Initial Structure of this Short Course

Date	Content
Feb. 21 (T)	Part-I (Katagiri): Introduction to OpenMP & MPI
Feb. 22 (W)	
Feb. 23 (Th)	Part-II (Nakajima): Parallel FVM
Feb. 24 (F)	

New Structure of this Short Course

Date	Content
Feb. 21 (T)	**Part-II-1 (Nakajima): Introduction to FVM**
Feb. 21 (T) – Feb. 23 (Th)	**Part-I (Katagiri): Introduction to OpenMP & MPI**
Feb. 23 (Th) – Feb. 24 (F)	**Part-II-2 (Nakajima): Parallel FVM** **FX10 Supercomputer is not available on Feb.24**

Overview of the 2nd Part

- Target Application
  - 3D Finite Volume Method (FVM)
  - Poisson Equations
  - Conjugate Gradient Iterative Method (CG)
  - CRS (Compressed Row Storage) for Sparse Matrices
- Parallel Application
  - OpenMP on a Single Node
  - MPI, OpenMP/MPI Hybrid
  - Parallel Data Structure for Distributed Computation
- (Very Rough) Schedule
  - Tuesday: FVM (Part-II 1)
  - Thursday PM: OpenMP (Part-II 2)
  - Friday AM: MPI, Parallel Data Structure (Part-II 3)
  - Friday PM: OpenMP/MPI Hybrid (Part-4)

SMASH: Scientific Computing

- **Science**
- **Modeling**
- **Algorithm**
- **Software**
- **Hardware**

- **Target: Parallel FVM (Finite-Volume Method) using OpenMP/MPI**
- Science: 3D Poisson Equations
- Modeling: FVM
- Algorithm: Iterative Solvers etc.
- You have to know many components to learn FVM, although you have already learned each of these in undergraduate and high-school classes.

Introduction to Parallel Programming for Multicore/Manycore Clusters

Part II-1: FVM Code

Kengo Nakajima
Information Technology Center
The University of Tokyo

Files on Your PC

Files on WEB:
http://nkl.cc.u-tokyo.ac.jp/files/fvm.tar

```
>$ cd <$CUR> : go to a certain directory
copy fvm.tar
>$ tar xvf fvm.tar

>$ cd fvm     <$P-fvm>
```

Please confirm that following directories are created:

```
>$ ls
src-c src-f run
```

PC

Oakleaf-FX

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

Target of this Part

- Material: CG solver for sparse matrices derived from FVM applications (Finite Volume Method).
- Parallelization on a single node of Oakleaf-FX (FX10) using OpenMP
- Keywords
  - Finite Volume Method (FVM)
  - Sparse Matrices
  - CG Method

Target Application

- 3D Poisson Equations

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

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

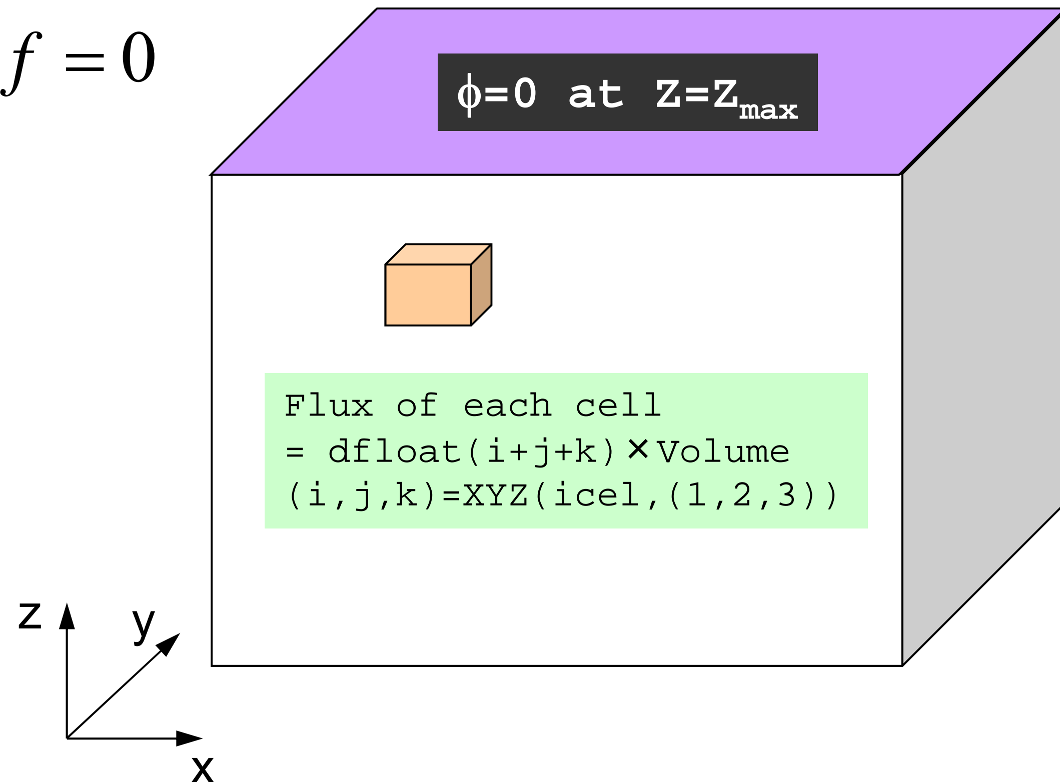
Target Problem: Variables are defined at cell-center's

Poisson Equation

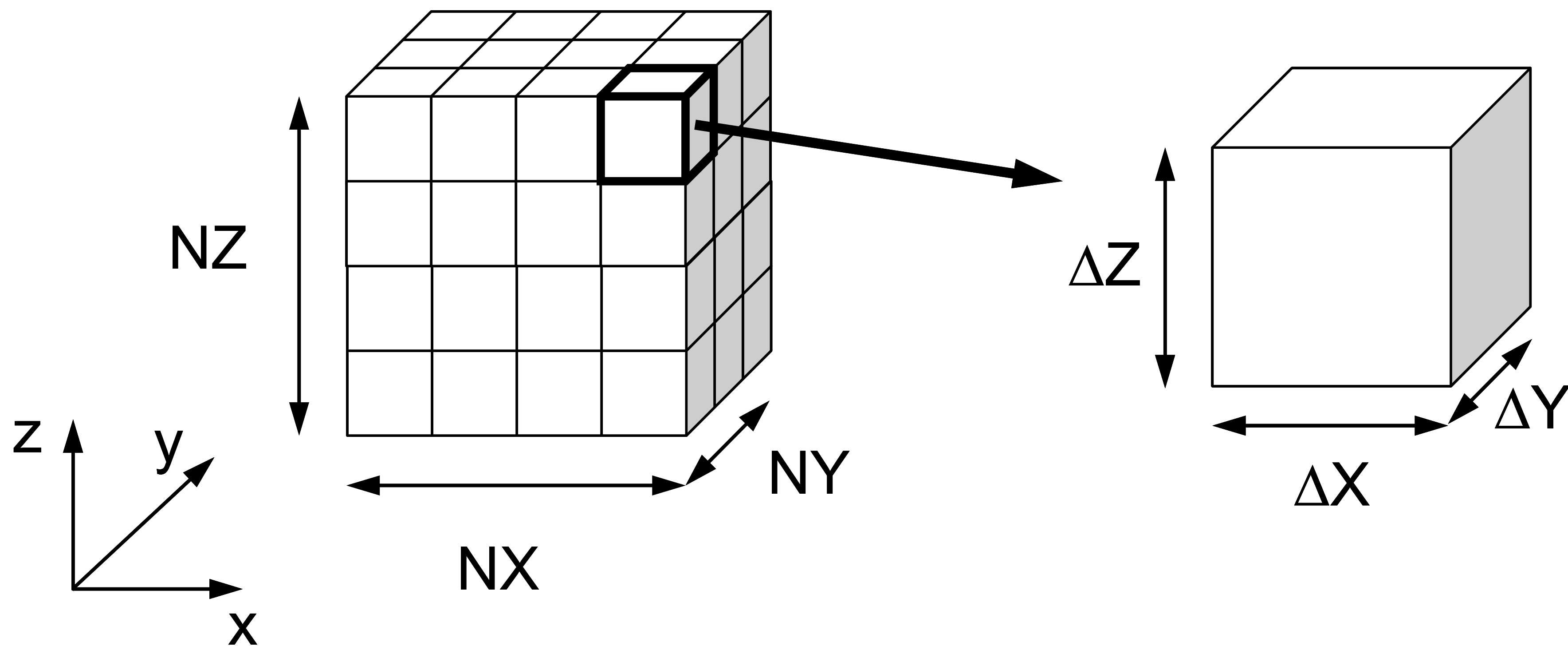
$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

B.C.

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



3D Structured Mesh
Internal data structure is "unstructured"



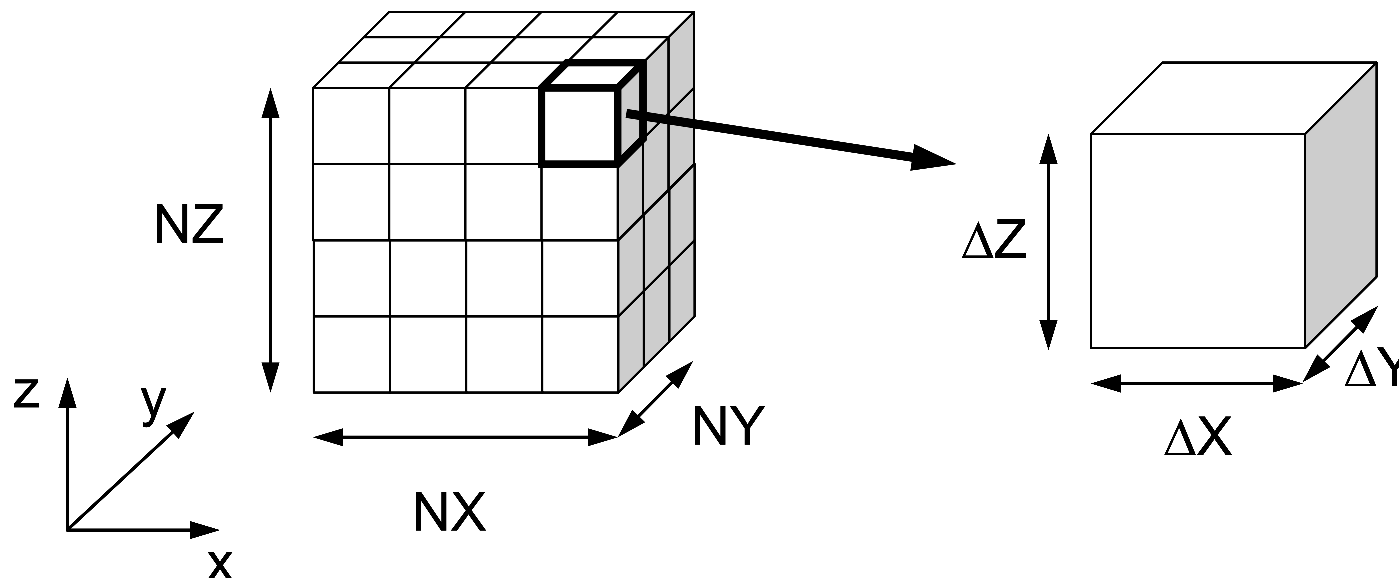
Volume Flux f

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

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

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

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



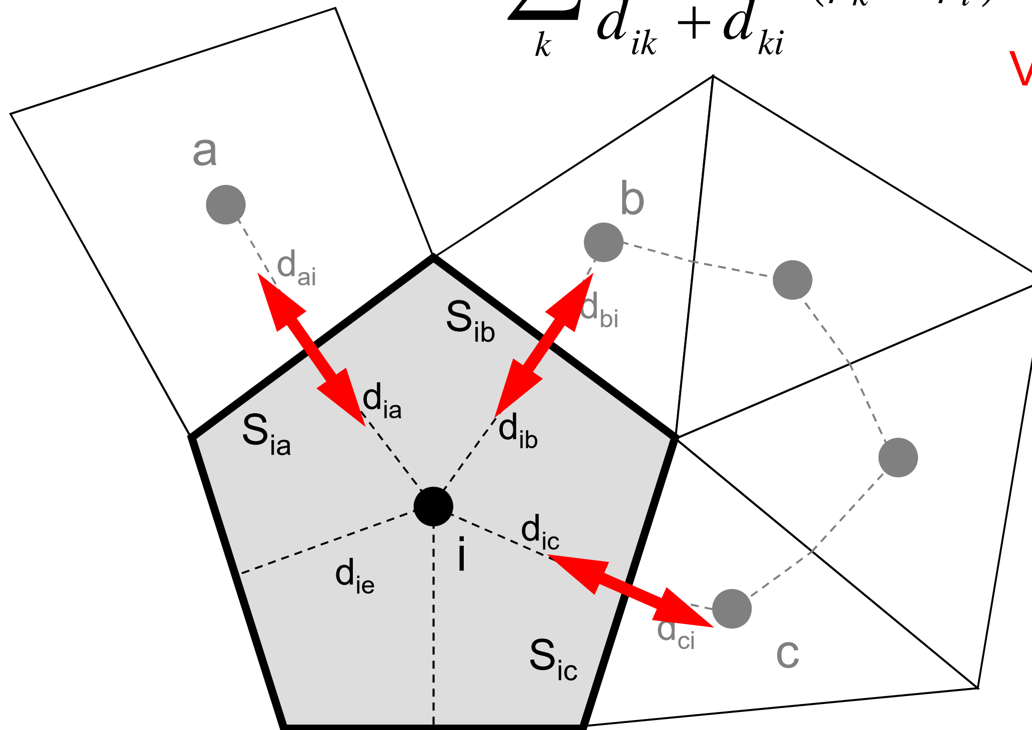
Finite Volume Method（FVM）

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

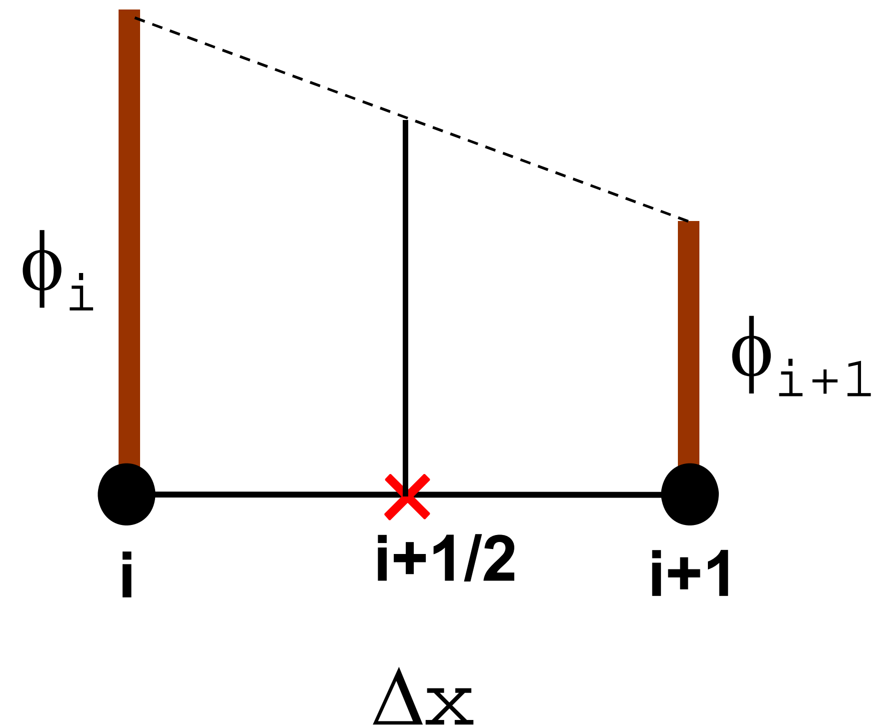


V_i : Volume
S : Surface Area
d_{ij} : Distance between Cell-Center & Surface
Q : Volume Flux

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

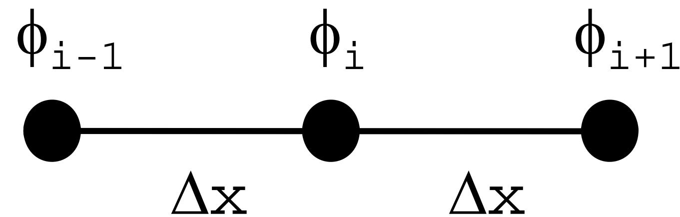
$$\left(\frac{d\phi}{dx}\right)_{i+1/2} \approx \frac{\phi_{i+1}-\phi_i}{\Delta x}$$

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



Finite Difference Method (FDM)
Taylor Series Expansion
2nd-Order Central Difference

$$\left(\frac{d^2\phi}{dx^2}\right)_i + Q = 0$$



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

$$= \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

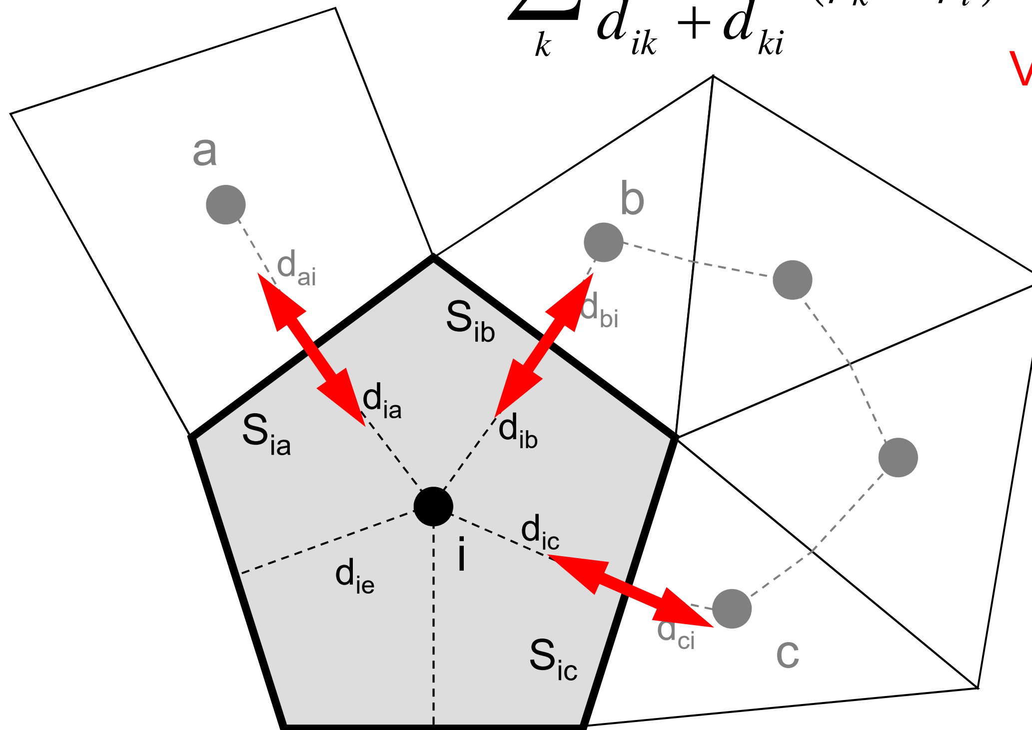
Finite Volume Method (FVM)

