0) - RHS_Aij
            endif
```

j<i

```
            if (j.gt.i .and. IW2(j).ne.0) then
                  Akj= AUlu0(kcon)
              RHS_Aij= Aik * DkINV * Akj

                      ij0 = IW2(j)
              AUlu0(ij0)= AUlu0(ij0) - RHS_Aij
            endif

          enddo
        enddo

        do k0= indexL(i-1)+1, indexL(i)
          IW1(itemL(k0))= 0
        enddo

        do k0= indexU(i-1)+1, indexU(i)
          IW2(itemU(k0))= 0
        enddo
      enddo

      do i= 1, N
        Dlu0(i)= 1.d0 / Dlu0(i)
      enddo
      deallocate (IW1, IW2)
!C===
      end subroutine FORM_ILU0
```

j>i

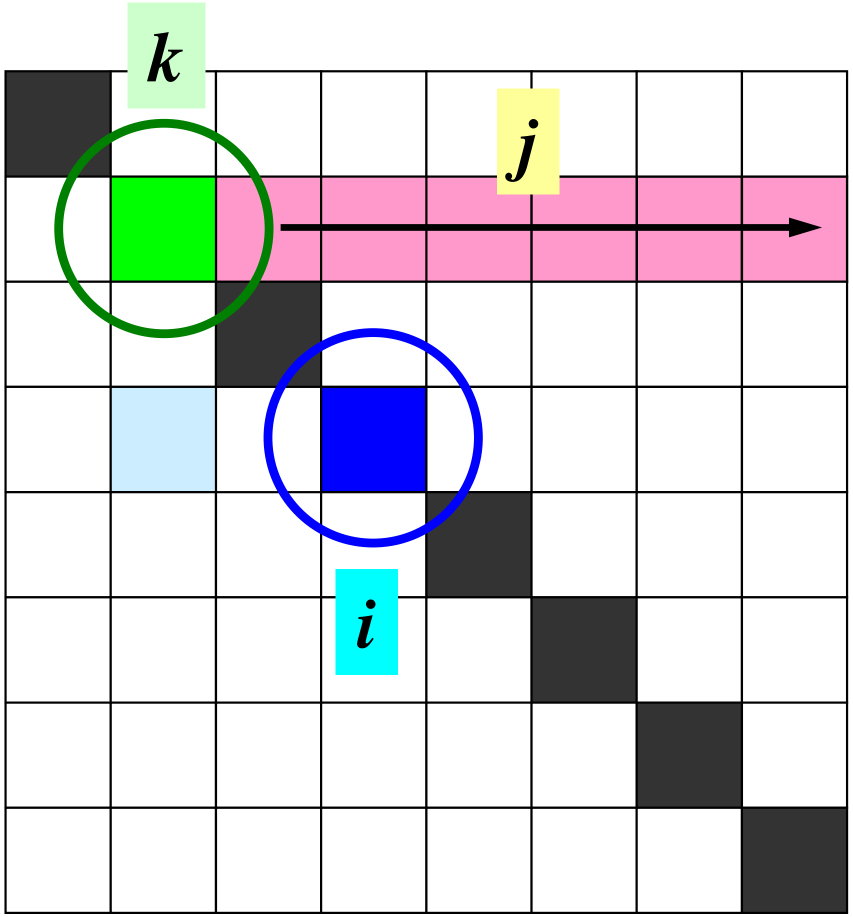
These if –then clauses never applied, therefore:

ALlu0= AL

AUlu0= AU

Dlu0 = W(i,DD)

j=i, j<i, j>i (1/3)



○: Mesh i

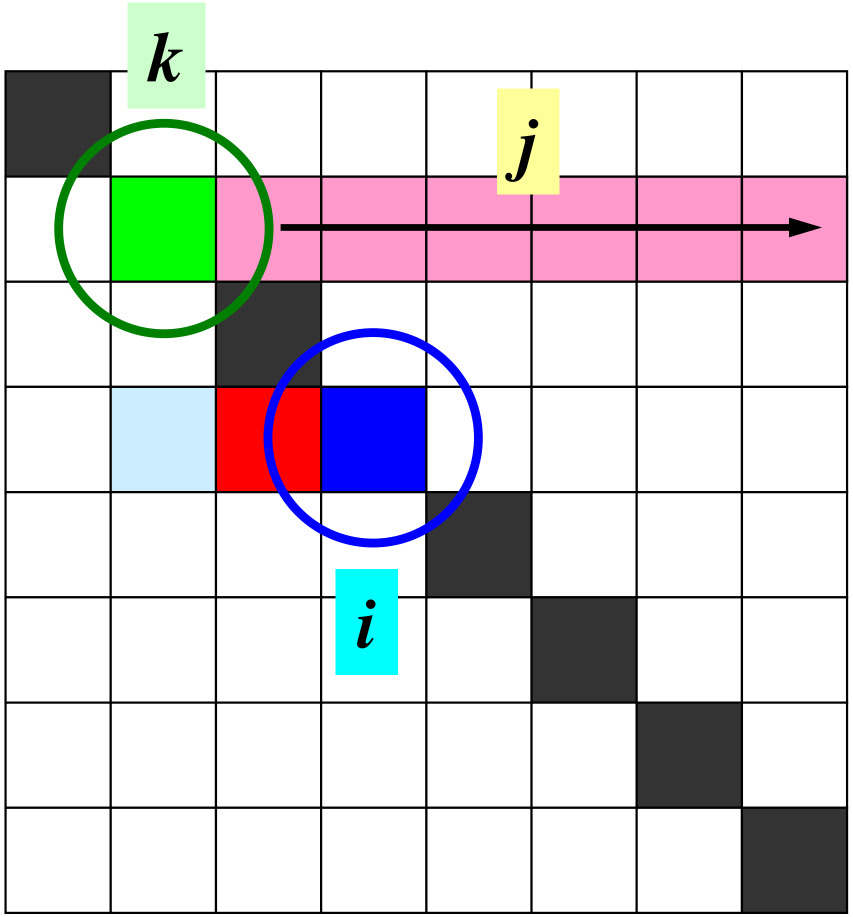
■○: Mesh k (Lower Triangular Component of i)

■: Mesh j (Upper Triangular Component of k)

if j=i Dlu(■) is updated

$$
\begin{cases}
