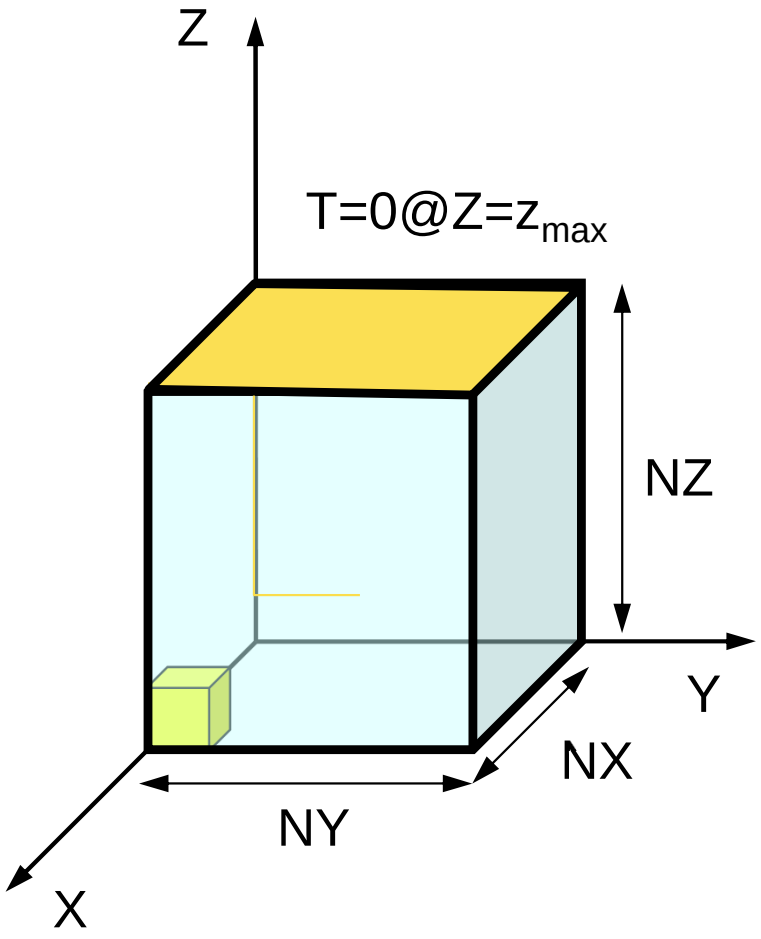
3D-FEM in C: Steady State Heat Conduction