Conservation of Fluxes through Surfaces

Diffusion:
Interaction with Neighbors

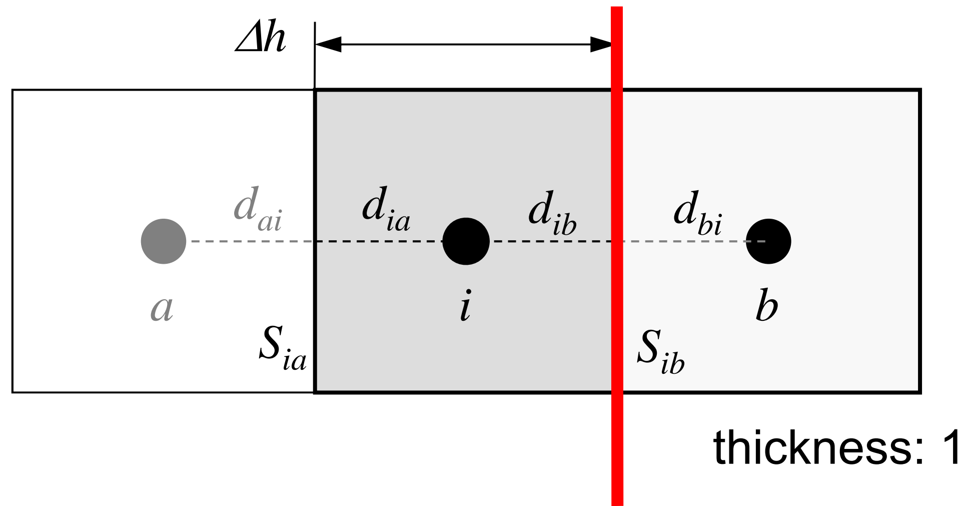
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

Volume Flux




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

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): $d_{ij} = \Delta h/2$

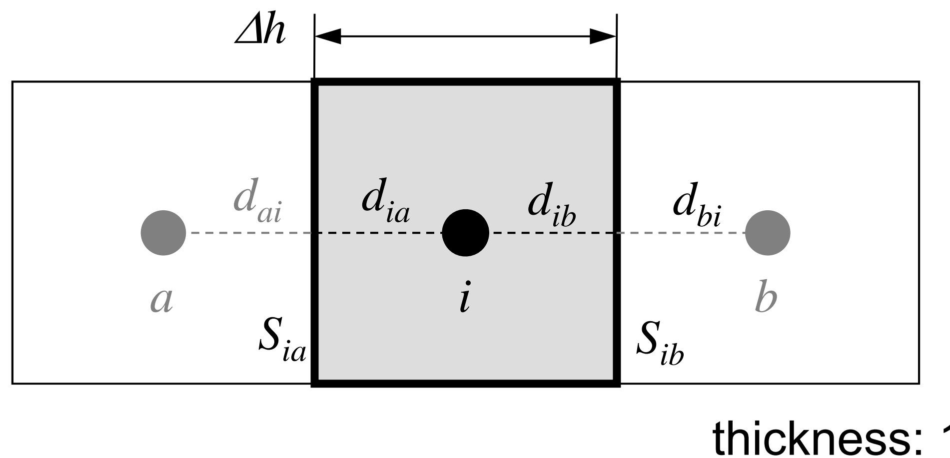
Flux through this surface: Qs_{ib}

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

Fourier's Law

Flux through a surface
= - (gradient of potential)

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

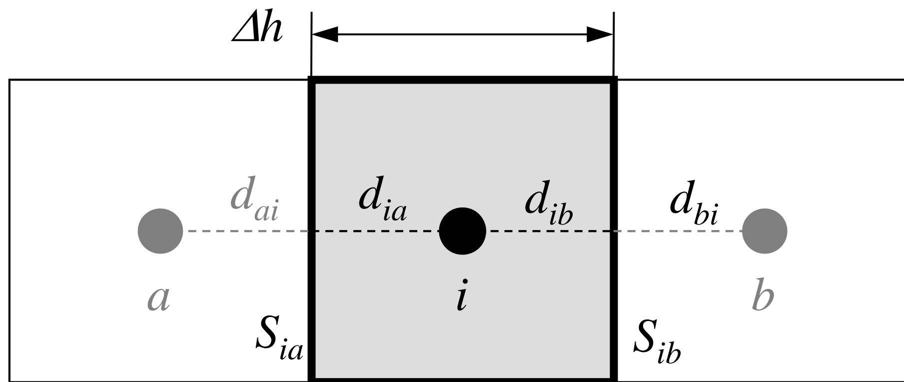
$$\sum_k \frac{S_{ik}}{d_{ik} + d_{ki}} (\phi_k - \phi_i) + V_i \dot{Q}_i = 0$$

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)



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

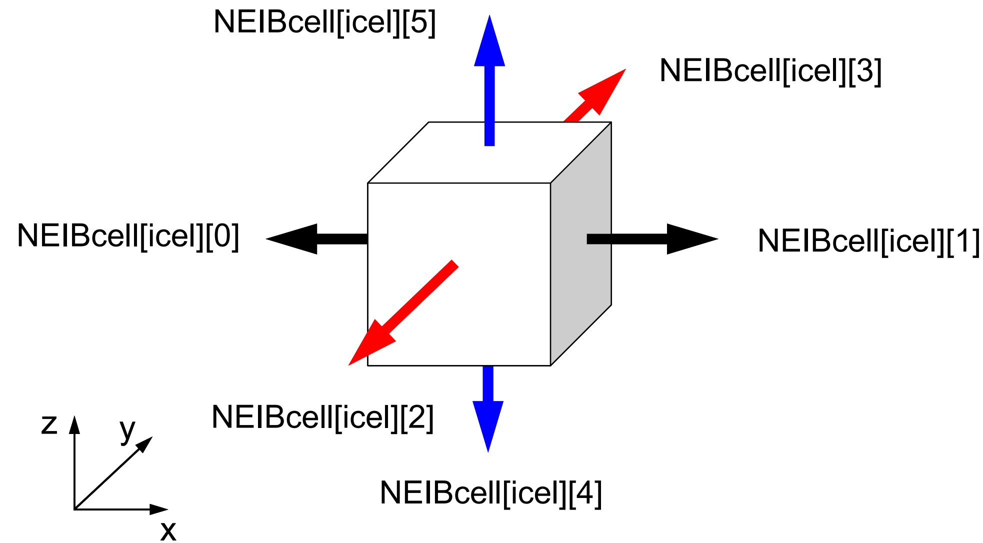
$$\frac{1}{V_i}\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)=\frac{1}{(\Delta h)^2}\sum_{k=a,b}\frac{\Delta h}{\frac{\Delta h}{2}+\frac{\Delta h}{2}}(\phi_k-\phi_i)$$

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

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

for i-th cell
linear equations

in 3D



$$\frac{\phi_{neib[icel][0]} - \phi_{icel}}{\Delta x} \Delta y \Delta z + \frac{\phi_{neib[icel][1]} - \phi_{icel}}{\Delta x} \Delta y \Delta z +$$

$$\frac{\phi_{neib[icel][2]} - \phi_{icel}}{\Delta y} \Delta z \Delta x + \frac{\phi_{neib[icel][3]} - \phi_{icel}}{\Delta y} \Delta z \Delta x +$$

$$\frac{\phi_{neib[icel][4]} - \phi_{icel}}{\Delta z} \Delta x \Delta y + \frac{\phi_{neib[icel][5]} - \phi_{icel}}{\Delta z} \Delta x \Delta y + f_{icel} \Delta x \Delta y \Delta z = 0$$

Linear Equations

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$
$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$
$$\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

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

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

Diagonal

Off-Diagonal

$$[A]\{\phi\}=\{f\}$$

Sparse Coef. Matrix in FEM
Many “0’s”

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

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

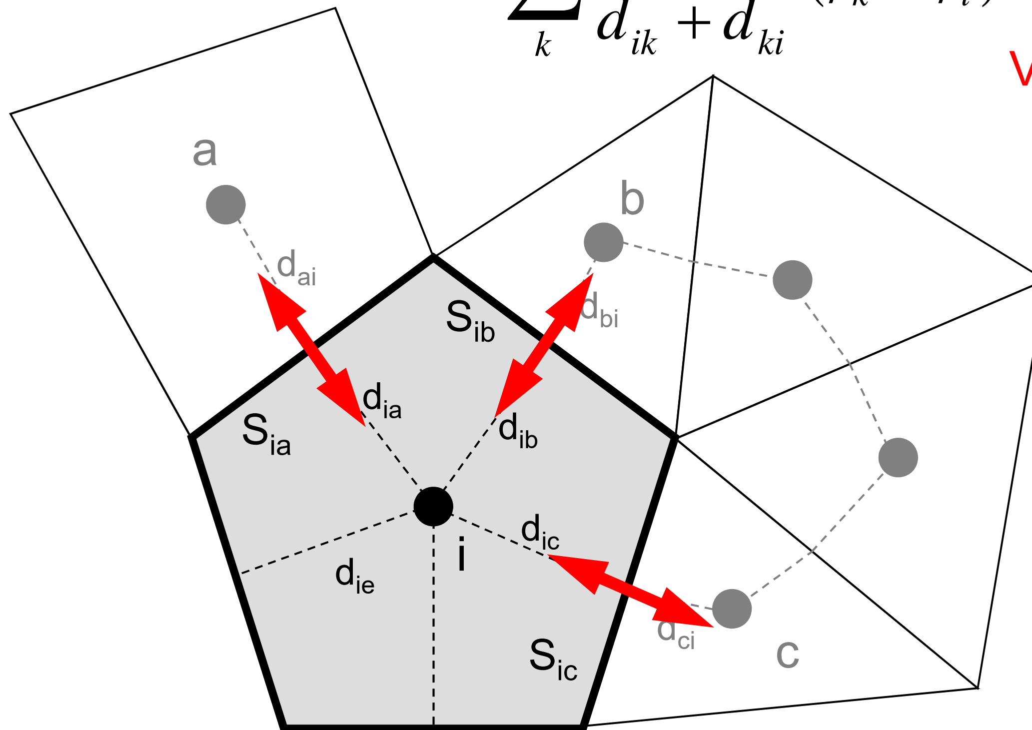
Coef. Matrices for FVM are sparse

Only neighboring cells are considered

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



V_i : Volume
S : Surface Area
d_{ij} : 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

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

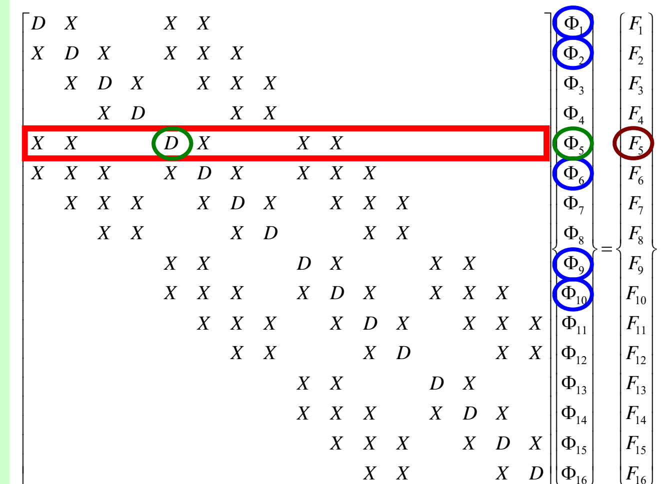
- Number of non-zero off-diagonal components is O(100) in FVM (only 6 in this case)
  - If number of unknowns is 10^8 :
    - $A(i,j)$: $O(10^{16})$ words
    - Actual Non-zero Components : $O(10^{10})$ words
- Only (really) non-zero off-diag. components should be stored on memory

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)	Off-Diagonal Components (Corresponding Column ID) (INT, k=1, index(N))
AMat(k)	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}

for(j=0;j<N;i++){
  Y[j]= 0.0;
  for (i=0;i<N;i++){
    Y[j]+= A[j][i]*X[i];
  }
}
```

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): C
Numbering starts from 0 in program

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

```
N= 8
```

Diagonal Components

```
Diag[0]=  1.1
Diag[1]=  3.6
Diag[2]=  5.7
Diag[3]=  9.8
Diag[4]= 11.5
Diag[5]= 12.4
Diag[6]= 23.1
Diag[7]= 51.3
```

Compressed Row Storage (CRS)

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

Compressed Row Storage (CRS)

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

NPLU= 25
(=Index[N])

(Index[i])th~(Index[i+1])th:
Non-Zero Off-Diag. Components corresponding to i-th row.

Compressed Row Storage (CRS)

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

NPLU= 25 (=Index[N])

(Index[i])th~(Index[i+1])th:
Non-Zero Off-Diag. Components corresponding to i-th row.

Compressed Row Storage (CRS)

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

```
Item[ 6]= 4, AMat[ 6]= 1.5
Item[18]= 2, AMat[18]= 2.5
```

Compressed Row Storage (CRS)

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

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

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

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

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

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, FDM, DEM, MD (solid), BEM w/FMM

Direct Method
直接法

- Gaussian Elimination/LU Factorization
  - compute A^{-1} directly.

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

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

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

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 Parallel FEM

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

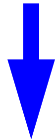
非定常法・クリロフ部分空間法

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

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

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

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



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

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

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

非定常法・クリロフ部分空間法

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

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

$\mathbf{z}_\mathbf{k}$ is a vector which belongs to k^{th} Krylov Subspace（クリロフ部分空間）, approximate solution vector $\mathbf{x}_\mathbf{k}$ 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: 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.
Assume that approximate solution: $x^{(0)}$, and
search direction vector $p^{(k)}$ is defined at k-th iteration.

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

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

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

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

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)

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

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

$\left(p^{(k+1)}, Ap^{(k)}\right) = 0$ $p^{(k)}$ and $p^{(k+1)}$ are "conjugate（共役）" for matrix A

```
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

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

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

if $i < k$

$$\left(r^{(k+1)}, r^{(i)}\right) = \left(r^{(i)}, r^{(k+1)}\right) \overset{(2)}{=} \left(r^{(i)}, r^{(k)} - \alpha_k Ap^{(k)}\right)$$
$$\overset{(*)}{=} -\alpha_k \left(r^{(i)}, Ap^{(k)}\right) \overset{(4)}{=} -\alpha_k \left(p^{(i)} - \beta_{i-1} p^{(i-1)}, Ap^{(k)}\right)$$
$$= -\alpha_k \left(p^{(i)}, Ap^{(k)}\right) + \alpha_k \beta_{i-1} \left(p^{(i-1)}, Ap^{(k)}\right) \overset{(*)}{=} 0$$

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

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

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

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

if $i < k$

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

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

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

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

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

α_k, β_k

Usually, we use simpler definitions of α_k, β_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