i = 1,2,\cdots,n \\
\begin{cases}
j = 1,2,\cdots,i-1 \\
l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk} \\
\boxed{d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{\ -1}}
\end{cases}
\end{cases}
$$

j=*i*, *j*<*i*, *j*>*i* (2/3)



○: Mesh i

■○: Mesh k (Lower Triangular Component of i)

■: Mesh j (Upper Triangular Component of k)

if $j<i$ ALlu0(i-j)(■) is updated

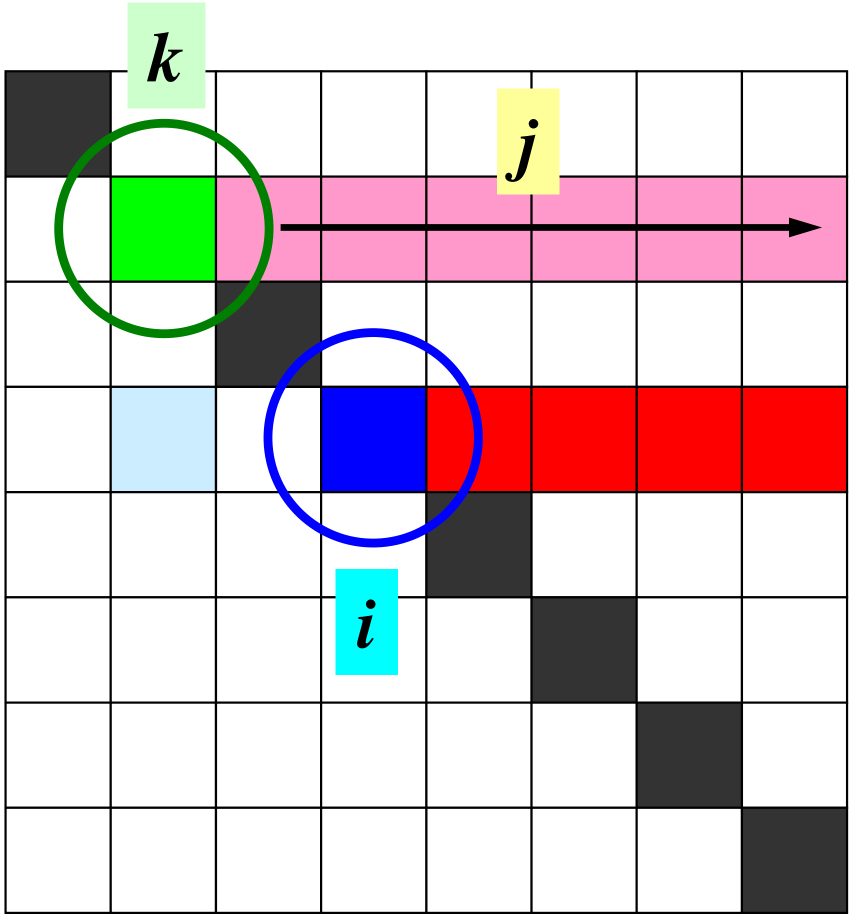
$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{-1}$$

$j=i$, $j<i$, $j>i$ (3/3)



○: Mesh i

■ ○: Mesh k (Lower Triangular Component of i)

■: Mesh j (Upper Triangular Component of k)

if $j>i$ AUlu0(i-j)(■) is updated

$$
i=1,2,\cdots,n
$$

$$
j=1,2,\cdots,i-1
$$

$$
l_{ij}=a_{ij}-\sum_{k=1}^{j-1} l_{ik}\cdot d_k \cdot l_{jk}
$$

$$
d_i=\left(a_{ii}-\sum_{k=1}^{i-1} l_{ik}{}^2\cdot d_k\right)^{-1}=l_{ii}{}^{-1}
$$

Actually, there are no cases for:

- **$j<i$**
- **$j>i$**

solve_ICCG2 (3/3): METHOD= 2

Fortran ONLY