Kengo Nakajima
RIKEN R-CCS

3D Steady-State Heat Conduction

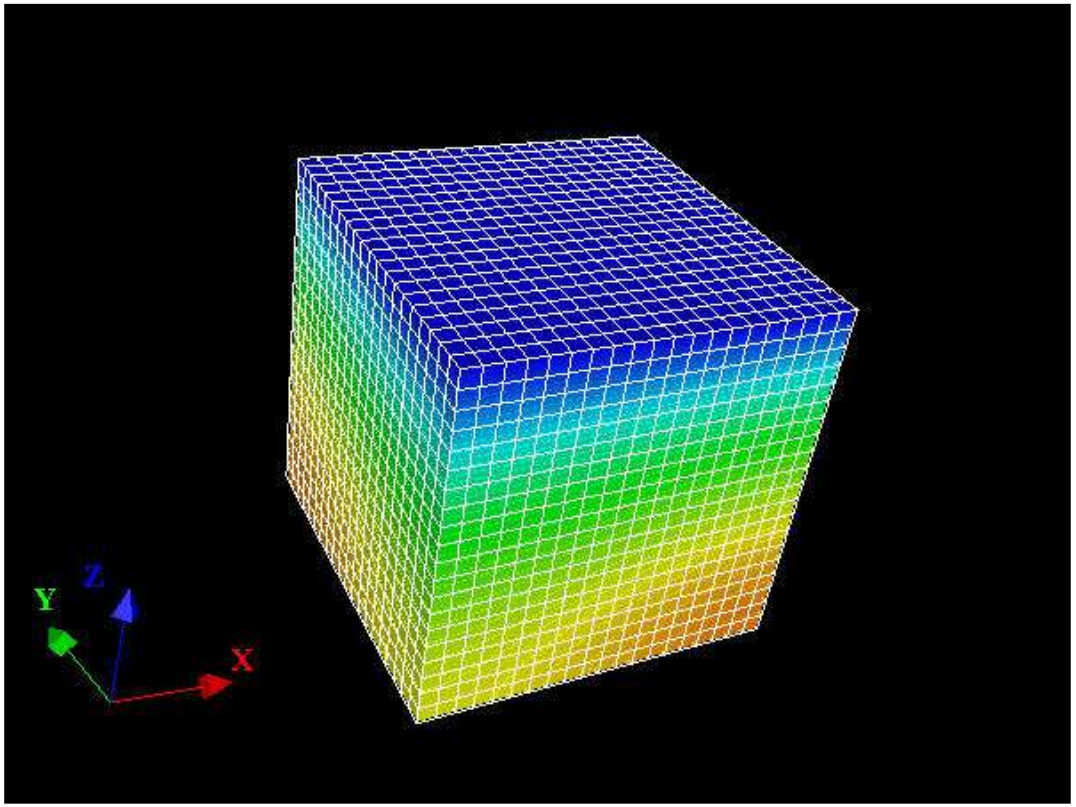
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\dot{Q}(x,y,z)=0$$



- Heat Generation
- Uniform thermal conductivity λ
- HEX meshes
  - 1x1x1 cubes
  - NX, NY, NZ cubes in each direction
- Boundary Conditions
  - T=0@Z=z_{max}
- Heat Gen. Rate is a function of location (cell center: x_c,y_c)
  - $\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$

3D Steady-State Heat Conduction

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



movie

- Higher temperature at nodes far from the origin.
- Heat Gen. Rate is a function of location (cell center: x_c,y_c)

$$\dot{Q}(x,y,z)=\left|x_C+y_C\right|$$

Finite-Element Procedures

- Governing Equations
- Galerkin Method: Weak Form
- Element-by-Element Integration
  - Element Matrix
- Global Matrix
- Boundary Conditions
- Linear Solver

FEM Procedures: Program

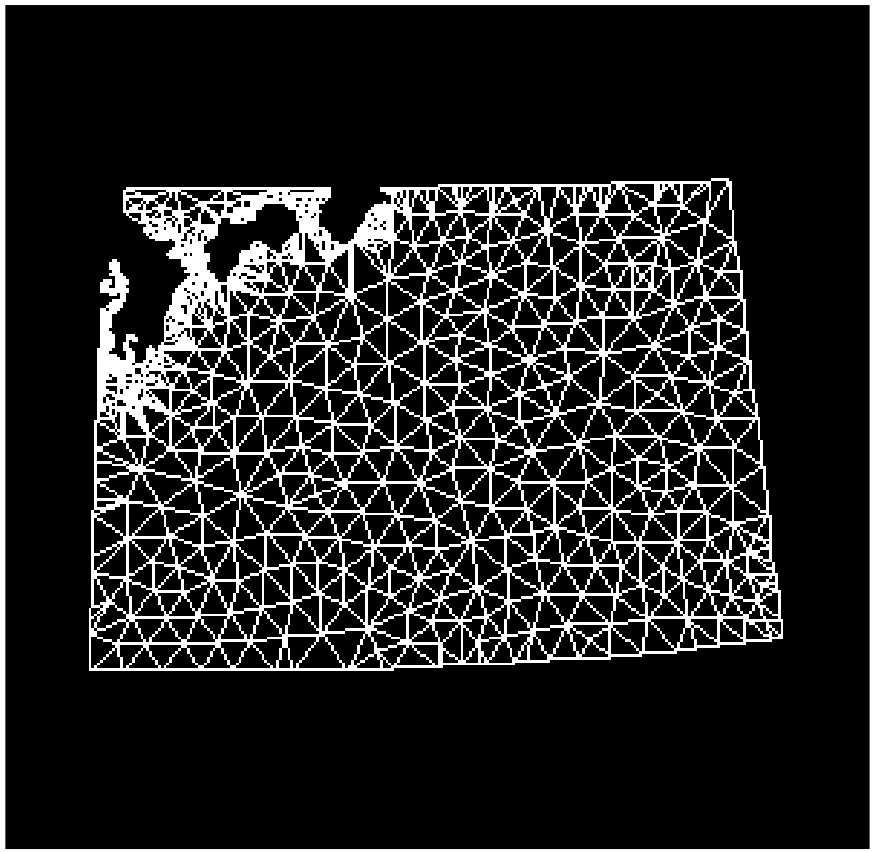
- Initialization
  - Control Data
  - Node, Connectivity of Elements (N: Node#, NE: Elem#)
  - Initialization of Arrays (Global/Element Matrices)
  - Element-Global Matrix Mapping (Index, Item)
- Generation of Matrix
  - Element-by-Element Operations (do icel= 1, NE)
    - Element matrices
    - Accumulation to global matrix
  - Boundary Conditions
- Linear Solver
  - Conjugate Gradient Method