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

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

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
```

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

$[A']x' = b'$

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

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

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

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

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

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

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

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

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

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)= p(i-1) + βi-1 z(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

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

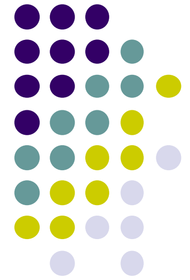
- **`solve [M]z(i-1)= r(i-1)`** is very easy.
- Provides fast convergence for simple problems.

ILU(0), IC(0)

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

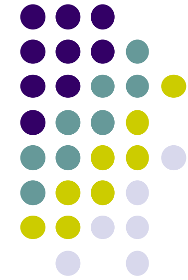
- Incomplete Direct Method
  - Even if original matrix is sparse, inverse matrix is not necessarily sparse.
  - **fill-in**
  - ILU(0)/IC(0) without fill-in have same non-zero pattern with the original (sparse) matrices

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

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
- **CG Solver for Poisson Equations**
  - **How to run**
    - **Data Structure**
  - Program
    - Initialization
    - Coefficient Matrices
    - CG

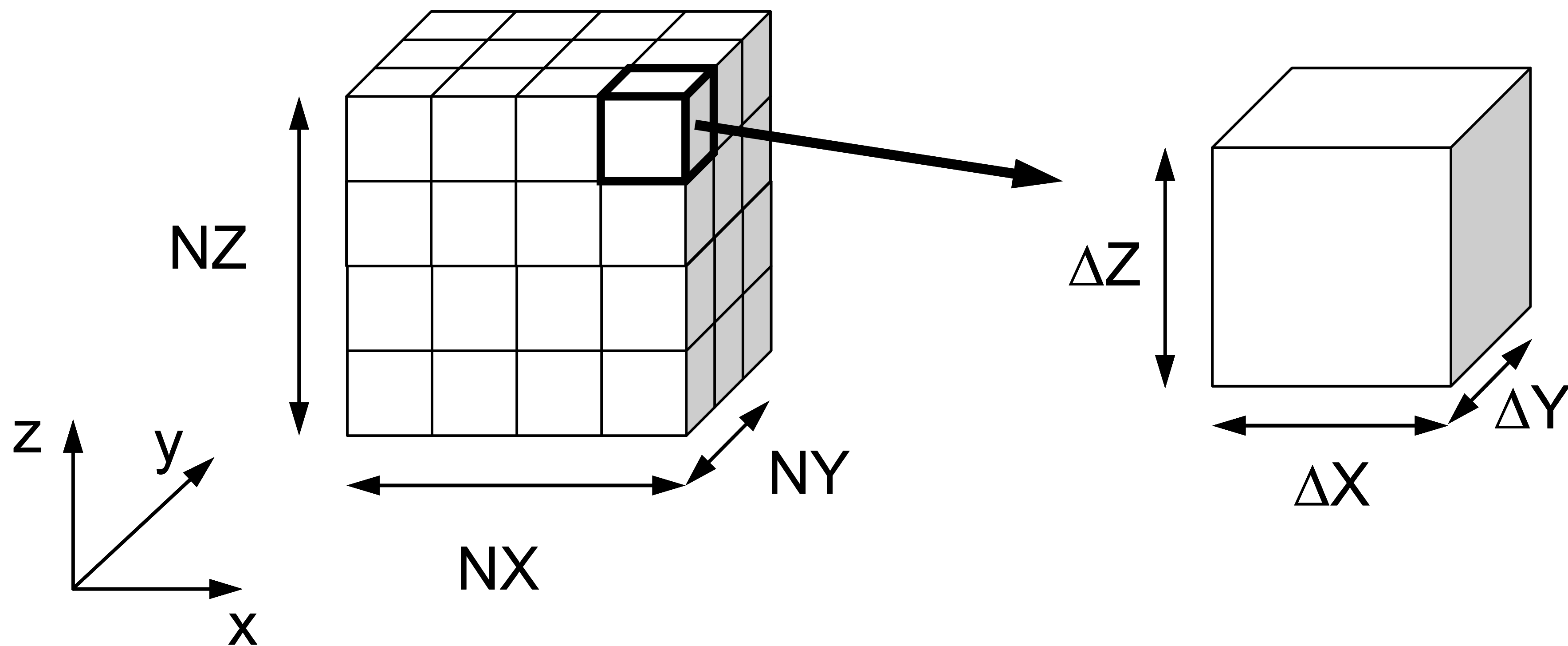
Target Application

- 3D Poisson Equations

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

- Finite Volume Method (FVM)
  - Arbitrary Shape Elements, Cell-Centered
  - “Direct” Finite Difference Method
- Boundary Conditions
  - Dirichlet B.C., Volume Flux
- Preconditioned Iterative Solvers
  - Conjugate Gradient + Preconditioner (Diagonal Scaling/Point Jacobi)

3D Structured Mesh
Internal data structure is "unstructured"



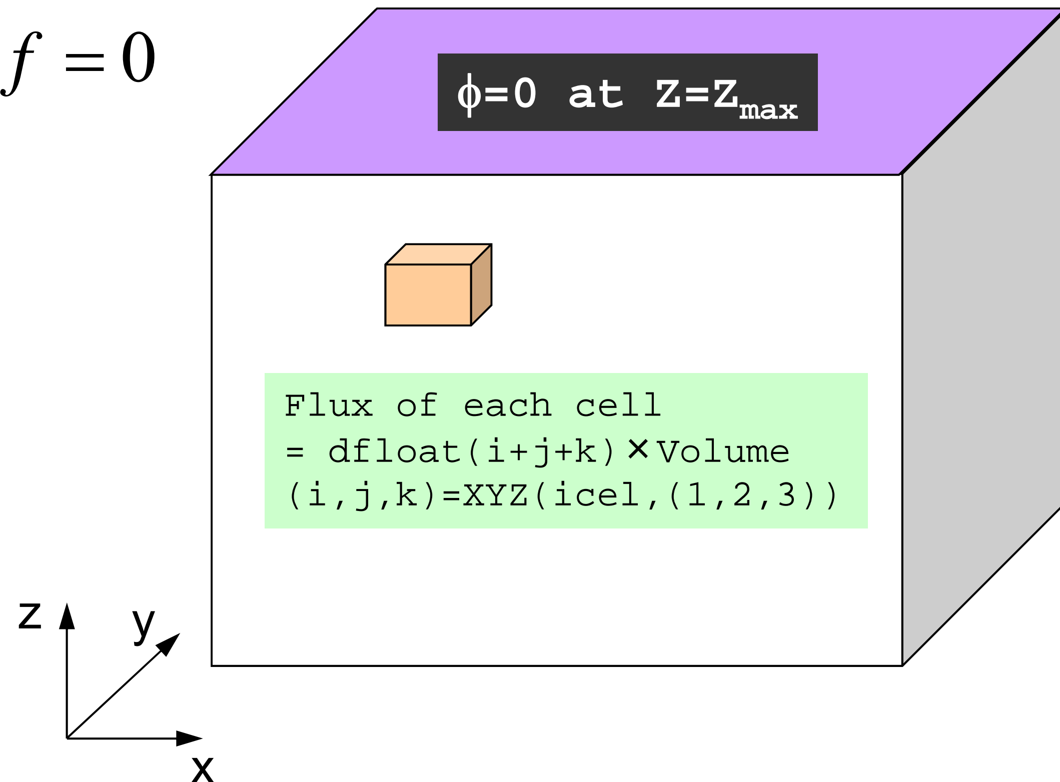
Target Problem: Variables are defined at cell-center'

Poisson Equation

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

B.C.

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



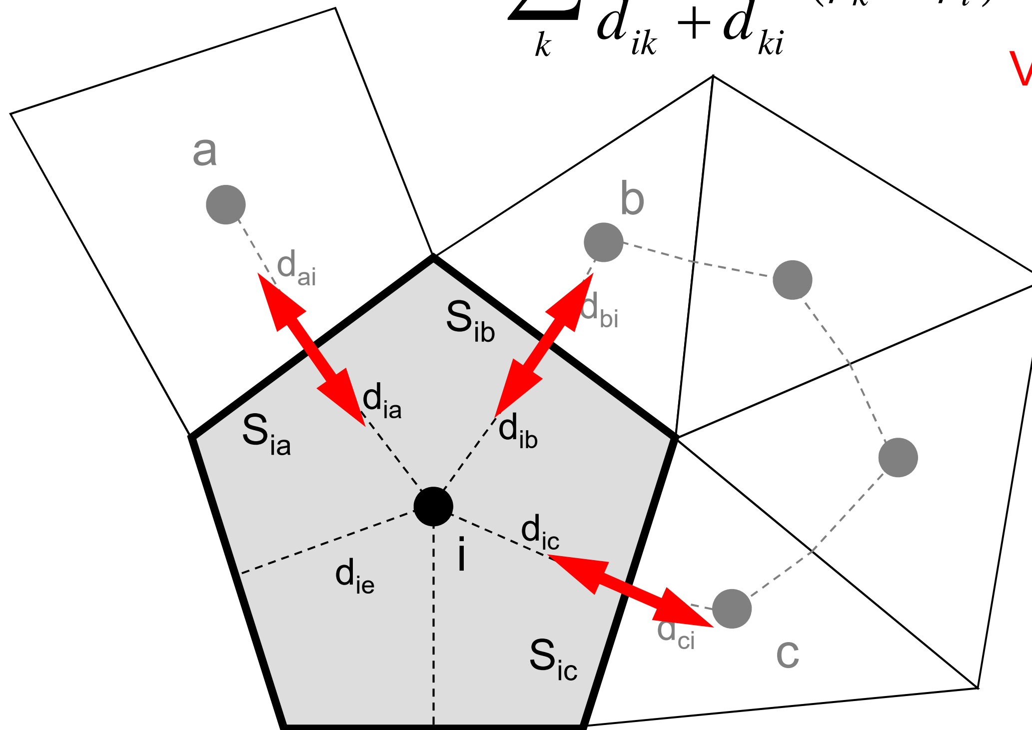
Finite Volume Method (FVM)

Conservation of Fluxes through Surfaces

Diffusion:
Interaction with Neighbors

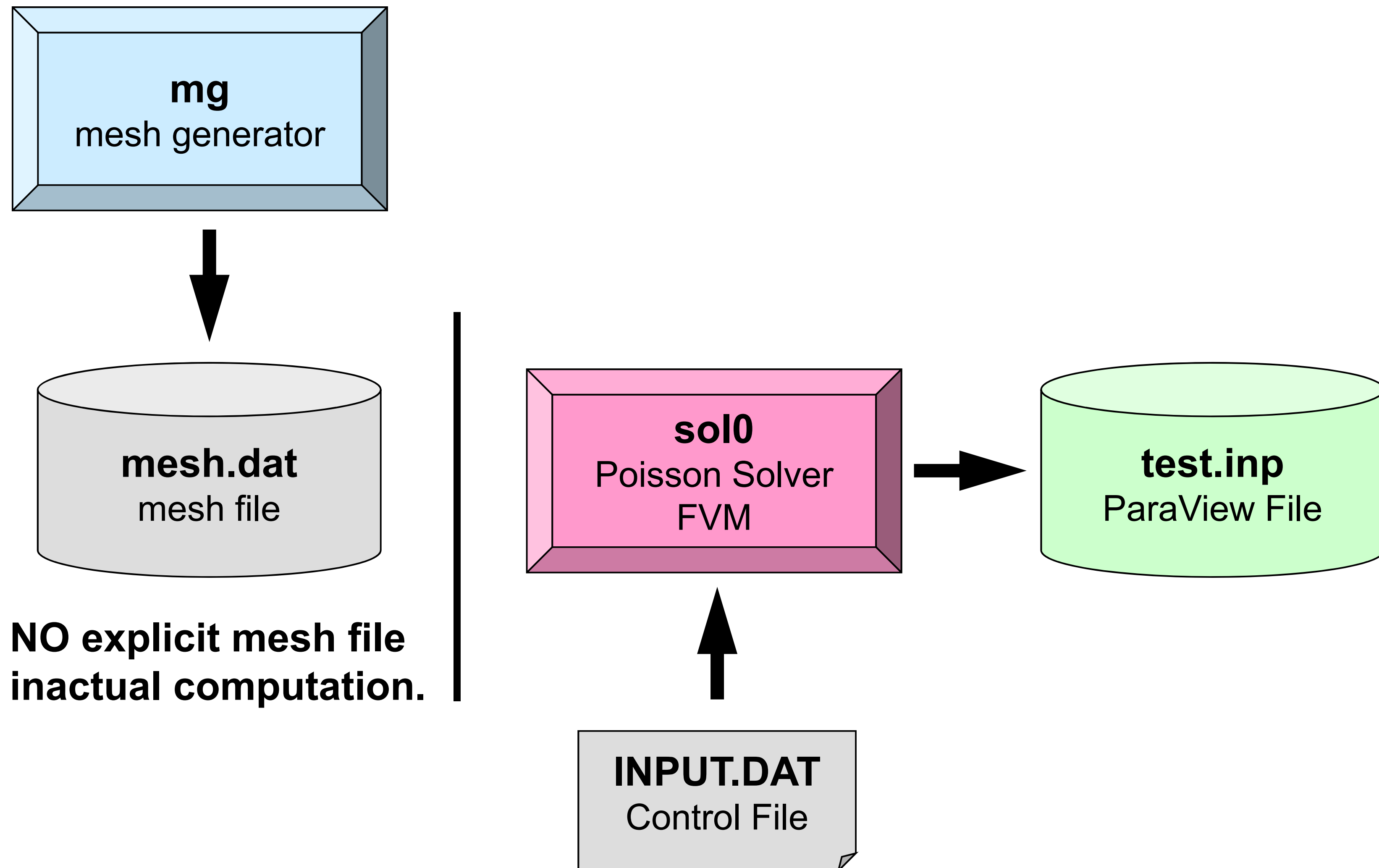
$$\sum_k \frac{S_{ik}}{d_{ik} + d_{ki}} (\phi_k - \phi_i) + V_i \dot{Q}_i = 0$$

Volume Flux



V_i : Volume
S : Surface Area
d_{ij} : Distance between Cell-Center & Surface
Q : Volume Flux

Running the Program: <$P-fvm>/run



Running the Program

Compiling

```
$> cd <$P-L1>/run

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

$> cd ../src-c
$> make
$> ls ../run/sol0
     sol0
```

Mesh Generator: **mg**

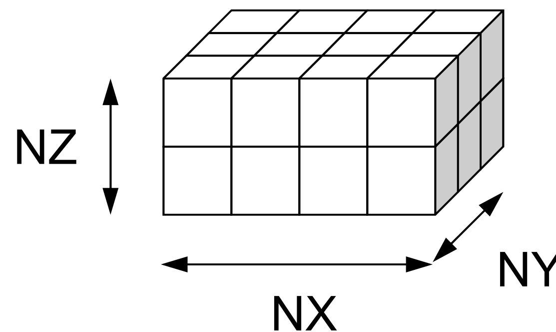
Poisson Solver (FVM): **L1-sol**

Running the Program

Mesh Generation

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

NX, NY, NZ



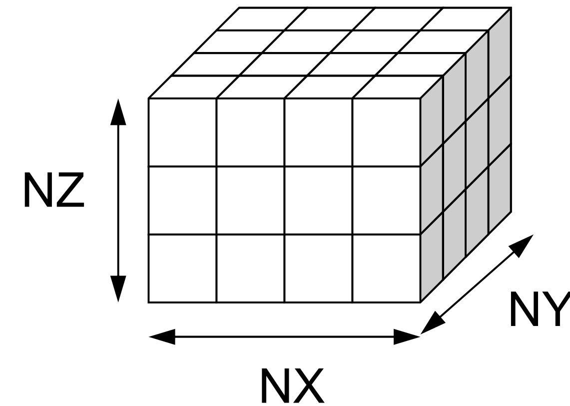
mesh.dat (1/5)

```
    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)

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

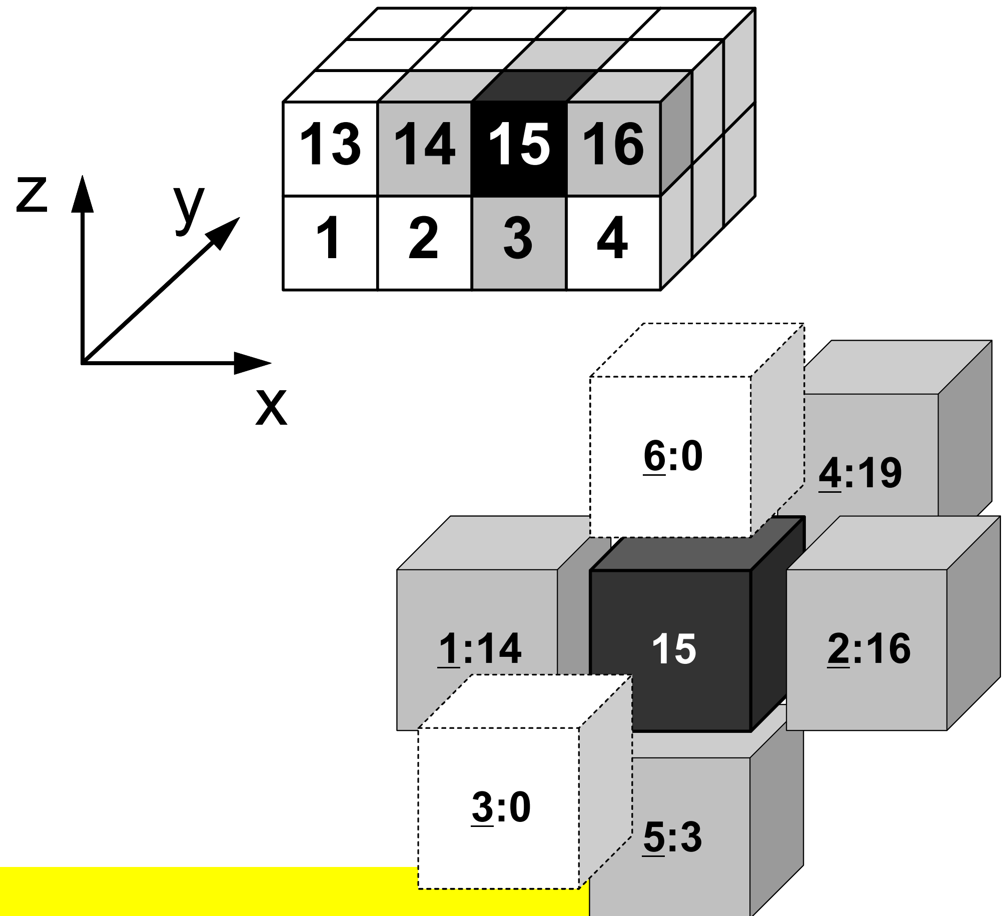
```
   4   3   2
  24
   1   0   2   0   5   0  13   1   1   1
   2   1   3   0   6   0  14   2   1   1
   3   2   4   0   7   0  15   3   1   1
   4   3   0   0   8   0  16   4   1   1
   5   0   6   1   9   0  17   1   2   1
   6   5   7   2  10   0  18   2   2   1
   7   6   8   3  11   0  19   3   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 (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
```