```
!C
!C***************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!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 -  ALlu0(k) * W(itemL(k),Z)
        enddo
        W(i,Z)= WVAL * Dlu0(i)
      enddo

      do i= N, 1, -1
        SW  = 0.0d0
        do k= indexU(i-1)+1, indexU(i)
          SW= SW + AUlu0(k) * W(itemU(k),Z)
        enddo
        W(i,Z)= W(i,Z) - Dlu0(i)*SW
      enddo
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$
for $i= 1, 2, \ldots$
    solve $[M]z^{(i-1)}= r^{(i-1)}$
    $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
    if $i=1$
        $p^{(1)}= z^{(0)}$
    else
        $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
        $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
    endif
    $q^{(i)}= [A]p^{(i)}$
    $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
    $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
    $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
    check convergence $|r|$
end

Other parts are as same as those in “solve_ICCG”

solve_ICCG2 (3/3): METHOD= 2

Fortran ONLY

```
!C
!C***************************************************  ITERATION
      ITR= N

      do L= 1, ITR
!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 -  ALlu0(k) * W(itemL(k),Z)
        enddo
        W(i,Z)= WVAL * Dlu0(i)
      enddo

      do i= N, 1, -1
        SW  = 0.0d0
        do k= indexU(i-1)+1, ind
          SW= SW + AUlu0(k) * W(itemU(k),Z)
        enddo
        W(i,Z)= W(i,Z) - Dlu0(i)*SW
      enddo
!C===
```

$$(M)\{z\}=(LDL^T)\{z\}=\{r\}$$

Forward Substitution

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

Backward Substitution

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

ALlu0=AL, AUlu0=AU, Dlu0=W(i,DD): Therefore, iterations for convergence for METHOD=1, and those for METHOD=2 are same.

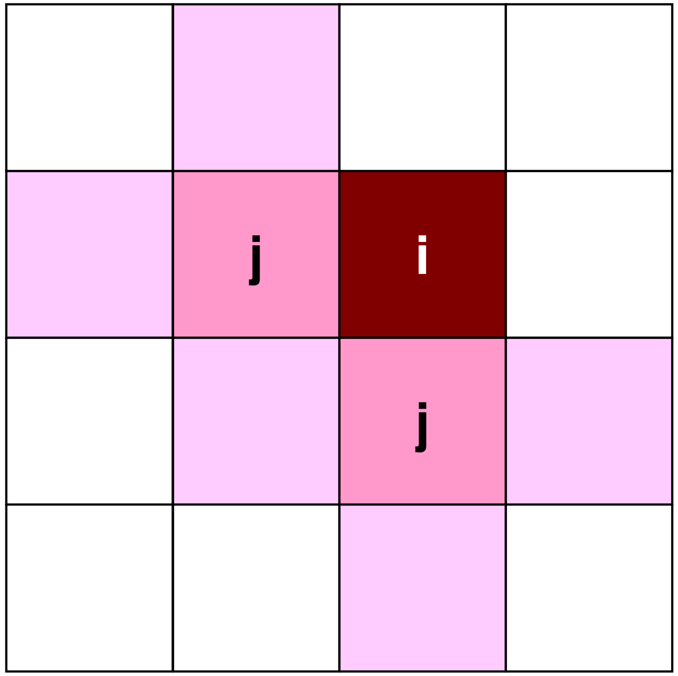
Incomplete Modified Cholesky Fact. Structured Meshes