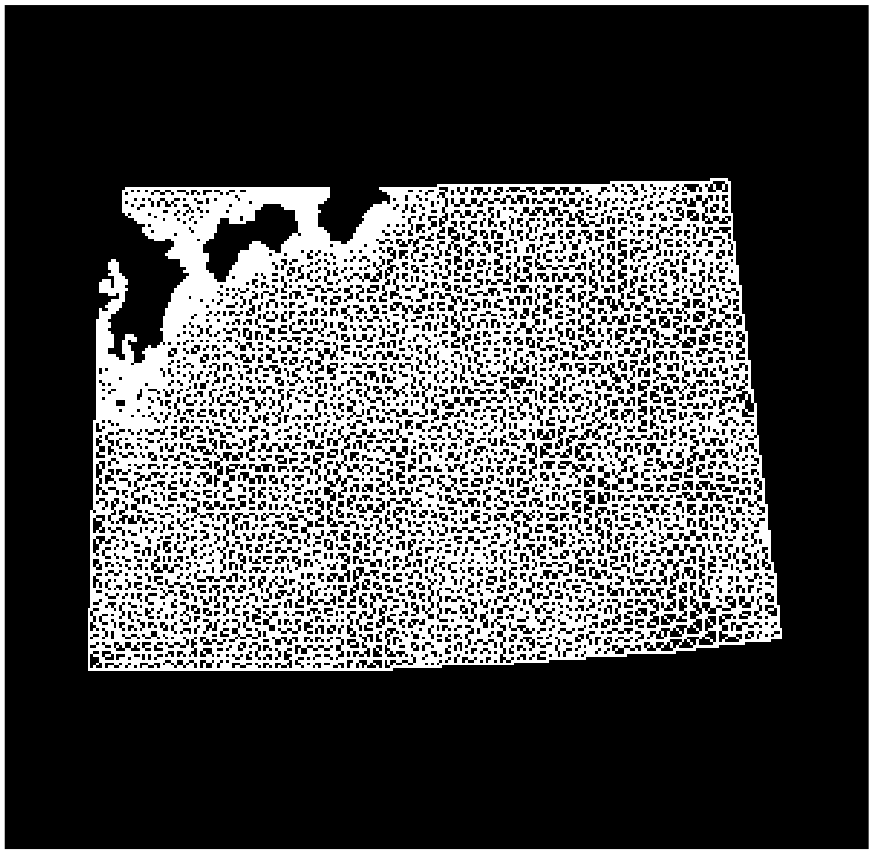
- Formulation of 3D Element
- 3D Heat Equations
  - Galerkin Method
  - Element Matrices