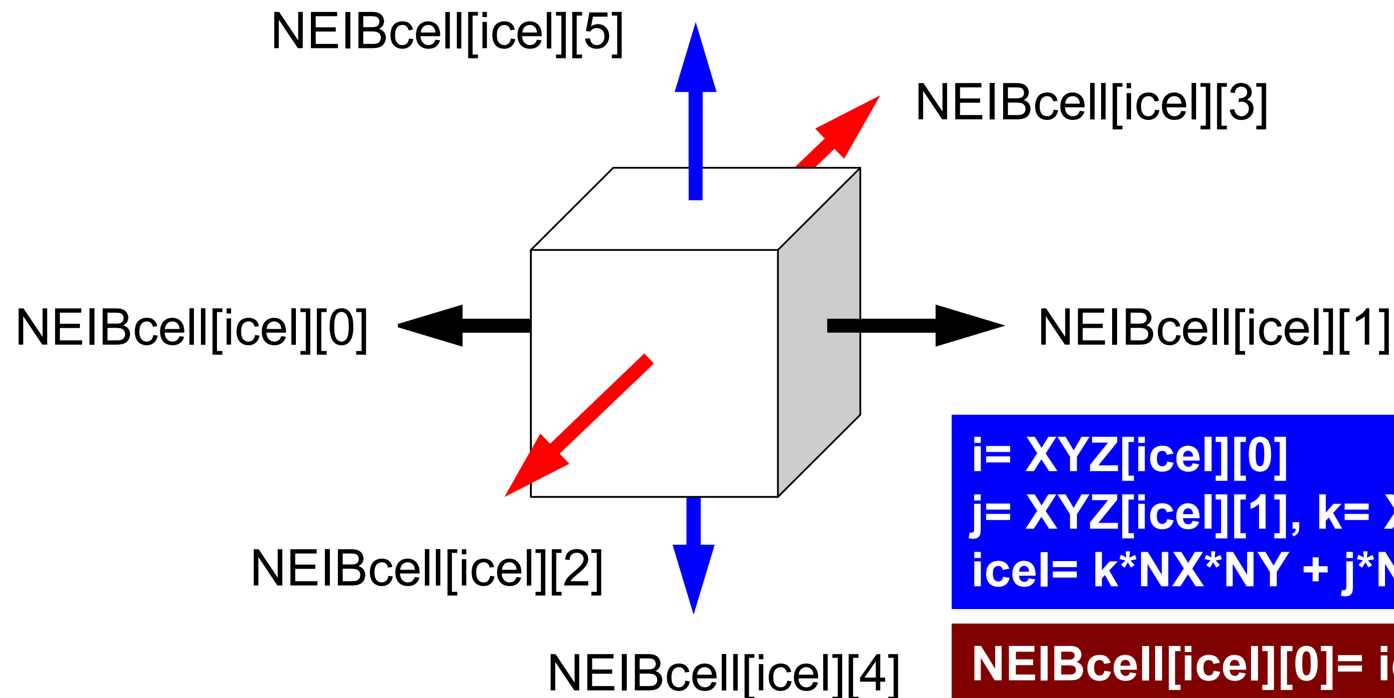
Neighboring Cells: NEIBcell(i,k)




```
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



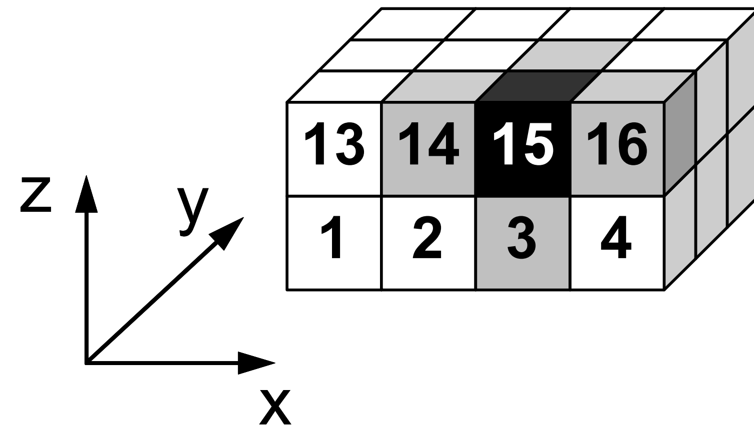
i= XYZ[icel][0]
j= XYZ[icel][1], k= XYZ[icel][2]
icel= k*NX*NY + j*NX + i

NEIBcell[icel][0]= icel – 1 + 1
NEIBcell[icel][1]= icel + 1 + 1
NEIBcell[icel][2]= icel – NX + 1
NEIBcell[icel][3]= icel + NX + 1
NEIBcell[icel][4]= icel – NX*NY + 1
NEIBcell[icel][5]= icel + NX*NY + 1

mesh.dat (5/5)

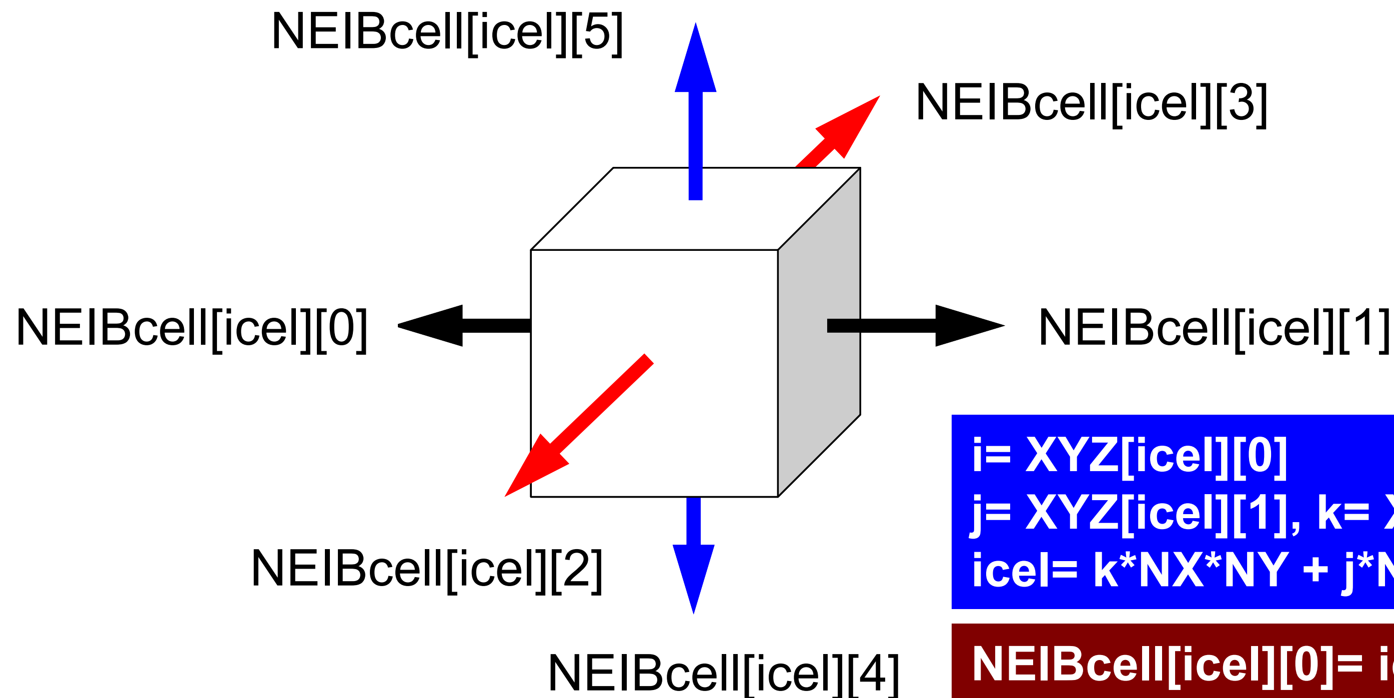
Location in X,Y,Z-directions: XYZ(i,j)

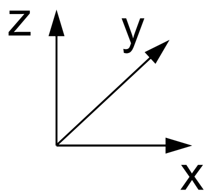
```
   4   3   2
  24
   1   0   2   0   5   0  13   1   1   1
   2   1   3   0   6   0  14   2   1   1
   3   2   4   0   7   0  15   3   1   1
   4   3   0   0   8   0  16   4   1   1
   5   0   6   1   9   0  17   1   2   1
   6   5   7   2  10   0  18   2   2   1
   7   6   8   3  11   0  19   3   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][0]
j= XYZ[icel][1], k= XYZ[icel][2]
icel= k*NX*NY + j*NX + i

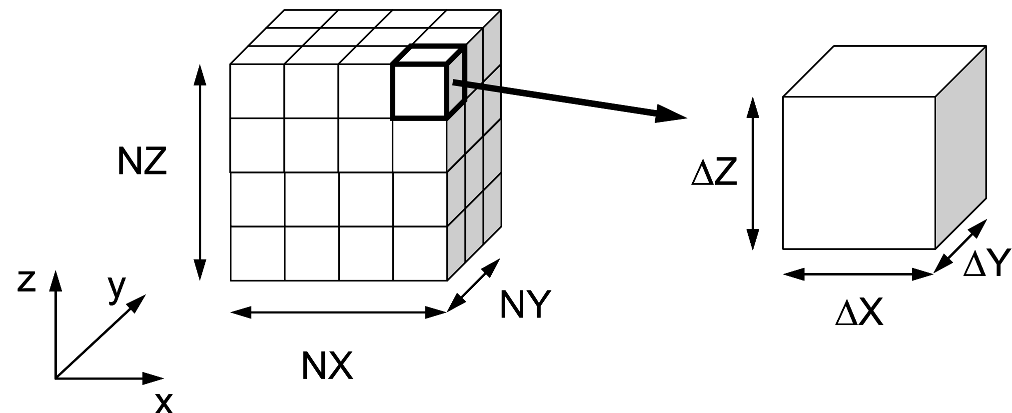
NEIBcell[icel][0]= icel – 1 + 1
NEIBcell[icel][1]= icel + 1 + 1
NEIBcell[icel][2]= icel – NX + 1
NEIBcell[icel][3]= icel + NX + 1
NEIBcell[icel][4]= icel – NX*NY + 1
NEIBcell[icel][5]= icel + NX*NY + 1

Running the Program

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

```
32 32 32                                  NX/NY/NZ
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.
- DX, DY, DZ
  - Size of meshes
- EPSICCG
  - Convergence Criteria for ICCG

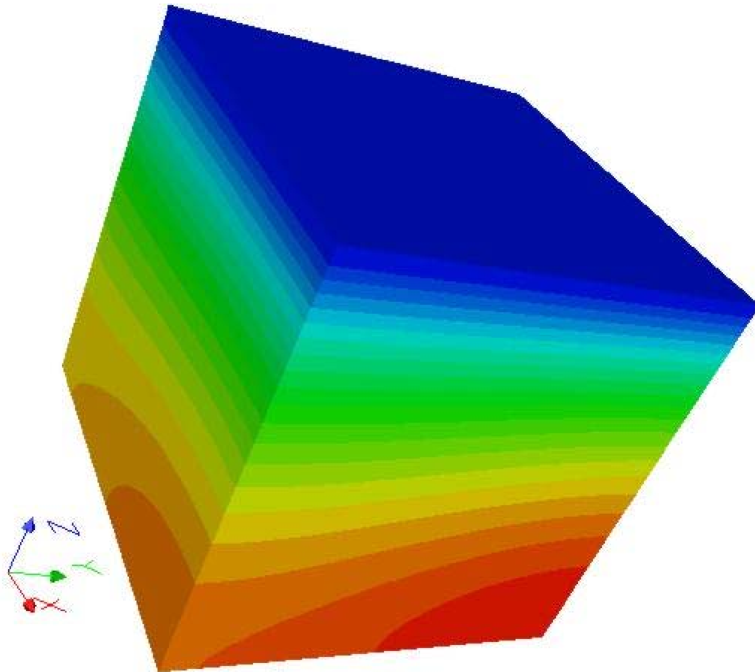


Running the Program

Running, Post Processing by ParaView

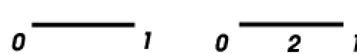
http://nkl.cc.u-tokyo.ac.jp/class/HowtouseParaViewE.pdf

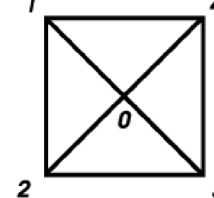
```
$> cd <$P-fvm>/run
$> ./sol0

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

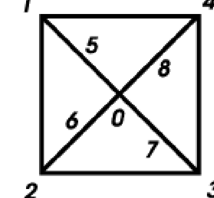


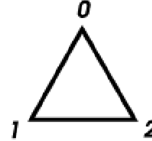
UCD Format (1/2) Unstructured Cell Data

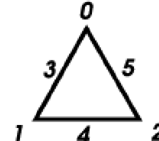
要素の種類	キーワード
点	pt
線	line
三角形	tri
四角形	quad
四面体	tet
角錐	pyr
三角柱	prism
六面体	hex
二次要素	
線2	line2
三角形2	tri2
四角形2	quad2
四面体2	tet2
角錐2	pyr2
三角柱2	prism2
六面体2	hex2

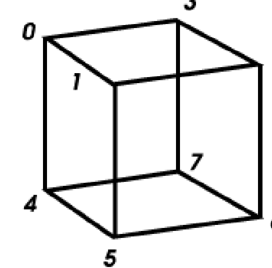


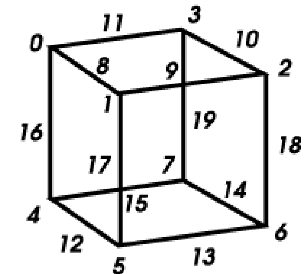


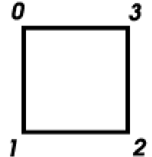


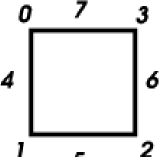


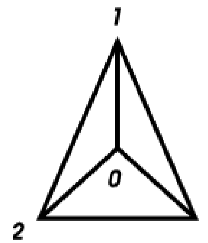


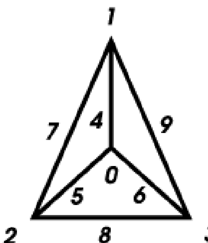


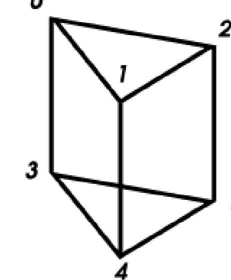


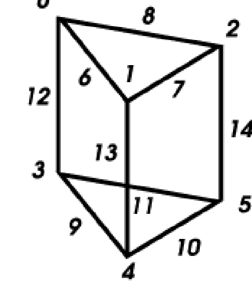












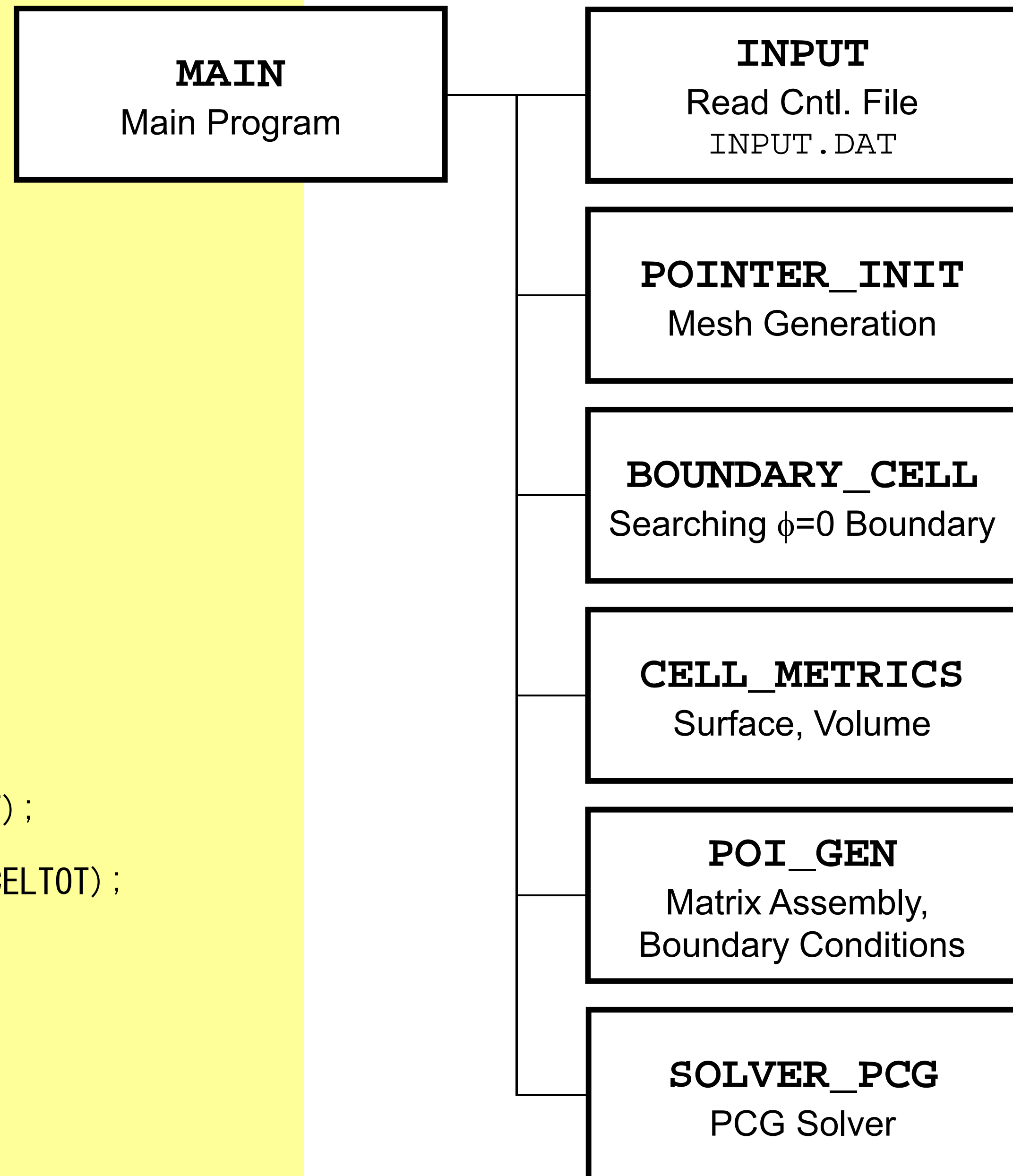
UCD Format (2/2)

- 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
- **CG Solver for Poisson Equations**
  - How to run
    - Data Structure
  - **Program**
    - **Initialization**
    - **Coefficient Matrices**
    - CG

Structure of the Program

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct.h"
#include "pcg.h"
#include "input.h " ...

int
main()
{
  double *WK;
  int NPLU; ISET, ITR, IER; icel, ic0, i;
  double xN, xL, xU; Stime, Etime;

  if(INPUT()) goto error;
  if(POINTER_INIT()) goto error;
  if(BOUNDARY_CELL()) goto error;
  if(CELL_METRICS()) goto error;
  if(POI_GEN()) goto error;

  memset(PHI, 0.0, sizeof(double)*ICELTOT);
  ISET = 0;
  WK = (double *)malloc(sizeof(double)*ICELTOT);

  if(solve_PCG(...)) goto error;

  if(OUTUCD()) goto error;
  return 0;
  error:
  return -1;
}
```



struct.h

```
#ifndef __H_STRUCT
#define __H_STRUCT

#include <omp.h>

int ICELTOT, ICELTOTp, N;
int NX, NY, NZ, NXP1, NYP1, NZP1, IBNODTOT;
int NXc, NYc, NZc;

double DX, DY, DZ, XAREA, YAREA, ZAREA;
double RDX, RDY, RDZ, RDX2, RDY2, RDZ2, R2DX, R2DY, R2DZ;
double *VOLCEL, *VOLNOD, *RVC, *RVN;

int **XYZ, **NEIBcell;

int ZmaxCELtot;
int *BC_INDEX, *BC_NOD;
int *ZmaxCEL;

int **IWKX;
double **FCV;

int my_rank, PETOT, PEsmpTOT;

#endif /* __H_STRUCT */
```

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

N:
Number of modes

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

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

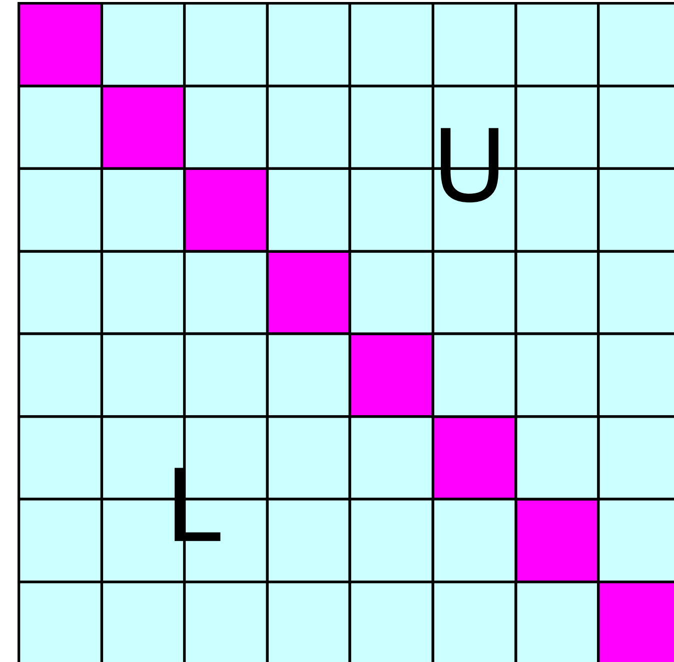
IBNODTOT:
= NXP1 x NYP1

XYZ[ICELTOT][3]:
Location of meshes

NEIBcell[ICELTOT][6]:
Neighboring meshes

pcg.h (1/5)