$$i = 1,2,\cdots,n$$

$$j = 1,2,\cdots,i-1$$

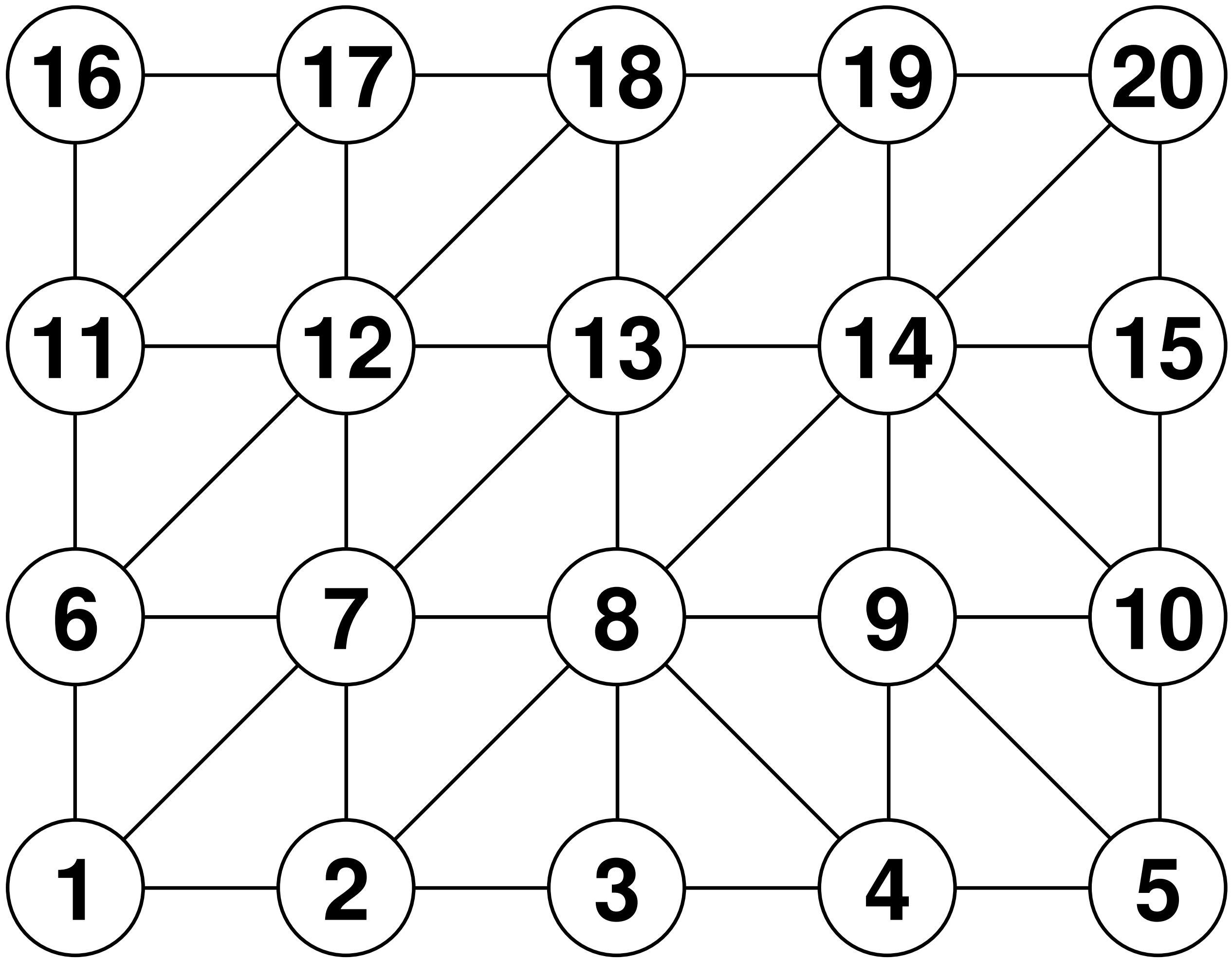
$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot d_k \cdot l_{jk}$$

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^{\ 2} \cdot d_k \right)^{-1} = l_{ii}^{\ -1}$$



There are no k-mesh which is adjacent to both of i and j simultaneously. Therefore, $l_{ij} = a_{ij}$.