- Running the Code
- Data Structure
- Overview of the Program

Extension to 2D Prob.: Triangles
三角形要素

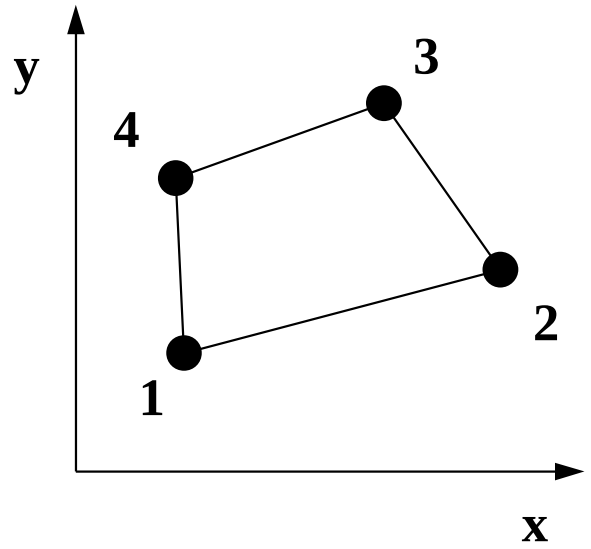
- Triangles can handle arbitrarily shaped object
- “Linear” triangular elements provide low accuracy, therefore they are not used in practical applications.





Extension to 2D Prob.: Quadrilaterals
四角形要素

- Formulation of quad. elements is possible if same shape functions in 1D elements are applied along X- and Y- axis.
  - More accurate than triangles
- Each edge must be “parallel” with X- and Y- axis.
  - Similar to FDM

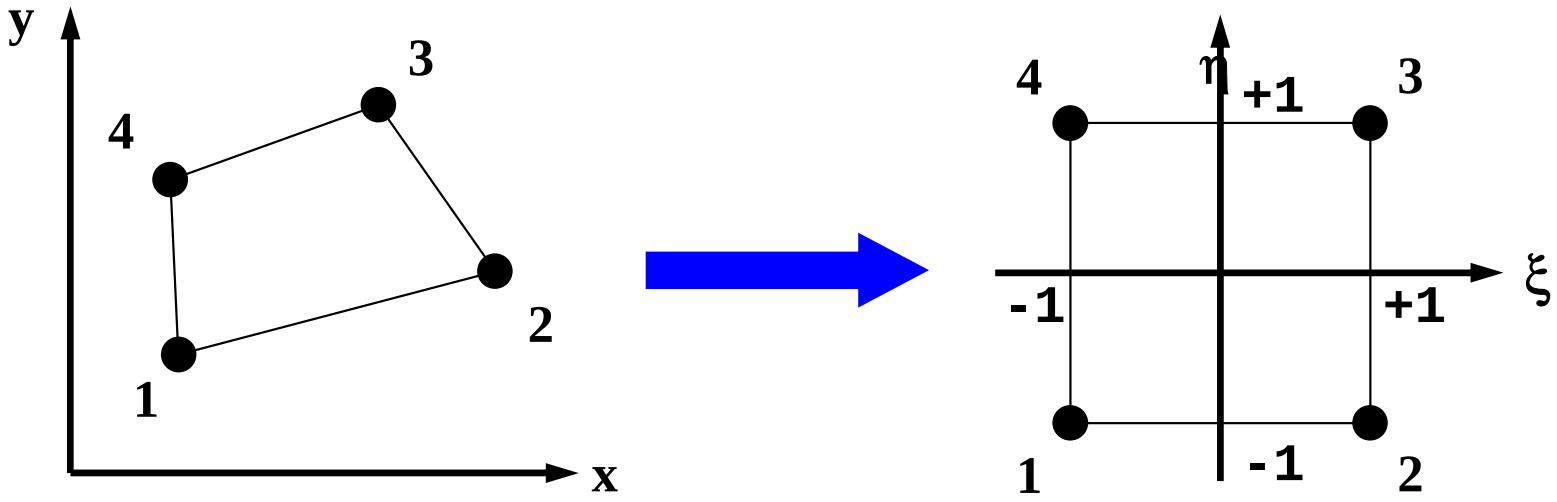


- This type of elements cannot be considered.