```
#ifndef __H_PCG
#define __H_PCG
        static int N2 = 256;
        int NLUmax, NCOLORtot, NCOLORk, NLU;
        int METHOD, ORDER_METHOD;
        double EPSICCG;

        double *D, *PHI, *BFORCE;
        double *AMAT;

        int *INLU, *COLORindex, *indexLU;
        int *OLDtoNEW, *NEWtoOLD;
        int **IALU, *itemLU, NPLU;
#endif /* __H_PCG */
```



- Sparse Matrix
- Only non-zero off-diagonal components (CRS)
- Diagonal/Off-Diagonal components are stored separately

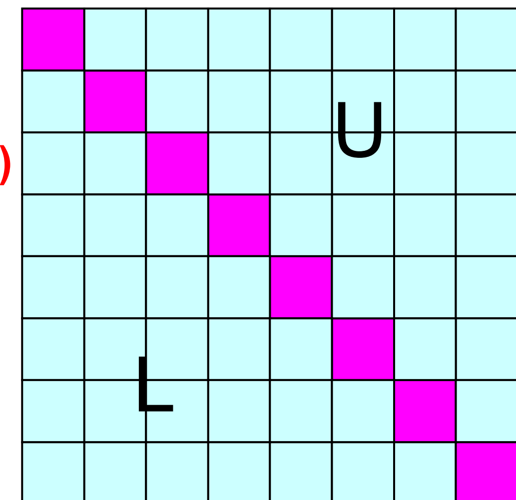
pcg.h (2/5)

```
#ifndef __H_PCG
#define __H_PCG
        static int N2 = 256;
        int NLUmax, NCOLORtot, NCOLORk, NLU;
        int METHOD, ORDER_METHOD;
        double EPSICCG;

        double *D, *PHI, *BFORCE;
        double *AMAT;

        int *INLU, *COLORindex, *indexLU;
        int *OLDtoNEW, *NEWtoOLD;
        int **IALU, *itemLU, NPLU;
#endif /* __H_PCG */
```

Auxiliary Arrays

Off-Diagonal Components (Column ID)
`IALU[i][icou]`

`INLU[ICELTOT]`	# Non-zero off-diag. components
`IALU[ICELTOT][NLU]`	**Col. ID: non-zero off-diag. comp.**
`NLU`	**Max # of L/U non-zero off-diag. comp.s (=6)**
`indexLU[ICELTOT+1]`	# Non-zero off-diag. comp. (CRS)
`NPLU`	Total # of L/U non-zero off-diag. comp.
`itemLU[NPLU]`	Col. ID: non-zero off-diag. comp. (CRS)



pcg.h (3/5)

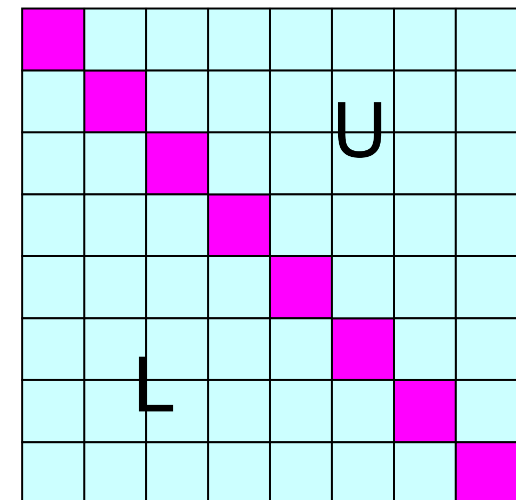
```
#ifndef __H_PCG
#define __H_PCG
        static int N2 = 256;
        int NLUmax, NCOLORtot, NCOLORk, NLU;
        int METHOD, ORDER_METHOD;
        double EPSICCG;

        double *D, *PHI, *BFORCE;
        double *AMAT;

        int *INLU, *COLORindex, *indexLU;
        int *OLDtoNEW, *NEWtoOLD;
        int **IALU, *itemLU, NPLU;
#endif /* __H_PCG */
```

Auxiliary Arrays

Off-Diagonal Components (Column ID)

- `IALU[i][icou]`
- `INLU[i]`: Number@each row

`INLU[ICELTOT]`	**# Non-zero off-diag. components**
`IALU[ICELTOT][NLU]`	Col. ID: non-zero off-diag. comp.
`NLU`	Max # of L/U non-zero off-diag. comp.s (=6)
`indexLU[ICELTOT+1]`	# Non-zero off-diag. comp. (CRS)
`NPLU`	Total # of L/U non-zero off-diag. comp.
`itemLU[NPLU]`	Col. ID: non-zero off-diag. comp. (CRS)



pcg.h (4/5)

```
#ifndef __H_PCG
#define __H_PCG
        static int N2 = 256;
        int NLUmax, NCOLORtot, NCOLORk, NLU;
        int METHOD, ORDER_METHOD;
        double EPSICCG;

        double *D, *PHI, *BFORCE;
        double *AMAT;

        int *INLU, *COLORindex, *indexLU;
        int *OLDtoNEW, *NEWtoOLD;
        int **IALU, *itemLU, NPLU;
#endif /* __H_PCG */
```

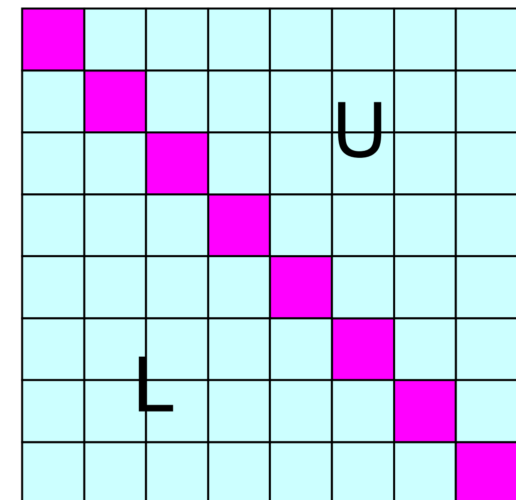
Auxiliary Arrays

Off-Diagonal Components (Column ID)

`IALU[i][icou]`

`INLU[i]`: Number@each row

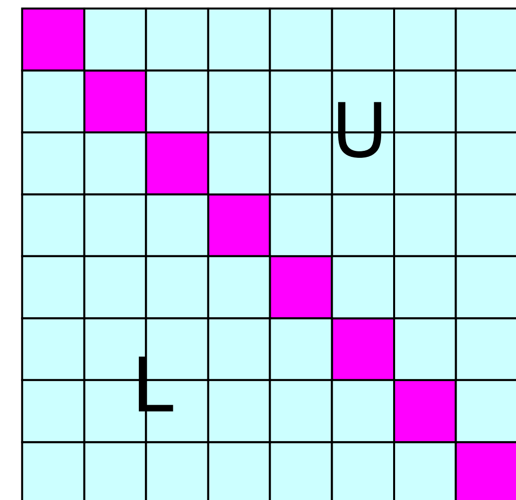
INLU[ICELTOT]	# Non-zero off-diag. components
IALU[ICELTOT][NLU]	Col. ID: non-zero off-diag. comp.
NLU	Max # of L/U non-zero off-diag. comp.s (=6)
indexLU[ICELTOT+1]	**# Non-zero off-diag. comp. (CRS)**
NPLU	**Total # of L/U non-zero off-diag. comp.**
itemLU[NPLU]	**Col. ID: non-zero off-diag. comp. (CRS)**



pcg.h (5/5)

```
#ifndef __H_PCG
#define __H_PCG
        static int N2 = 256;
        int NLUmax, NCOLORtot, NCOLORk, NLU;
        int METHOD, ORDER_METHOD;
        double EPSICCG;

        double *D, *PHI, *BFORCE;
        double *AMAT;

        int *INLU, *COLORindex, *indexLU;
        int *OLDtoNEW, *NEWtoOLD;
        int **IALU, *itemLU, NPLU;
#endif /* __H_PCG */
```

EPSICCG	Convergence criteria for ICCG
D [ICELTOT]	Diagonal components of the matrix
PHI [ICLETOT]	Unknown vector
BFORCE[ICELTOT]	RHS vector
AMAT[NPLU]	Non-zero off-diagonal L/U components of the matrix (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
indexLU[N+1]	**I**	Number of L/U non-zero off-diag. comp. (CRS)
NPLU	**I**	Total number of L/U non-zero off-diag. comp. (CRS)
itemLU[NPLU]	**I**	Column ID of L/U non-zero off-diag. comp. (CRS)
AMAT[NPLU]	**R**	L/U non-zero off-diag. comp. (CRS)

Variables/Arrays for Matrix Auxiliary Arrays

Name	Type	Content
NLU	I	MAX. number of Lower/Upper non-zero off-diag. comp. for each mesh/row (=6 in this case)
INLU[N]	I	Number of L/U non-zero off-diag. comp.
IALU[N][NLU]	I	Column ID of L/Unon-zero off-diag. comp.

Why Auxiliary Arrays ?

① NPLU is unknown before computation.
② CRS is not suitable for reordering.

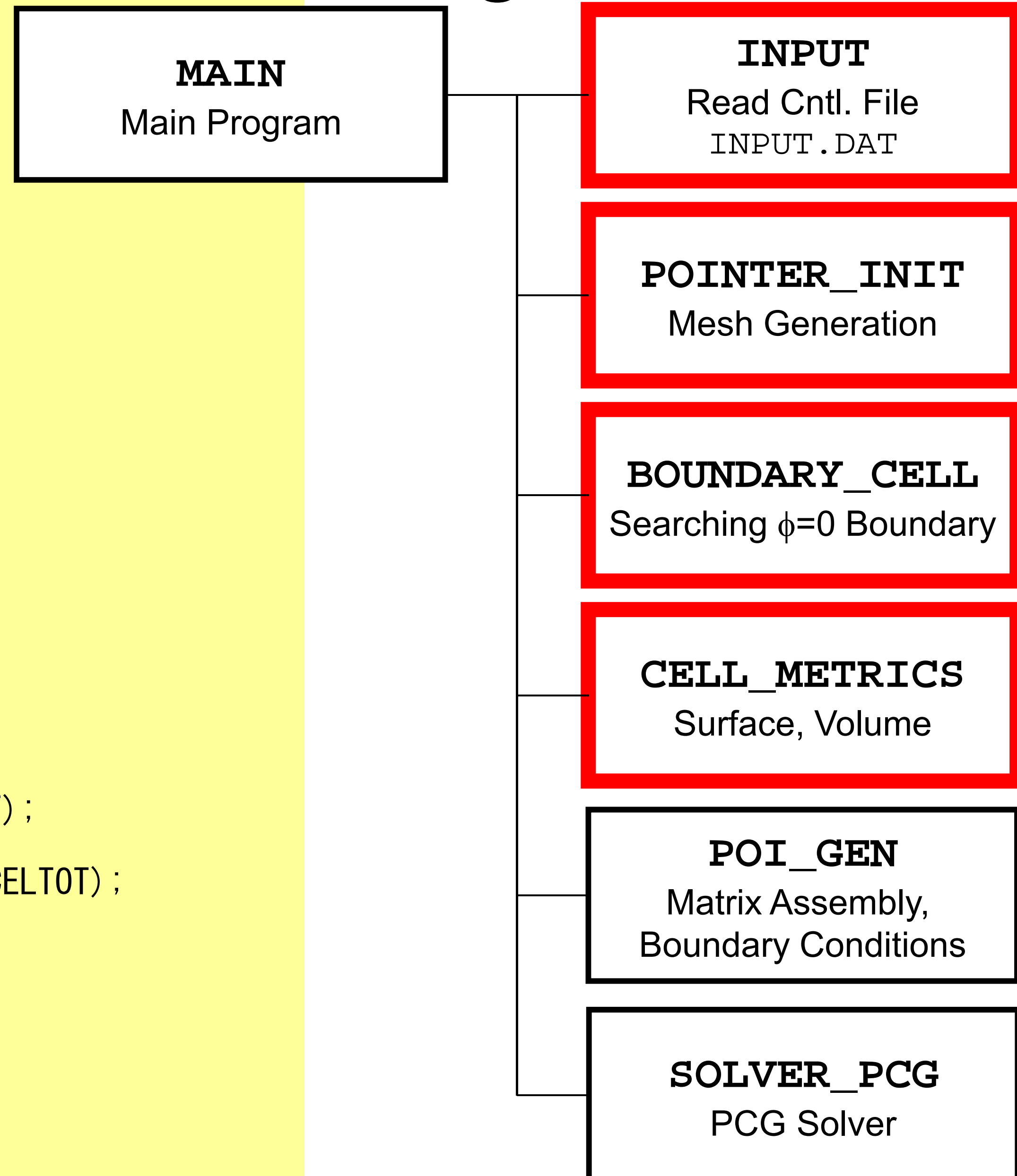
Mat-Vec Multiplication: {q}=[A]{p}

```
for (i=0; i<N; i++) {
    q[i]= D[i] * p[i];
    for (j=indexLU[i]; j<indexLU[i+1]; j++) {
        q[i] += AMAT[j] * p[itemLU[j]-1];
    }
}
```

In this program numbering in itemLU starts from “1” (not 0)

Structure of the Program

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct.h"
#include "pcg.h"
#include "input.h " ...

int
main()
{
  double *WK;
  int NPLU; ISET, ITR, IER; icel, ic0, i;
  double xN, xL, xU; Stime, Etime;

  if(INPUT()) goto error;
  if(POINTER_INIT()) goto error;
  if(BOUNDARY_CELL()) goto error;
  if(CELL_METRICS()) goto error;
  if(POI_GEN()) goto error;

  memset(PHI, 0.0, sizeof(double)*ICELTOT);
  ISET = 0;
  WK = (double *)malloc(sizeof(double)*ICELTOT);

  if(solve_PCG(...)) goto error;

  if(OUTUCD()) goto error;
  return 0;
  error:
  return -1;
}
```



input: reading “INPUT.DAT”

```
#include <stdio.h>; <stdlib.h>; <string.h>; <errno.h>
#include "struct_ext.h "; "pcg_ext.h "; "input.h"

extern int
INPUT(void)
{
#define BUF_SIZE 1024
        char line[BUF_SIZE];
        char CNTFIL[81];
        double OMEGA;
        FILE *fp11;

        if((fp11 = fopen("INPUT.DAT", "r")) == NULL) {
            fprintf(stderr, "Error: %s¥n", strerror(errno));
            return -1;
        }
        fgets(line, BUF_SIZE, fp11); sscanf(line, "%d%d%d", &NX, &NY, &NZ);
        fgets(line, BUF_SIZE, fp11); sscanf(line, "%le%le%le", &DX, &DY, &DZ);
        fgets(line, BUF_SIZE, fp11); sscanf(line, "%le", &EPSICCG);
        fgets(line, BUF_SIZE, fp11);

        fclose(fp11);
        return 0;
}
```

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

pointer_init (1/3): “mesh.dat”

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct_ext.h"
#include "pcg_ext.h"
#include "pointer_init.h"
#include "allocate.h"

extern int
POINTER_INIT(void)
{

        int icel, ipe, i, j, k;

/*
 * INIT.
 */

  ICELTOT = NX * NY * NZ;

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


  NEIBcell =
    (int **)allocate_matrix(sizeof(int),ICELTOT,6);

  XYZ      =
    (int **)allocate_matrix(sizeof(int),ICELTOT,3);
```

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]:

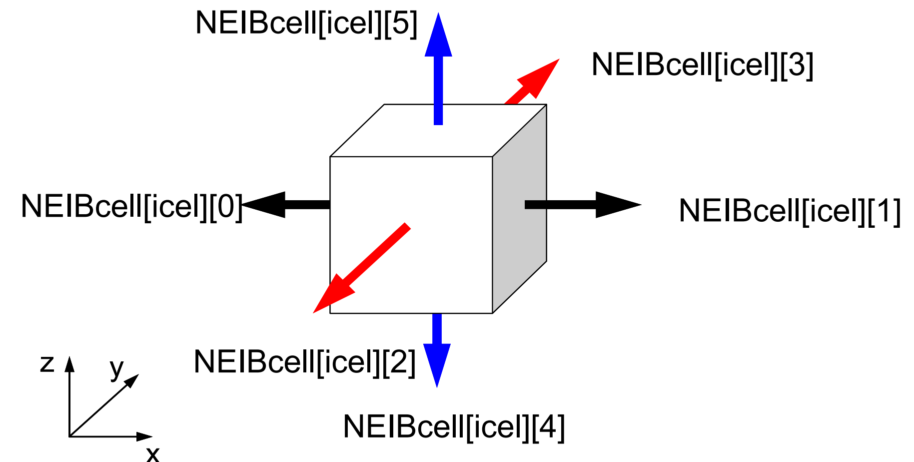
Location of meshes

NEIBcell[ICELTOT][6]:

Neighboring meshesc

pointer_init (2/3): “mesh.dat”

```
for(k=0; k<NZ; k++) {
    for(j=0; j<NY; j++) {
        for(i=0; i<NX; i++) {
            icel = k * NX * NY + j * NX + i;
            NEIBcell[icel][0] = icel - 1       + 1;
            NEIBcell[icel][1] = icel + 1       + 1;
            NEIBcell[icel][2] = icel - NX      + 1;
            NEIBcell[icel][3] = icel + NX      + 1;
            NEIBcell[icel][4] = icel - NX * NY + 1;
            NEIBcell[icel][5] = icel + NX * NY + 1;
            if(i == 0)    NEIBcell[icel][0] = 0;
            if(i == NX-1) NEIBcell[icel][1] = 0;
            if(j == 0)    NEIBcell[icel][2] = 0;
            if(j == NY-1) NEIBcell[icel][3] = 0;
            if(k == 0)    NEIBcell[icel][4] = 0;
            if(k == NZ-1) NEIBcell[icel][5] = 0;

            XYZ[icel][0] = i + 1;
            XYZ[icel][1] = j + 1;
            XYZ[icel][2] = k + 1;
        }
    }
}
```



i= XYZ[icel][0]
j= XYZ[icel][1], k= XYZ[icel][2]
icel= k*NX*NY + j*NX + i

“icel” starts at 0

12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3

“NEIBcell” starts at 1

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

NEIBcell[icel][0]= icel – 1 + 1
NEIBcell[icel][1]= icel + 1 + 1
NEIBcell[icel][2]= icel – NX + 1
NEIBcell[icel][3]= icel + NX + 1
NEIBcell[icel][4]= icel – NX*NY + 1
NEIBcell[icel][5]= icel + NX*NY + 1

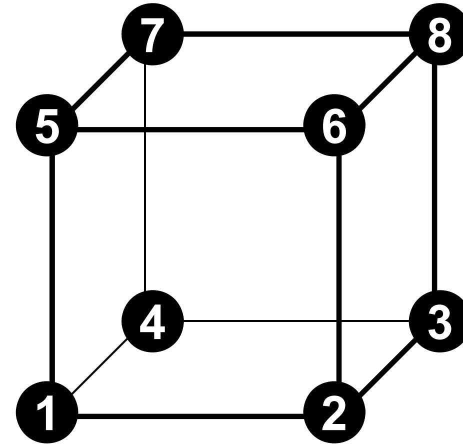
pointer_init (3/3): “mesh.dat”

```
        if(DX <= 0.0) {
                DX = 1.0 / (double)NX;
                DY = 1.0 / (double)NY;
                DZ = 1.0 / (double)NZ;
        }