In this case, ALlu0/AUlu0 could be changed



Parallelize ICCG Method

- Dot Product: OK
- DAXPY: OK
- Matrix-Vector Multiply: OK
- Preconditioning

How about the preconditioning ? Point Jacobi is easy: but slow

```
do i= 1, N
  W(i,Z)= W(i,R)*W(i,DD)
enddo
```

```
!$omp parallel do private(i)
  do i = 1, N
    W(i,Z)= W(i,R)*W(i,DD)
  enddo
!$omp end parallel do
```

```
!$omp parallel do private(ip,i)
  do ip= 1, PEsmpTOT
  do i = INDEX(ip-1)+1, INDEX(ip)
    W(i,Z)= W(i,R)*W(i,DD)
  enddo
  enddo
!$omp end parallel do
```

```
64*64*64
METHOD= 1
1      6.543963E+00
101    1.748392E-05
146    9.731945E-09

real    0m14.662s
```

```
METHOD= 3
1      6.299987E+00
101    1.298539E+00
201    2.725948E-02
301    3.664216E-05
401    2.146428E-08
413    9.621688E-09

real    0m19.660s
```

How about the preconditioning ?

IC Factorization

```
do i= 1, N
  VAL= D(i)
  do k= indexL(i-1)+1, indexL(i)
    VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
  enddo
  W(i,DD)= 1.d0/VAL
enddo
```

Forward Substitution

```
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
```

Data Dependency

Conflict of reading from/writing to memory
Difficult to be parallelized

IC Factorization

```
do i= 1, N
  VAL= D(i)
  do k= indexL(i-1)+1, indexL(i)
    VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
  enddo
  W(i,DD)= 1.d0/VAL
enddo
```

Forward Substitution

```
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
```

Matrix-Vector Multiply: Easy to be Parallelized {q}=[A]{p}

{q}: LHS: Updated

{p}: RHS: No change

```
!$omp parallel do private(i,VAL,k)
  do i = 1, N
    VAL= D(i)*W(i,P)
    do k= indexL(i-1)+1, indexL(i)
      VAL= VAL + AL(k)*W(itemL(k),P)
    enddo
    do k= indexU(i-1)+1, indexU(i)
      VAL= VAL + AU(k)*W(itemU(k),P)
    enddo
    W(i,Q)= VAL
  enddo
!$omp end parallel do
```

IC Factorization
Four Thread Parallel Operation

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

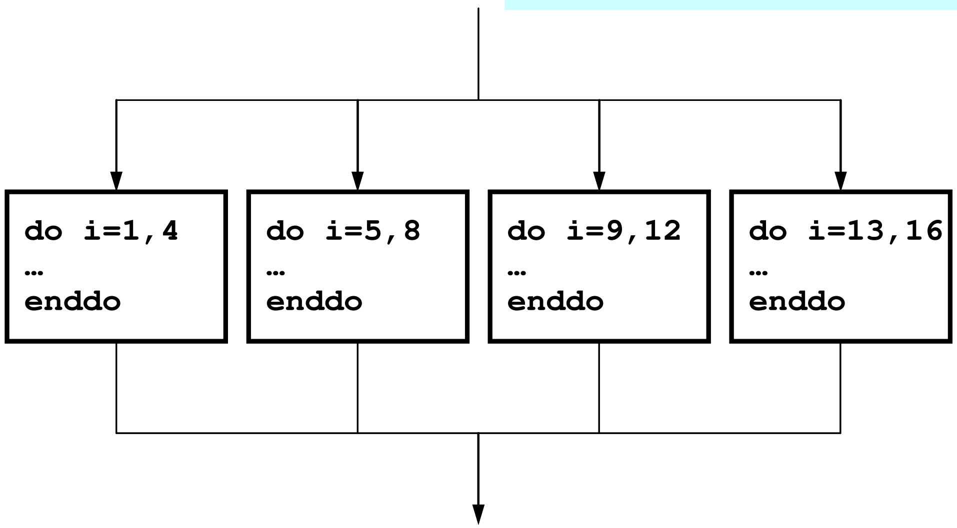
```
do i= 1, N
  WVAL= W(i,Z)
  do k= indexL(i-1)+1, indexL(i)
    WVAL= WVAL -  AL(k) * W(itemL(k),Z)
  enddo
  W(i,Z)= WVAL * W(i,DD)
enddo
```