Natural/Local/Element Coordinate (1/2)

自然/局所/要素座標系

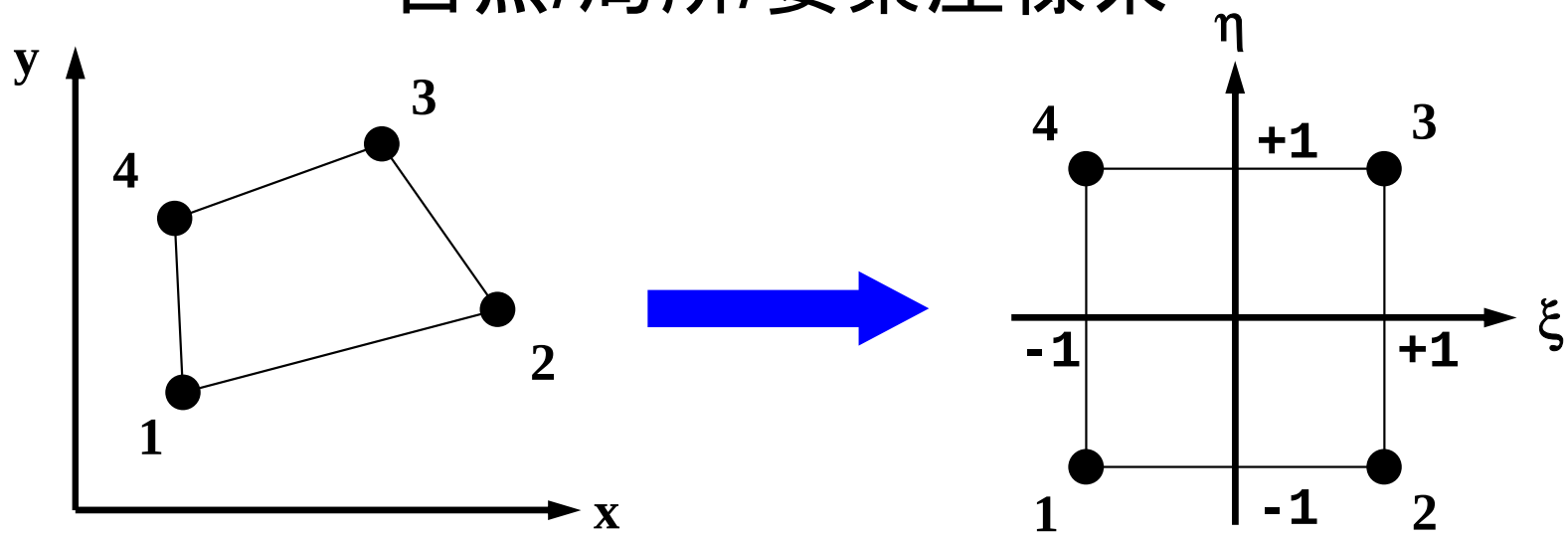
- Each element is mapped to square element $[\pm 1, \pm 1]$ on natural/local/element coordinate (ξ,η)



- Components of global coordinate system of each node (x,y) for certain kinds of elements are defined by shape functions $[N]$ on natural/local coordinate system, where shape functions $[N]$ are also used for interpolation of dependent variables.