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

        IBNODTOT = NXP1 * NYP1;
        N        = NXP1 * NYP1 * NZP1;

        return 0;
}
```

if DX is no larger than 0.0

pointer_init (3/3): “mesh.dat”

```
        if(DX <= 0.0) {
                DX = 1.0 / (double)NX;
                DY = 1.0 / (double)NY;
                DZ = 1.0 / (double)NZ;
        }

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

        IBNODTOT = NXP1 * NYP1;
        N        = NXP1 * NYP1 * NZP1;

        return 0;
}
```



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

IBNODTOT:
= NXP1 x NYP1

N:
Number of modes meshes (for visualization)

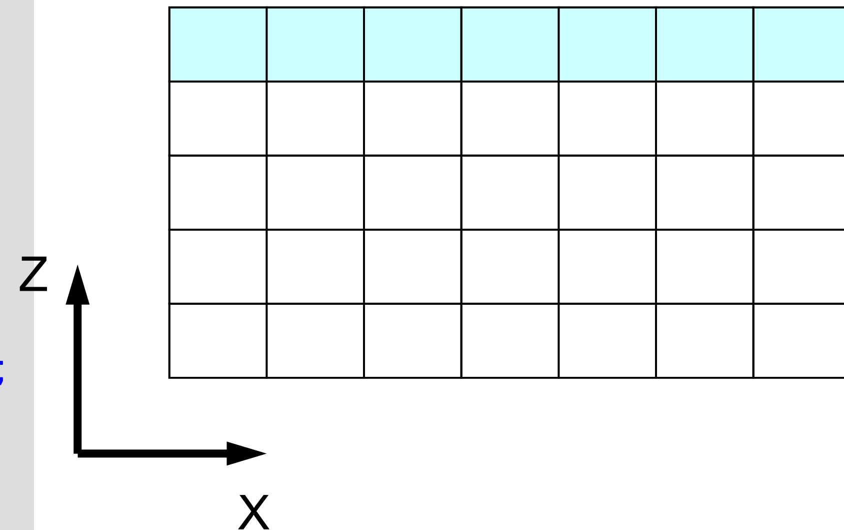
boundary_cell

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct_ext.h"
#include "boundary_cell.h"
#include "allocate.h"

extern int
BOUNDARY_CELL(void)
{
 int IFACTOT;
 int icou, icel, i, j, k;

 IFACTOT = NX * NY;
 ZmaxCELtot = IFACTOT;

 ZmaxCEL =
    (int *)allocate_vector(sizeof(int),ZmaxCELtot);

 icou = 0;
 k    = NZ - 1;

 for(j=0; j<NY; j++) {
     for(i=0; i<NX; i++) {
         icel = k*IFACTOT + j*NX + i+1;
         ZmaxCEL[icou] = icel;
         icou++;
     }
 }

 return 0;
}
```

Meshes @ $Z=Z_{max}$

Number: ZmaxCELtot

Mesh ID: ZmaxCEL[:]



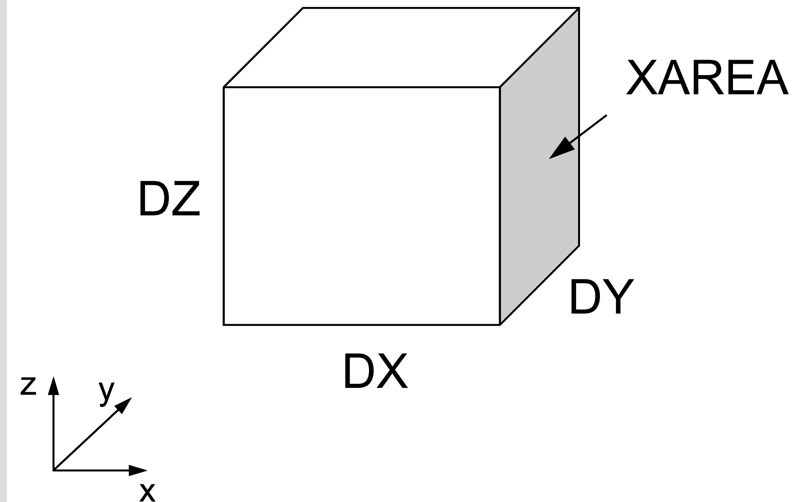
allocate.c

```
/*************************
  allocate vector
*************************/

void* allocate_vector(int size,int m)
{
  void *a;
  if ( ( a=(void * )malloc( m * size ) ) == NULL ) {
     fprintf(stdout,"Error:Memory does not enough! in vector ¥n");
     exit(1);
  }
  return a;
}
```

cell_metrics

Parameters for Computations

```
#include <stdio.h> ...

extern int
CELL_METRICS(void)
{       double V0, RV0;
        int i;
VOLCEL =
(double*)allocate_vector(sizeof(double),ICELTOT);
RVC    =
(double*)allocate_vector(sizeof(double),ICELTOT);

XAREA = DY * DZ;
YAREA = DZ * DX;
ZAREA = DX * DY;

RDX = 1.0 / DX;
RDY = 1.0 / DY;
RDZ = 1.0 / DZ;

RDX2 = 1.0 / (pow(DX, 2.0));
RDY2 = 1.0 / (pow(DY, 2.0));
RDZ2 = 1.0 / (pow(DZ, 2.0));
R2DX = 1.0 / (0.5 * DX);
R2DY = 1.0 / (0.5 * DY);
R2DZ = 1.0 / (0.5 * DZ);

V0  = DX * DY * DZ;
RV0 = 1.0 / V0;

for(i=0; i<ICELTOT; i++) {
    VOLCEL[i] = V0;
    RVC[i]    = RV0;
}
return 0; }
```



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

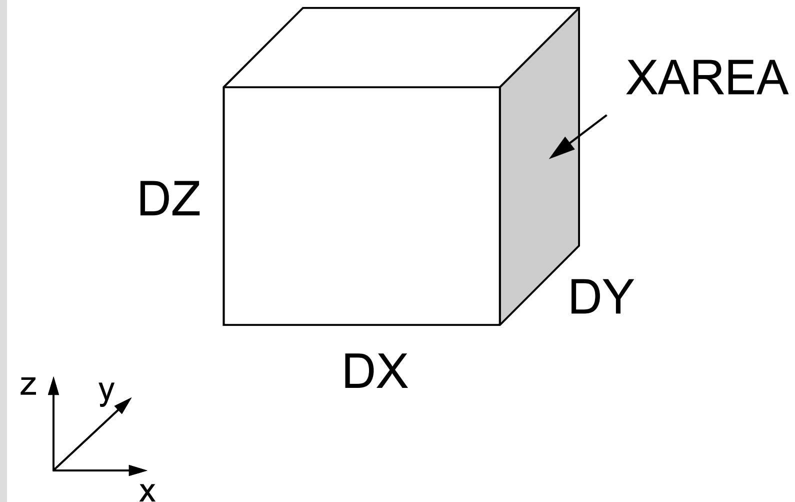
$$ZAREA = \Delta X \times \Delta Y$$

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

cell_metrics

Parameters for Computations

```
#include <stdio.h> ...

extern int
CELL_METRICS(void)
{       double V0, RV0;
        int i;
VOLCEL =
(double*)allocate_vector(sizeof(double),ICELTOT);
RVC    =
(double*)allocate_vector(sizeof(double),ICELTOT);

XAREA = DY * DZ;
YAREA = DZ * DX;
ZAREA = DX * DY;

RDX = 1.0 / DX;
RDY = 1.0 / DY;
RDZ = 1.0 / DZ;

RDX2 = 1.0 / (pow(DX, 2.0));
RDY2 = 1.0 / (pow(DY, 2.0));
RDZ2 = 1.0 / (pow(DZ, 2.0));
R2DX = 1.0 / (0.5 * DX);
R2DY = 1.0 / (0.5 * DY);
R2DZ = 1.0 / (0.5 * DZ);

V0  = DX * DY * DZ;
RV0 = 1.0 / V0;

for(i=0; i<ICELTOT; i++) {
    VOLCEL[i] = V0;
    RVC[i]    = RV0;
}
return 0; }
```



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

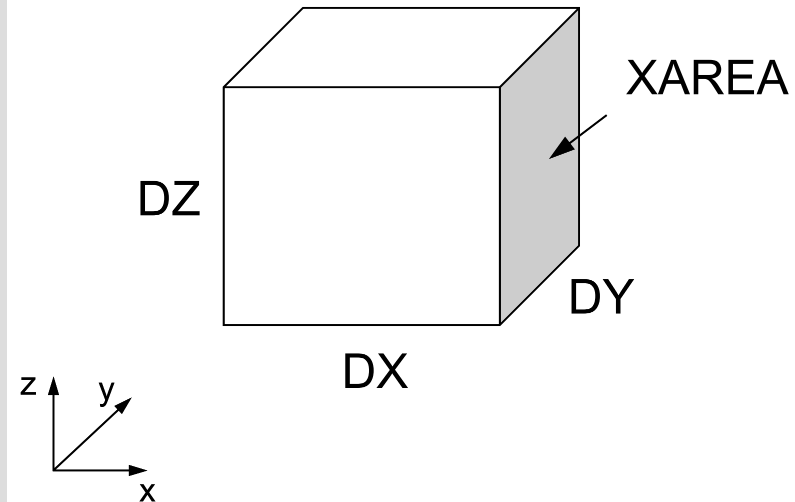
$$R2DX = \frac{1}{0.5 \times \Delta X}, \quad R2DY = \frac{1}{0.5 \times \Delta Y},$$

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

cell_metrics

Parameters for Computations

```
#include <stdio.h> ...

extern int
CELL_METRICS(void)
{       double V0, RV0;
        int i;
VOLCEL =
(double*)allocate_vector(sizeof(double),ICELTOT);
RVC    =
(double*)allocate_vector(sizeof(double),ICELTOT);

XAREA = DY * DZ;
YAREA = DZ * DX;
ZAREA = DX * DY;

RDX = 1.0 / DX;
RDY = 1.0 / DY;
RDZ = 1.0 / DZ;

RDX2 = 1.0 / (pow(DX, 2.0));
RDY2 = 1.0 / (pow(DY, 2.0));
RDZ2 = 1.0 / (pow(DZ, 2.0));
R2DX = 1.0 / (0.5 * DX);
R2DY = 1.0 / (0.5 * DY);
R2DZ = 1.0 / (0.5 * DZ);

V0  = DX * DY * DZ;
RV0 = 1.0 / V0;

for(i=0; i<ICELTOT; i++) {
    VOLCEL[i] = V0;
    RVC[i]    = RV0;
}
return 0; }
```

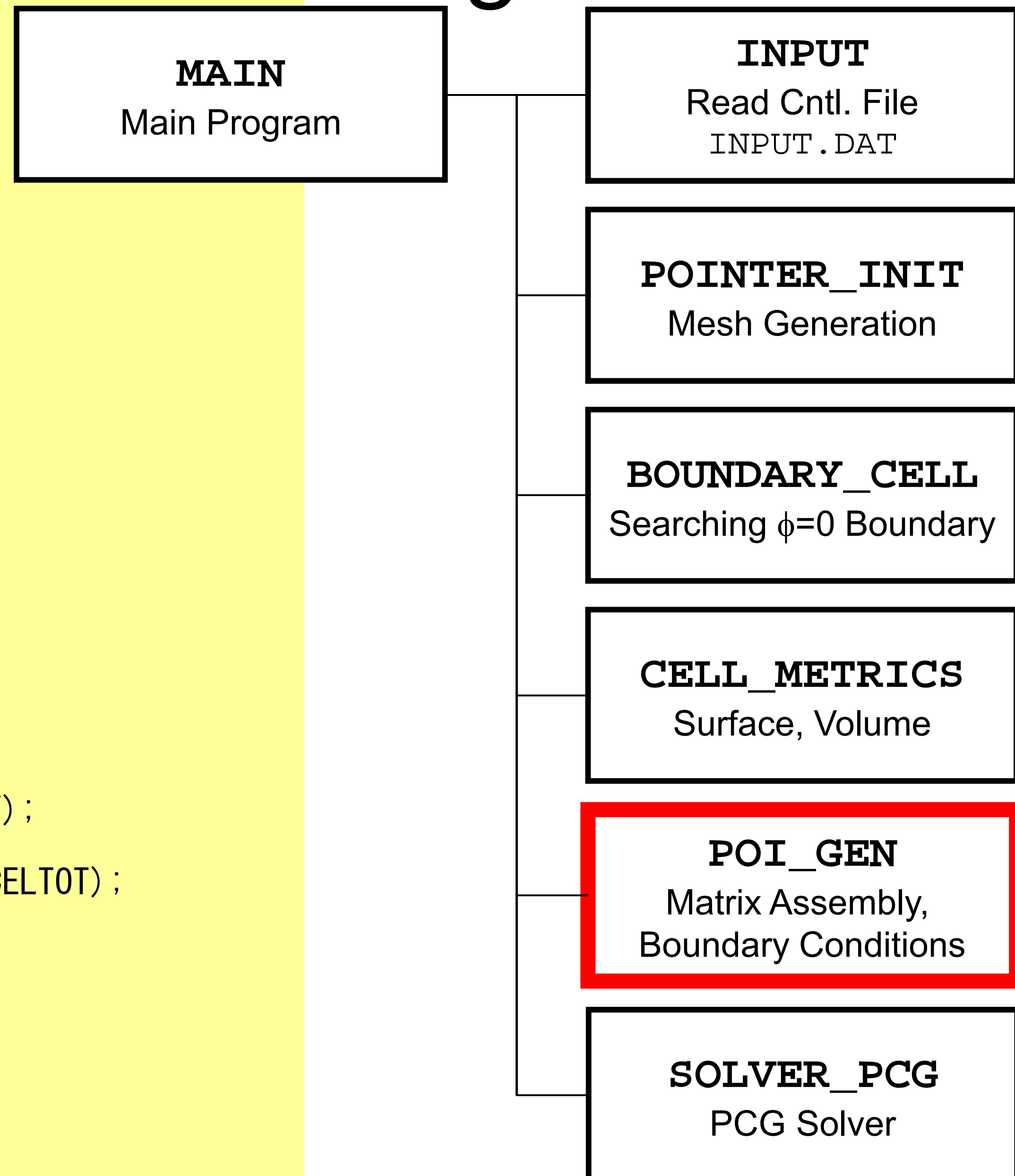


$$VOLCEL = V0 = \Delta X \times \Delta Y \times \Delta Z$$

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

Structure of the Program

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct.h"
#include "pcg.h"
#include "input.h " ...

int
main()
{
  double *WK;
  int NPLU; ISET, ITR, IER; icel, ic0, i;
  double xN, xL, xU; Stime, Etime;

  if(INPUT()) goto error;
  if(POINTER_INIT()) goto error;
  if(BOUNDARY_CELL()) goto error;
  if(CELL_METRICS()) goto error;
  if(POI_GEN()) goto error;

  memset(PHI, 0.0, sizeof(double)*ICELTOT);
  ISET = 0;
  WK = (double *)malloc(sizeof(double)*ICELTOT);

  if(solve_PCG(...)) goto error;

  if(OUTUCD()) goto error;
  return 0;
  error:
  return -1;
}
```



poi_gen (1/7)

```
#include "allocate.h"
extern int
POI_GEN(void)
{ int nn;
  int ic0, icN1, icN2, icN3, icN4, icN5, icN6;
  int i, j, k, ib, ic, ip, icel, icou, icol, icouG;
  int ii, jj, kk, nn1, num, nr, j0, j1;
  double coef, VOL0, S1t, E1t;
  int isL, ieL, isU, ieU;
  NL=6; NU= 6;
  IALU = (int **)allocate_matrix(sizeof(int),ICELTOT,NL);
  BFORCE = (double *)allocate_vector(sizeof(double),ICELTOT);
  D      = (double *)allocate_vector(sizeof(double),ICELTOT);
  PHI    = (double *)allocate_vector(sizeof(double),ICELTOT);
  INLU = (int *)allocate_vector(sizeof(int),ICELTOT);

  for (i = 0; i <ICELTOT ; i++) {
       BFORCE[i]=0.0;
       D[i]  =0.0; PHI[i]=0.0;
       INLU[i] = 0;
       for(j=0;j<6;j++){
           IALU[i][j]=0;
       }
  }
  for (i = 0; i <=ICELTOT ; i++) {
       indexLU[i] = 0;
  }
```

allocate.c

```
/**************************
  allocate matrix
**************************/
void** allocate_matrix(int size,int m,int n)
{
  void **aa;
  int i;
  if ( ( aa=(void ** )malloc( m * sizeof(void*) ) ) == NULL ) {
     fprintf(stdout,"Error:Memory does not enough! aa in matrix ¥n");
     exit(1);
  }
  if ( ( aa[0]=(void * )malloc( m * n * size ) ) == NULL ) {
     fprintf(stdout,"Error:Memory does not enough! in matrix ¥n");
     exit(1);
  }
         for(i=1;i<m;i++) aa[i]=(char*)aa[i-1]+size*n;
  return aa;
}
```

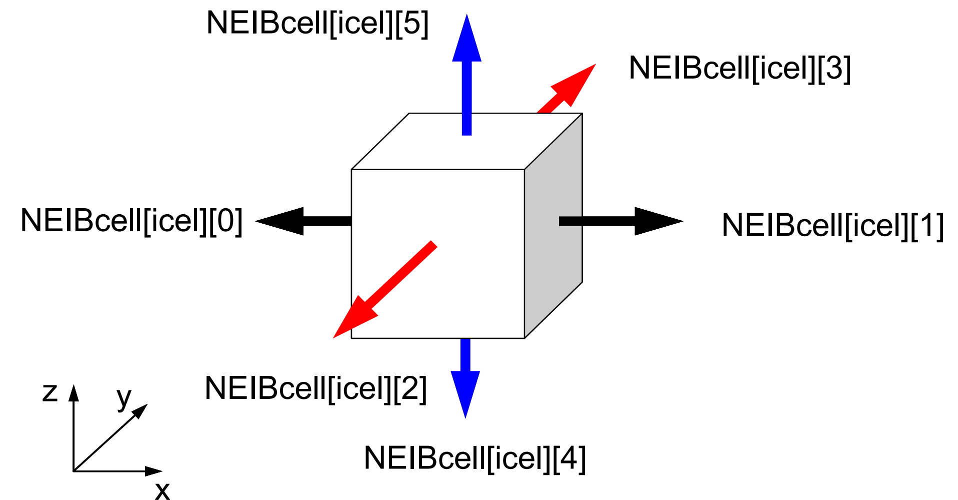
Variables/Arrays for Matrix

Name	Type	Content
D[N]	**R**	Diagonal components of the matrix (N= ICELTOT)
BFORCE[N]	**R**	RHS vector
PHI[N]	**R**	Unknown vector
indexLU[N+1]	**I**	Number of L/U non-zero off-diag. comp. (CRS)
NPLU	**I**	Total number of L/U non-zero off-diag. comp. (CRS)
itemLU[NPLU]	**I**	Column ID of L/U non-zero off-diag. comp. (CRS)
AMAT[NPLU]	**R**	L/U non-zero off-diag. comp. (CRS)

Name	Type	Content
NLU	**I**	MAX. number of Lower/Upper non-zero off-diag. comp. for each mesh/row (=6 in this case)
INLU[N]	**I**	Number of L/U non-zero off-diag. comp.
IALU[N][NLU]	**I**	Column ID of L/Unon-zero off-diag. comp.

poi_gen (2/7)