IC Factorization
Four Thread Parallel Operation

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

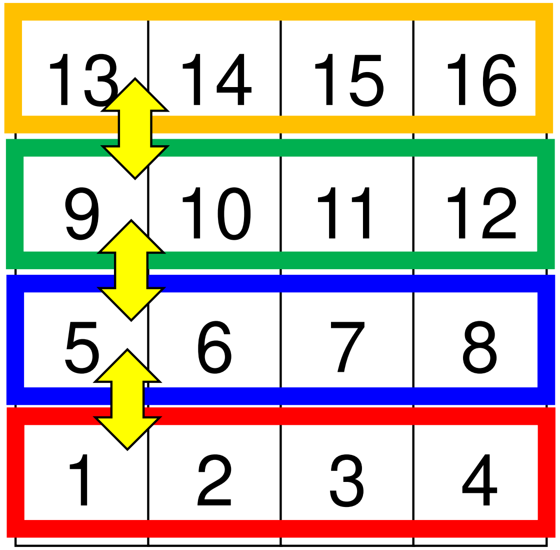
```
!$omp parallel do private (ip, i, k, VAL)
  do ip= 1, 4
  do  i= INDEX(ip-1)+1, INDEX(ip)
    WVAL= W(i,Z)
    do k= indexL(i-1)+1, indexL(i)
      WVAL= WVAL -  AL(k) * W(itemL(k),Z)
    enddo
    W(i,Z)= WVAL * W(i,DD)
  enddo
  enddo
!$omp parallel enddo
```

```
INDEX(0)= 0
INDEX(1)= 4
INDEX(2)= 8
INDEX(3)=12
INDEX(4)=16
```



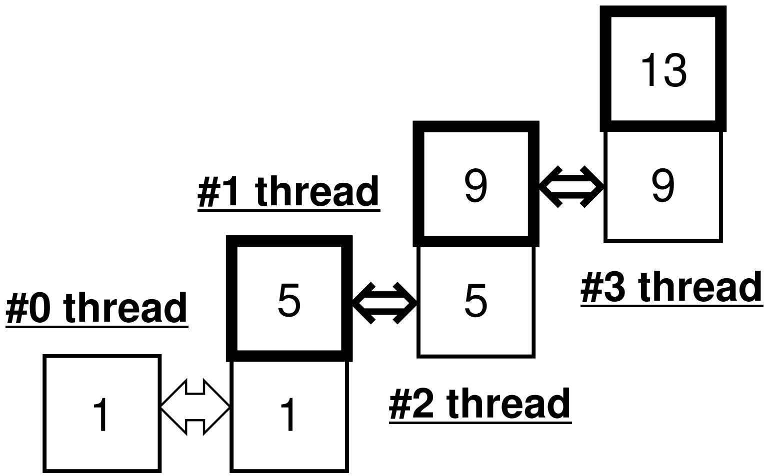
These four threads are executed simultaneously.

Data Dependency: Conflict of reading from/writing to memory




```
!$omp parallel do private (ip,I,k,VAL)
  do ip= 1, 4
  do  i= INDEX(ip-1)+1, INDEX(ip)
    WVAL= W(i,Z)
    do k= indexL(i-1)+1, indexL(i)
      WVAL= WVAL -  AL(k) * W(itemL(k),Z)
    enddo
    W(i,Z)= WVAL * W(i,DD)
  enddo
  enddo
!$omp parallel enddo
```

```
INDEX(0)= 0
INDEX(1)= 4
INDEX(2)= 8
INDEX(3)=12
INDEX(4)=16
```



⇔: Data Dependency

Parallelize ICCG Method

- Dot Product: OK
- DAXPY: OK
- Matrix-Vector Multiply: OK
- Preconditioning: Something special needed !
  - Just inserting OpenMP directive is not enough