Natural/Local/Element Coordinate (2/2)

自然/局所/要素座標系

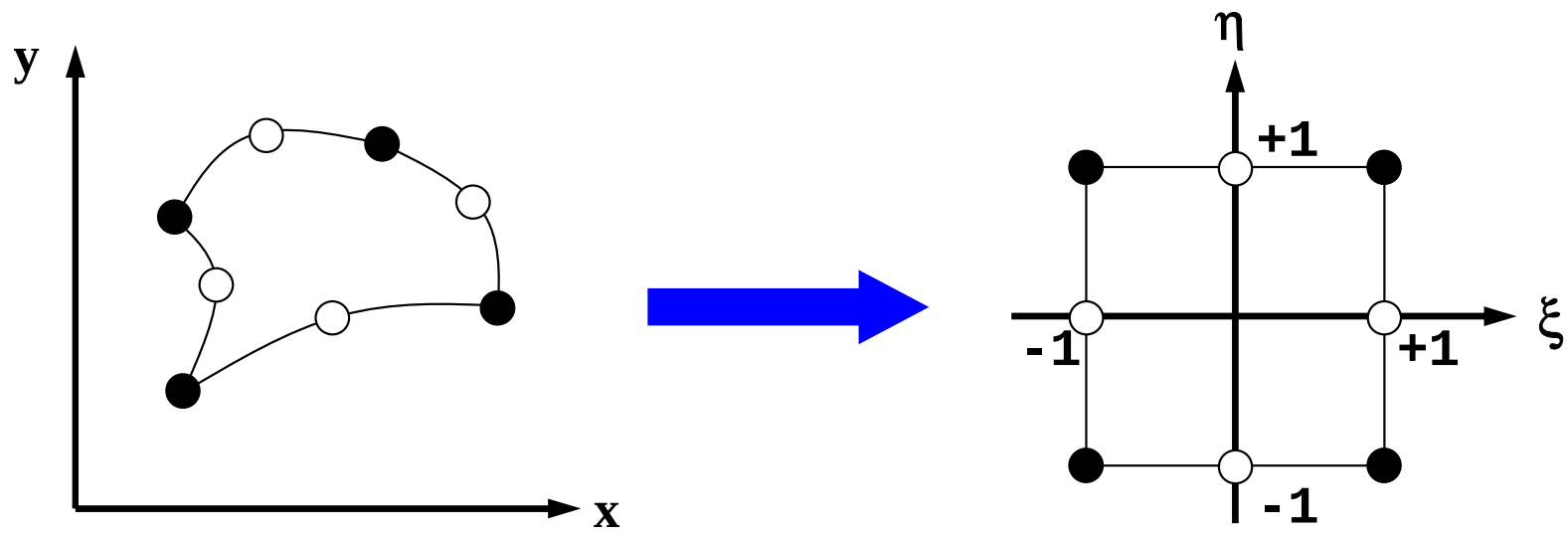


- Coordinate of each node: (x_1,y_1), (x_2,y_2), (x_3,y_3), (x_4,y_4)
- Temperature at each node: T_1, T_2, T_3, T_4

$$T = \sum_{i=1}^{4} N_i(\xi,\eta)\cdot T_i, \quad x = \sum_{i=1}^{4} N_i(\xi,\eta)\cdot x_i,\ y = \sum_{i=1}^{4} N_i(\xi,\eta)\cdot y_i$$

- Isoparametric Elements: N_i for (x_i,y_i) and N_i for T_i are same

Isoparametric Element

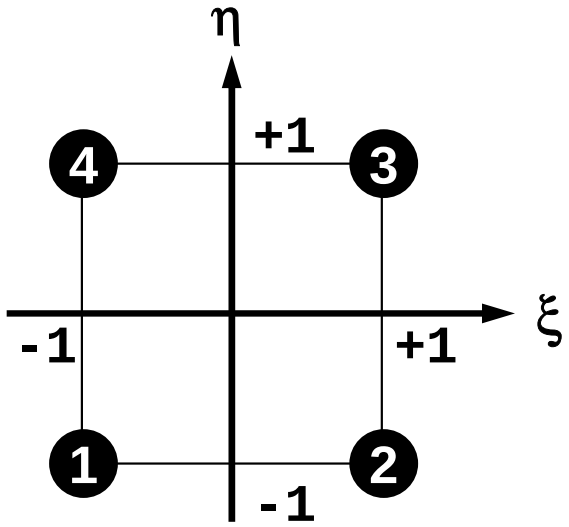


- Higher-order shape function can handle curved lines/surfaces.
- “Natural” coordinate system
- Super-Parametric: Higher-Order N_i for (x,y)
- Sub-Parametric: Lower-Order N_i for (x,y)