```
for(icel=0; icel<ICELTOT; icel++) {

    icN1 = NEIBcell[icel][0];
    icN2 = NEIBcell[icel][1];
    icN3 = NEIBcell[icel][2];
    icN4 = NEIBcell[icel][3];
    icN5 = NEIBcell[icel][4];
    icN6 = NEIBcell[icel][5];

    if(icN5 != 0) {
       icou = INLU[icel] + 1;
       IALU[icel][icou-1] = icN5;
       INLU[icel]         = icou;
     }

     if(icN3 != 0) {
       icou = INLU[icel] + 1;
       IALU[icel][icou-1] = icN3;
       INLU[icel]         = icou;
     }

     if(icN1 != 0) {
       icou = INLU[icel] + 1;
       IALU[icel][icou-1] = icN1;
       INLU[icel]         = icou;
     }
```



Lower Triangular Part

NEIBcell[icel][4]= icel – NX*NY + 1
NEIBcell[icel][2]= icel – NX + 1
NEIBcell[icel][0]= icel – 1 + 1

“icel” starts at 0

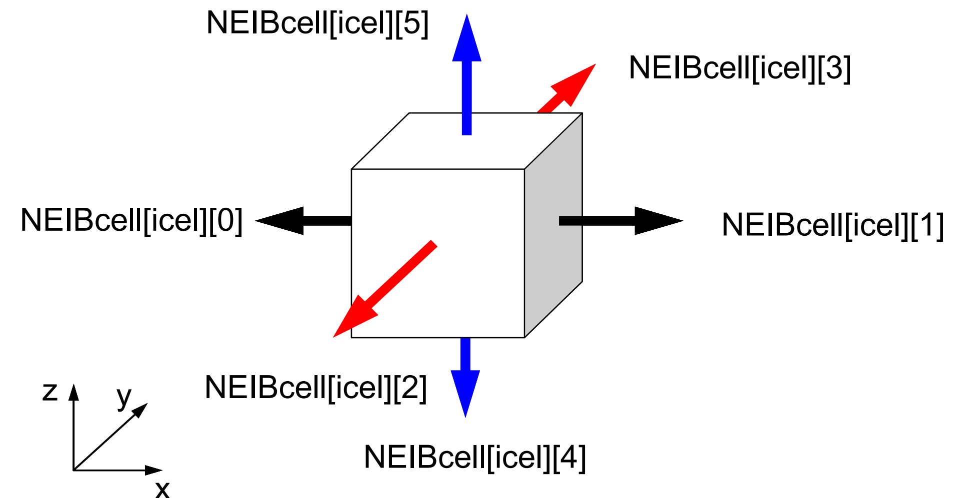
12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3

“IALU” starts at 1

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

poi_gen (3/7)

```
 for(icel=0; icel<ICELTOT; icel++) {

        icN1 = NEIBcell[icel][0];
        icN2 = NEIBcell[icel][1];
        icN3 = NEIBcell[icel][2];
        icN4 = NEIBcell[icel][3];
        icN5 = NEIBcell[icel][4];
        icN6 = NEIBcell[icel][5];
....
          if(icN2 != 0) {
             icou = INLU[icel] + 1;
             IALU[icel][icou-1] = icN2;
             INLU[icel]         = icou;
          }

          if(icN4 != 0) {
             icou = INLU[icel] + 1;
             IALU[icel][icou-1] = icN4;
             INLU[icel]         = icou;
          }

          if(icN6 != 0) {
             icou = INLU[icel] + 1;
             IALU[icel][icou-1] = icN6;
             INLU[icel]         = icou;
          }
}
```



Upper Triangular Part

NEIBcell[icel][1]= icel + 1 + 1
NEIBcell[icel][3]= icel + NX + 1
NEIBcell[icel][5]= icel + NX*NY + 1

"icel" starts at 0

12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3

"IALU" starts at 1

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

poi_gen (4/7)

```
indexLU =
   (int *)allocate_vector(sizeof(int),ICELTOT+1);

for(i=0; i<ICELTOT; i++){
     indexLU[i+1]=indexLU[i]+INLU[i];
}
NPLU= indexLU[ICELTOT];

itemLU= (int *)allocate_vector(sizeof(int),NPLU);

AMAT=
(double *)allocate_vector(sizeof(double),NPLU);

memset(itemLU, 0, sizeof(int)*NPLU);
memset(AMAT, 0.0, sizeof(double)*NPLU);

for(i=0; i<ICELTOT; i++){
     for(k=0;k<INLU[i];k++){
          kk= k + indexLU[i];
          itemLU[kk]= IALU[i][k];
     }
}

free(INLU); free(IALU);
```

Name	Type	Content
D[N]	R	Diagonal components of the matrix (N= ICELTOT)
BFORCE[N]	R	RHS vector
PHI[N]	R	Unknown vector
indexLU[N+1]	I	Number of L/U non-zero off-diag. comp. (CRS)
NPLU	I	Total number of L/U non-zero off-diag. comp. (CRS)
itemLU[NPLU]	I	Column ID of L/U non-zero off-diag. comp. (CRS)
AMAT[NPLU]	R	L/U non-zero off-diag. comp. (CRS)

Name	Type	Content
NLU	I	MAX. number of Lower/Upper non-zero off-diag. comp. for each mesh/row (=6 in this case)
INLU[N]	I	Number of L/U non-zero off-diag. comp.
IALU[N][NLU]	I	Column ID of L/Unon-zero off-diag. comp.

"itemLU" starts at 1

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

```
for (i=0; i<N; i++) {
     q[i]= D[i] * p[i];
     for (j=indexLU[i]; j<indexLU[i+1]; j++) {
          q[i] += AMAT[j] * p[itemLU[j]-1];
     }
}
```

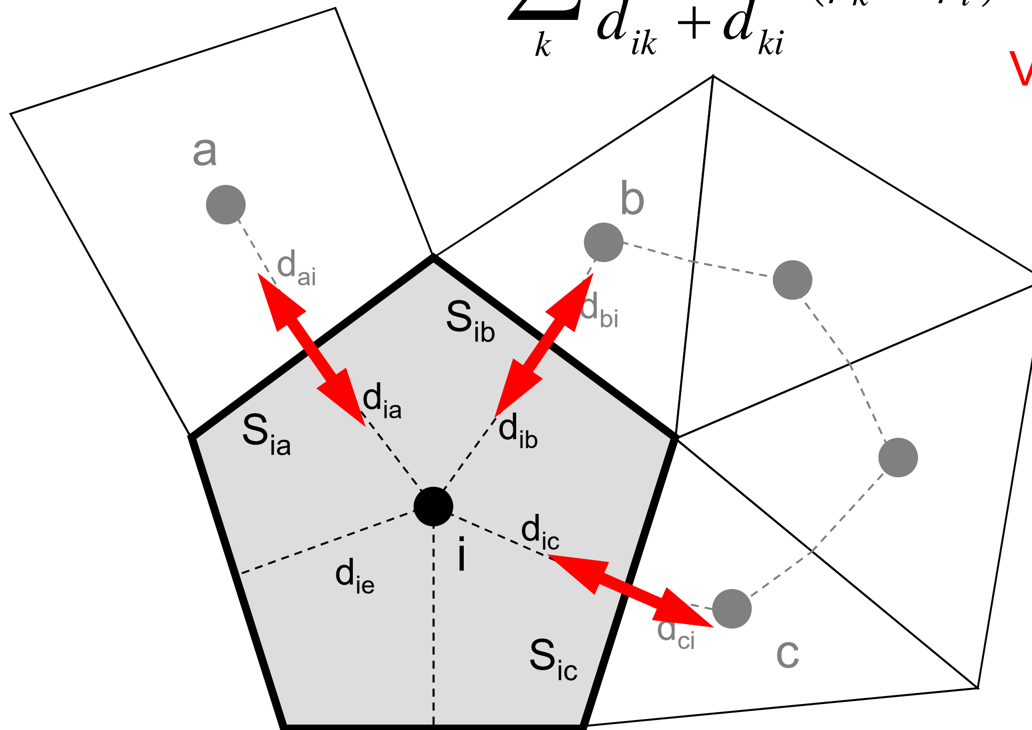
Finite Volume Method（FVM）

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



- V_i : Volume
- S : Surface Area
- d_{ij} : Distance between Cell-Center & Surface
- Q : Volume Flux

Constructing Coefficient Matrix

Conservation for i-th mesh

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

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

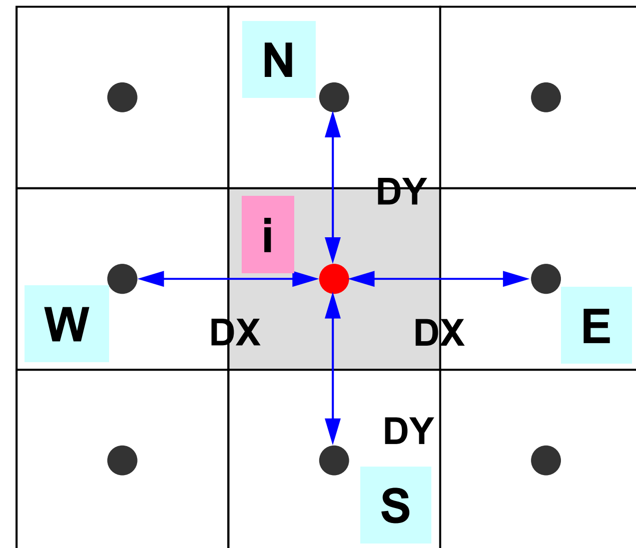
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal) **AMAT (off-diag.)** **BFORCE (RHS)**

poi_gen (5/7)

```
for(icel=0; icel<ICELTOT; icel++) {
    icN1 = NEIBcell[icel][0];
    icN2 = NEIBcell[icel][1];
    icN3 = NEIBcell[icel][2];
    icN4 = NEIBcell[icel][3];
    icN5 = NEIBcell[icel][4];
    icN6 = NEIBcell[icel][5];
    VOL0 = VOLCEL[icel];
    isLU =indexLU[icel  ];
    ieLU =indexLU[icel+1];

    if(icN5 != 0) {
      coef = RDZ * ZAREA;
      D[icel] -= coef;
      for(j=isLU; j<ieLU; j++) {
          if(itemLU[j] == icN5) {
             AMAT[j] = coef;
             break;}
      }
    }
     if(icN3 != 0) {
      coef = RDY * YAREA;
      D[icel] -= coef;
      for(j=isLU; j<ieLU; j++) {
          if(itemLU[j] == icN3) {
             AMAT[j] = coef;
             break;}
      }
    }
     if(icN1 != 0) {
      coef = RDX * XAREA;
      D[icel] -= coef;
      for(j=isLU; j<ieLU; j++) {
          if(itemLU[j] == icN1) {
             ALU[j] = coef;
             break;}
      }
    }
```

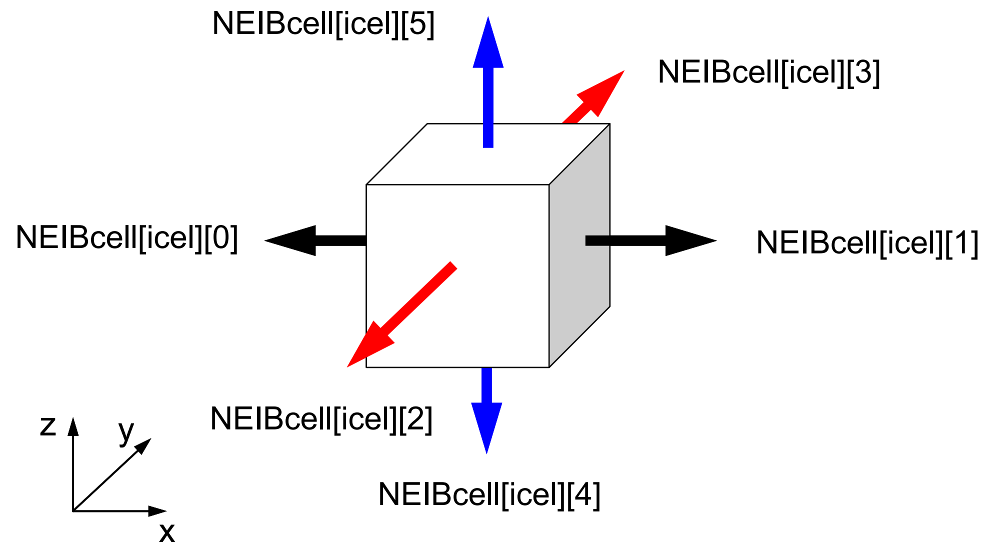
Calculation of Coefficients



$$\frac{\phi_E - \phi_i}{\Delta x}\Delta y \Delta z + \frac{\phi_W - \phi_i}{\Delta x}\Delta y \Delta z +$$

$$\frac{\phi_N - \phi_i}{\Delta y}\Delta x \Delta z + \frac{\phi_S - \phi_i}{\Delta y}\Delta x \Delta z + f_c \Delta x \Delta y \Delta z = 0$$

in 3D




```
if(icN5 != 0) {
   coef = RDZ * ZAREA;
   D[icel] -= coef;
   for(j=isLU; j<ieLU; j++) {
        if(itemLU[j] == icN5) {
           AMAT[j] = coef;
           break;
        }
     }
}
```

$$
\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+
$$

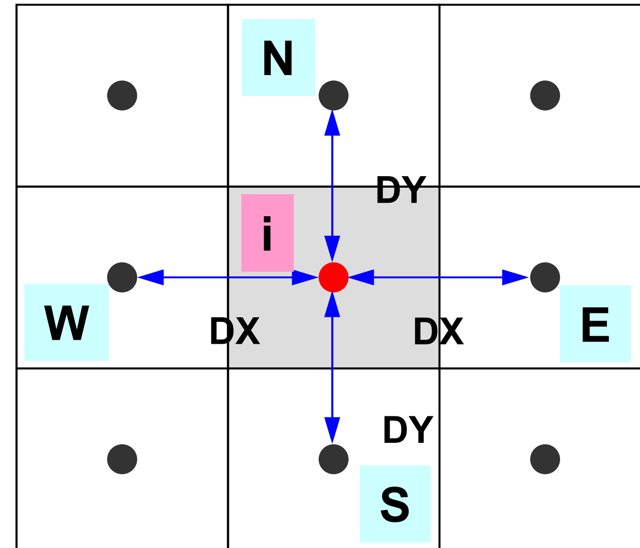
$$
\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+
$$

$$
\boxed{\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y}+\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0
$$

poi_gen (6/7)

```
      if(icN2 != 0) {
        coef = RDX * XAREA;
        D[icel] -= coef;
        for(j=isLU; j<ieLU; j++) {
            if(itemLU[j] == icN2) {
               AMAT[j] = coef;
               break;}
        }
      }

      if(icN4 != 0) {
        coef = RDY * YAREA;
        D[icel] -= coef;
        for(j=isLU; j<ieLU; j++) {
            if(itemLU[j] == icN4) {
               AMAT[j] = coef;
               break;}
        }
      }

      if(icN6 != 0) {
        coef = RDZ * ZAREA;
        D[icel] -= coef;
        for(j=isLU; j<ieLU; j++) {
            if(itemLU[j] == icN6) {
               AMAT[j] = coef;
               break;}
        }
      }

      ii = XYZ[icel][0];
      jj = XYZ[icel][1];
      kk = XYZ[icel][2];

      BFORCE[icel]= -(double)(ii+jj+kk) *
                           VOLCEL[icel];
}
```

Calculation of Coefficients



$$\frac{\phi_E-\phi_i}{\Delta x}\Delta y\Delta z+\frac{\phi_W-\phi_i}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_N-\phi_i}{\Delta y}\Delta x\Delta z+\frac{\phi_S-\phi_i}{\Delta y}\Delta x\Delta z+f_c\Delta x\Delta y\Delta z=0$$

poi_gen (6/7)

```
      if(icN2 != 0) {
        coef = RDX * XAREA;
        D[icel] -= coef;
        for(j=isLU; j<ieLU; j++) {
             if(itemLU[j] == icN2) {
                AMAT[j] = coef;
                break;}
        }
      }

      if(icN4 != 0) {
        coef = RDY * YAREA;
        D[icel] -= coef;
        for(j=isLU; j<ieLU; j++) {
             if(itemLU[j] == icN4) {
                AMAT[j] = coef;
                break;}
        }
      }

      if(icN6 != 0) {
        coef = RDZ * ZAREA;
        D[icel] -= coef;
        for(j=isLU; j<ieLU; j++) {
             if(itemLU[j] == icN6) {
                AMAT[j] = coef;
                break;}
        }
      }

      ii = XYZ[icel][0];
      jj = XYZ[icel][1];
      kk = XYZ[icel][2];

      BFORCE[icel]= -(double)(ii+jj+kk) *
                           VOLCEL[icel];
}
```

Volume Flux

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

$$i_0 = XYZ[icel][0],$$

$$j_0 = XYZ[icel][1],$$

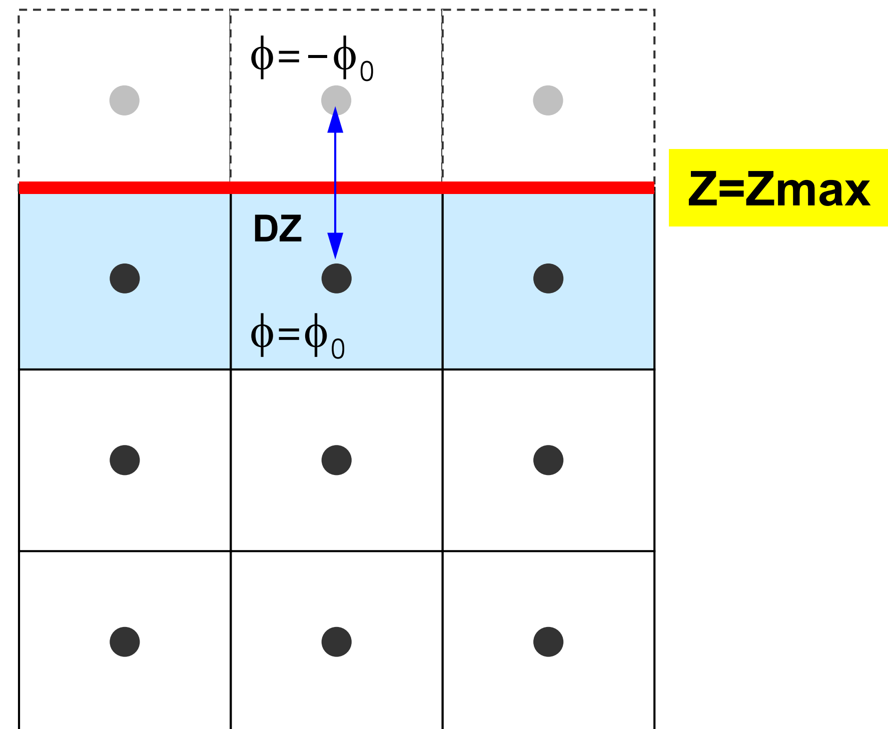
$$k_0 = XYZ[icel][2]$$

XYZ[icel][k](k=0,1,2)
Index for location of finite-difference mesh in X-/Y-/Z-axis.

poi_gen (7/7)

```
/* TOP SURFACE */

        for(ib=0; ib<ZmaxCELtot; ib++) {
            icel  = ZmaxCEL[ib];
            coef = 2.0 * RDZ * ZAREA;
            D[icel-1] -= coef;
        }


        return 0;
}
```

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



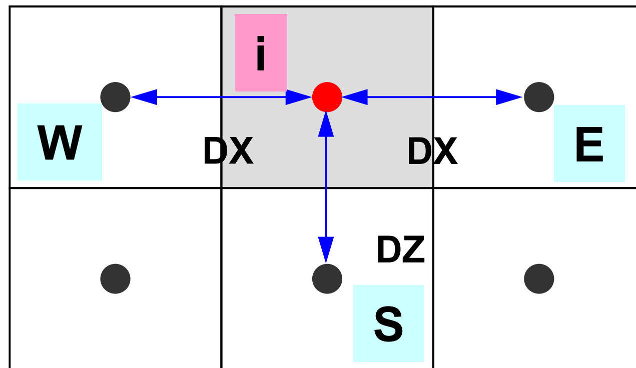
<u>1st Order Approximation:</u>

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.



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

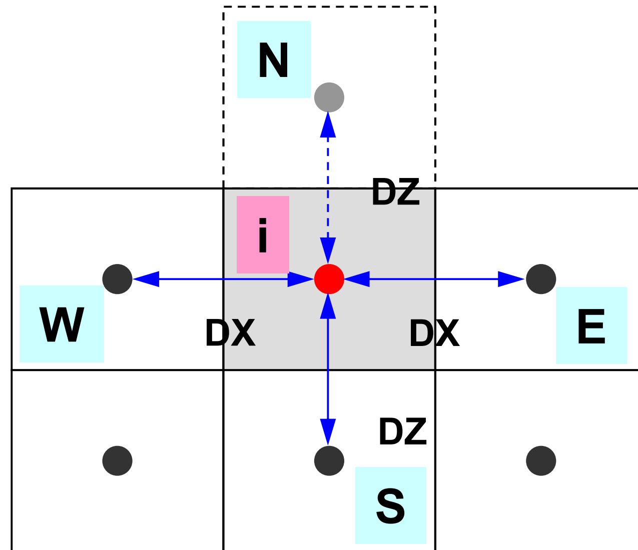
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal)

AMAT (off-diag.)

BFORCE (RHS)

Dirichlet B.C.



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

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

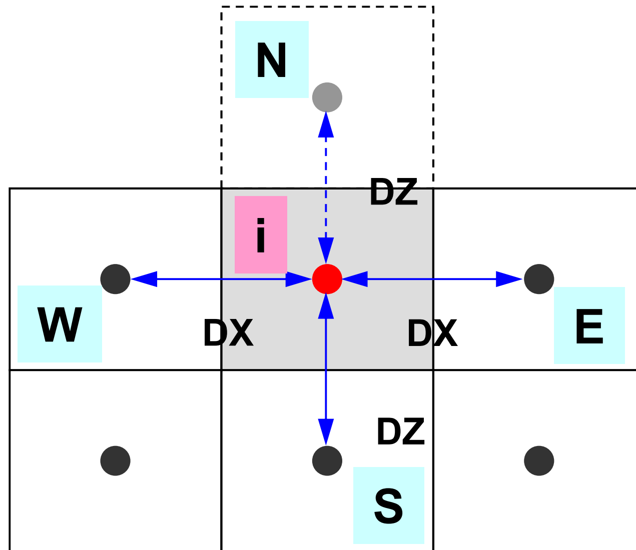
D (diagonal)

AMAT (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.



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

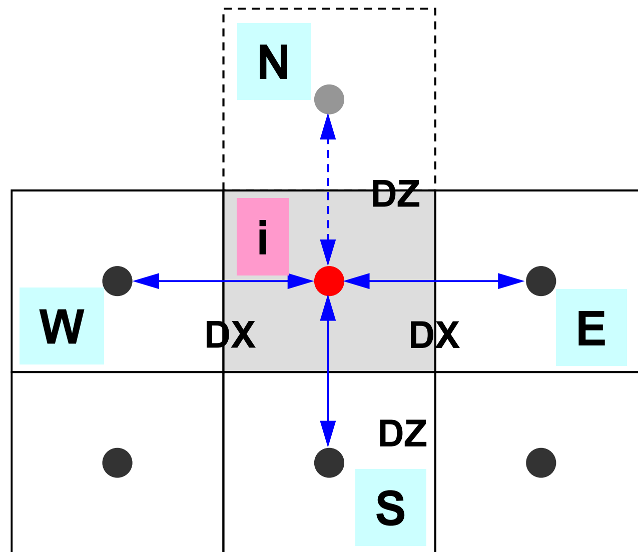
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]=-V_i\dot{Q}_i$$

D (diagonal) **AMAT (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.



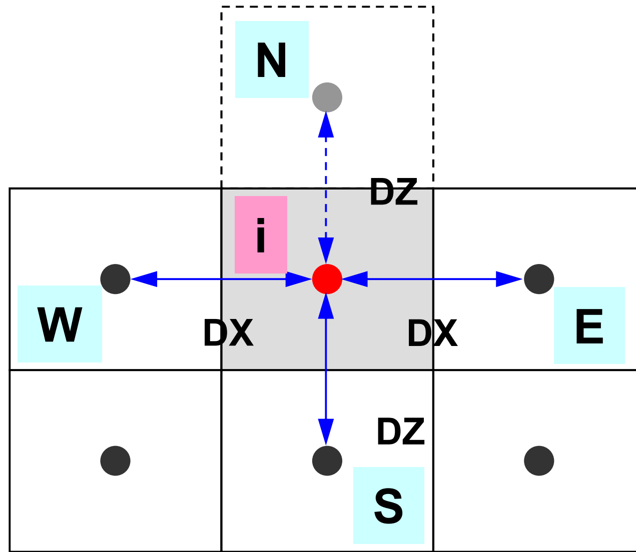
$$\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}(\phi_k-\phi_i)+V_i\dot{Q}_i=0$$

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

D (diagonal) **AMAT (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.



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

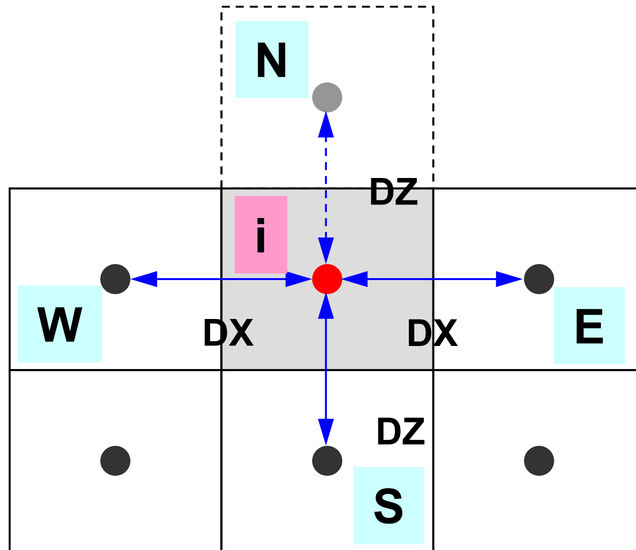
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i + \left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right] = -V_i \dot{Q}_i$$

D (diagonal) **AMAT (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) **AMAT (off-diag.)** **BFORCE (RHS)**

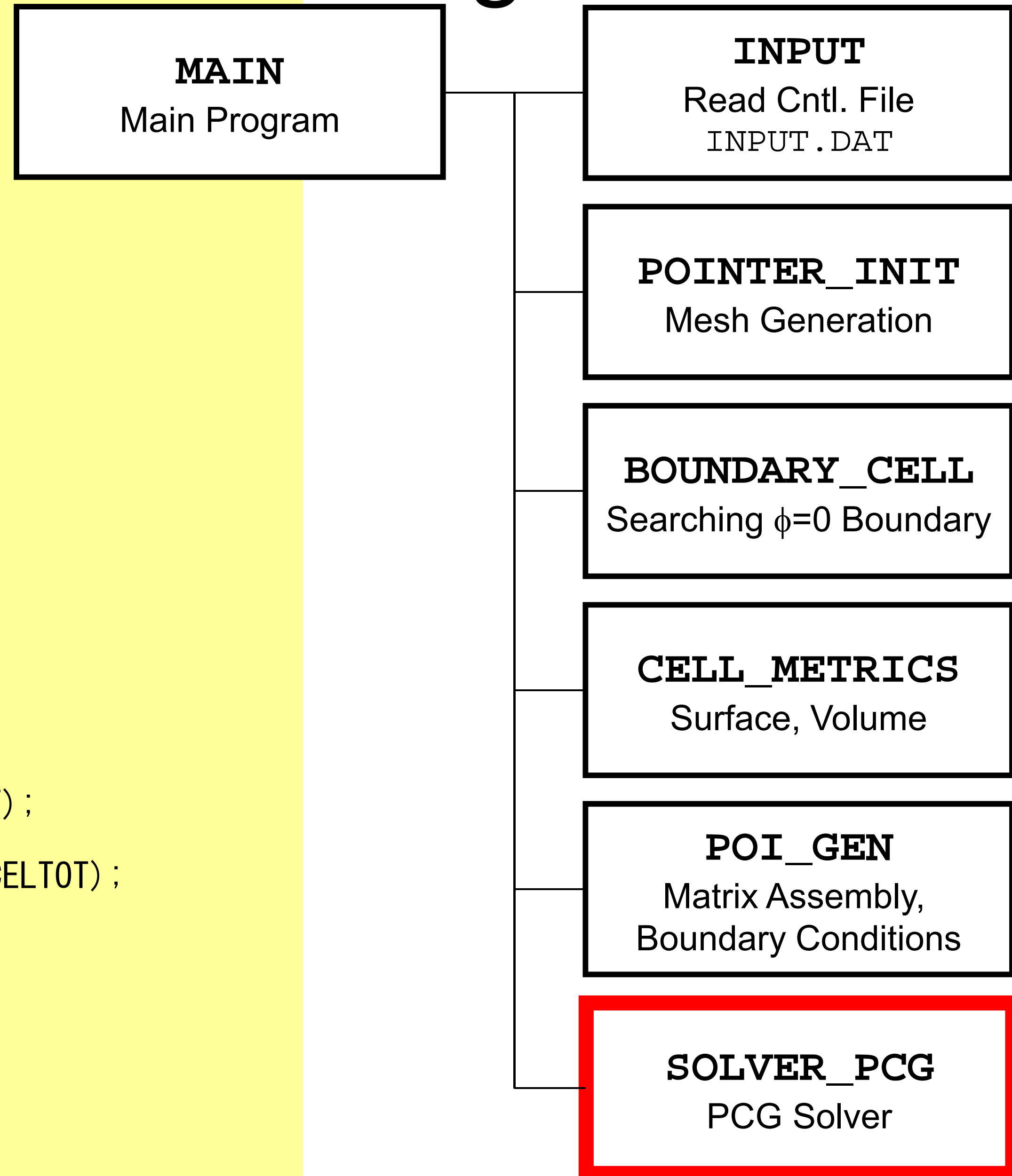
$$-\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\right]\phi_i+\left[\sum_k \frac{S_{ik}}{d_{ik}+d_{ki}}\phi_k\right]$$

```
for(ib=0; ib<ZmaxCELtot; ib++) {
     icel  = ZmaxCEL[ib];
     coef = 2.0 * RDZ * ZAREA;
     D[icel-1] -= coef;
}
```

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

Structure of the Program

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct.h"
#include "pcg.h"
#include "input.h “ ...

int
main()
{
  double *WK;
  int NPLU; ISET, ITR, IER; icel, ic0, i;
  double xN, xL, xU; Stime, Etime;

  if(INPUT()) goto error;
  if(POINTER_INIT()) goto error;
  if(BOUNDARY_CELL()) goto error;
  if(CELL_METRICS()) goto error;
  if(POI_GEN()) goto error;

  memset(PHI, 0.0, sizeof(double)*ICELTOT);
  ISET = 0;
  WK = (double *)malloc(sizeof(double)*ICELTOT);

  if(solve_PCG(...)) goto error;

  if(OUTUCD()) goto error;
  return 0;
  error:
  return -1;
}
```



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

Solving Linear Equations

- Conjugate Gradient, CG
- Point Jacobi/Diagonal Scaling Preconditioning

solve_PCG (1/6)

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>
#include <math.h> etc.

#include "solver_ICCG.h"

extern int
solve_ICCG (int N, int NLU, int *indexLU, int *itemLU,
            double *D, double *B, double *X,
            double *AMAT,
            double EPS, int *ITR, int *IER)
{
  double **W;
  double VAL, BNRM2, WVAL, SW, RHO, BETA, RHO1, C1, DNRM2;
  doble  ALPHA, ERR;

        int i, j, ic, ip, L, ip1;
        int R  = 0;
        int Z  = 1;
        int Q  = 1;
        int P  = 2;
        int DD = 3;
```

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

W[0][i]= W[R][i} ⇒ {r}
W[1][i]= W[Z][i} ⇒ {z}
W[1][i]= W[Q][i} ⇒ {q}
W[2][i]= W[P][i} ⇒ {p}

W[3][i]= W[DD][i} ⇒1/{D}

solve_PCG (2/6)

```
W = (double **)malloc(sizeof(double *)*4);
if(W == NULL) {
   fprintf(stderr, "Error: %s¥n", strerror(errno));
   return -1;
}

for(i=0; i<4; i++) {
    W[i] = (double *)malloc(sizeof(double)*N);
    if(W[i] == NULL) {
       fprintf(stderr, "Error: %s¥n",
strerror(errno));
       return -1;
    }
}

for(i=0; i<N; i++) {
    X[i] = 0.0;
    W[1][i] = 0.0;
    W[2][i] = 0.0;
    W[3][i] = 0.0;
}

for(i=0; i<N; i++) {
    W[DD][i] = 1.0 / D[i];
}
```

W[DD][i]= 1./D_i

multiplying "reciprocal(逆数)"

solve_PCG (3/6)

```
for(i=0; i<N; i++) {
    VAL = D[i] * X[i];
    for(j=indexLU[i]; j<indexLU[i+1]; j++) {
        VAL += AMAT[j] * X[itemLU[j]-1];
    }
    W[R][i] = B[i] - VAL;
}

BNRM2 = 0.0;
for(i=0; i<N; i++) {
    BNRM2 += B[i]*B[i];
}
```

BNRM2=|b|²
Convergence criteria

Compute $r^{(0)}= b-[A]x^{(0)}$
for i= 1, 2, …
  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_PCG (4/6)

```
*ITR = N;
for(L=0; L<(*ITR); L++) {


/*******************
 * {z} = [Minv]{r} *
 *******************/
    for(i=0; i<N; i++) {
        W[Z][i] = W[R][i]*W[DD][i];
    }


/****************
 * RHO = {r}{z} *
 ****************/
    RHO = 0.0;
    for(i=0; i<N; i++) {
        RHO += W[R][i] * W[Z][i];
    }
```

Compute $r^{(0)}= b-[A]x^{(0)}$
for i= 1, 2, …
  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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
  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_PCG (5/6)

```
/***********************************
 * {p}  = {z} if       ITER=0    *
 * BETA = RHO / RHO1  otherwise *
 ***********************************/

if(L == 0) {
   for(i=0; i<N; i++) {
       W[P][i] = W[Z][i];
   }
   } else {
   BETA = RHO / RHO1;
   for(i=0; i<N; i++) {
       W[P][i] = W[Z][i] + BETA * W[P][i];
   }
}

/****************
 * {q} = [A]{p} *
 ****************/

for(i=0; i<N; i++) {
    VAL = D[i] * W[P][i];
    for(j=indexLU[i]; j<indexLU[i+1]; j++) {
        VAL += AMAT[j] * W[P][itemLU[j]-1];
    }
    W[Q][i] = VAL;
}
```

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

<u>end</u>

solve_PCG (6/6)

```
/************************
 * ALPHA = RHO / {p}{q} *
 ************************/
C1 = 0.0;
for(i=0; i<N; i++) {
    C1 += W[P][i] * W[Q][i];
}
ALPHA = RHO / C1;

/***************************
 * {x} = {x} + ALPHA * {p} *
 * {r} = {r} - ALPHA * {q} *
 ***************************/
for(i=0; i<N; i++) {
    X[i]    += ALPHA * W[P][i];
    W[R][i] -= ALPHA * W[Q][i];
}

DNRM2 = 0.0;
for(i=0; i<N; i++) {
    DNRM2 += W[R][i]*W[R][i];
}

ERR = sqrt(DNRM2/BNRM2);
if((L+1)%100 ==1) {
   fprintf(stderr, "%5d%16.6e¥n", L+1, ERR);
}
if(ERR < EPS) {
   *IER = 0; goto N900;
  } else {
   RHO1 = RHO;
  }
}
*IER = 1;
```

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>
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1} p^{(i)}$
  <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_PCG (6/6)

```
/*************************
 * ALPHA = RHO / {p}{q} *
 *************************/
C1 = 0.0;
for(i=0; i<N; i++) {
    C1 += W[P][i] * W[Q][i];
}
ALPHA = RHO / C1;

/***************************
 * {x} = {x} + ALPHA * {p} *
 * {r} = {r} - ALPHA * {q} *
 ***************************/
for(i=0; i<N; i++) {
    X[i]    += ALPHA * W[P][i];
    W[R][i] -= ALPHA * W[Q][i];
}

DNRM2 = 0.0;
for(i=0; i<N; i++) {
    DNRM2 += W[R][i]*W[R][i];
}

ERR = sqrt(DNRM2/BNRM2);
if((L+1)%100 ==1) {
   fprintf(stderr, "%5d%16.6e¥n", L+1, ERR);
}
if(ERR < EPS) {
   *IER = 0; goto N900;
  } else {
   RHO1 = RHO;
  }
}
*IER = 1;
```

r= b-[A]x
DNRM2=|r|²
BNRM2=|b|²

ERR= |r|/|b|

```
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)
     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
```

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

$$Ax = b \Rightarrow \alpha Ax = \alpha b$$

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