Shape Fn's on 2D Natural Coord. (1/3)

- Polynomial shape functions on squares of natural coordinate:

$$T = \alpha_1 + \alpha_2 \xi + \alpha_3 \eta + \alpha_4 \xi \eta$$



- Coefficients are calculated as follows:

$$\alpha_1 = \frac{T_1 + T_2 + T_3 + T_4}{4}, \quad \alpha_2 = \frac{-T_1 + T_2 + T_3 - T_4}{4},$$

$$\alpha_3 = \frac{-T_1 - T_2 + T_3 + T_4}{4}, \quad \alpha_4 = \frac{T_1 - T_2 + T_3 - T_4}{4}$$

Shape Fn's on 2D Natural Coord. (2/3)

$$T = \alpha_1 + \alpha_2\xi + \alpha_3\eta + \alpha_4\xi\eta$$

$$= \frac{T_1+T_2+T_3+T_4}{4} + \frac{-T_1+T_2+T_3-T_4}{4}\xi +$$

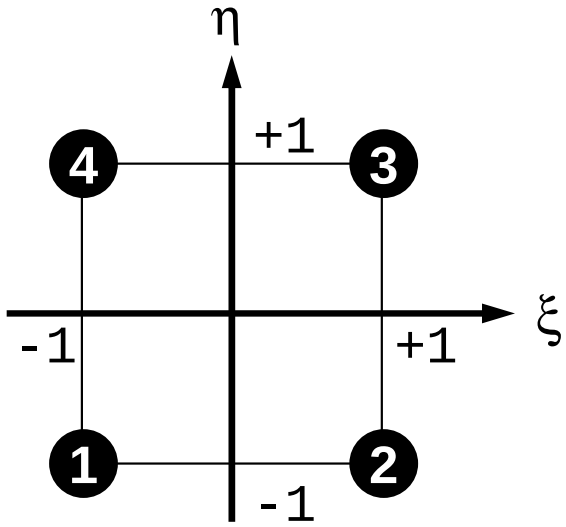
$$\frac{-T_1-T_2+T_3+T_4}{4}\eta + \frac{T_1-T_2+T_3-T_4}{4}\xi\eta$$

$$= \frac{1}{4}(1-\xi-\eta+\xi\eta)T_1 + \frac{1}{4}(1+\xi-\eta-\xi\eta)T_2 +$$

$$\frac{1}{4}(1+\xi+\eta+\xi\eta)T_3 + \frac{1}{4}(1-\xi+\eta-\xi\eta)T_4$$

$$= \frac{1}{4}(1-\xi)(1-\eta)T_1 + \frac{1}{4}(1+\xi)(1-\eta)T_2 +$$

$$\frac{1}{4}(1+\xi)(1+\eta)T_3 + \frac{1}{4}(1-\xi)(1+\eta)T_4$$



Shape Fn's on 2D Natural Coord. (2/3)

$$T = \alpha_1 + \alpha_2\xi + \alpha_3\eta + \alpha_4\xi\eta$$

$$= \frac{T_1+T_2+T_3+T_4}{4} + \frac{-T_1+T_2+T_3-T_4}{4}\xi +$$

$$\frac{-T_1-T_2+T_3+T_4}{4}\eta + \frac{T_1-T_2+T_3-T_4}{4}\xi\eta$$

$$= \frac{1}{4}(1-\xi-\eta+\xi\eta)T_1 + \frac{1}{4}(1+\xi-\eta-\xi\eta)T_2 +$$

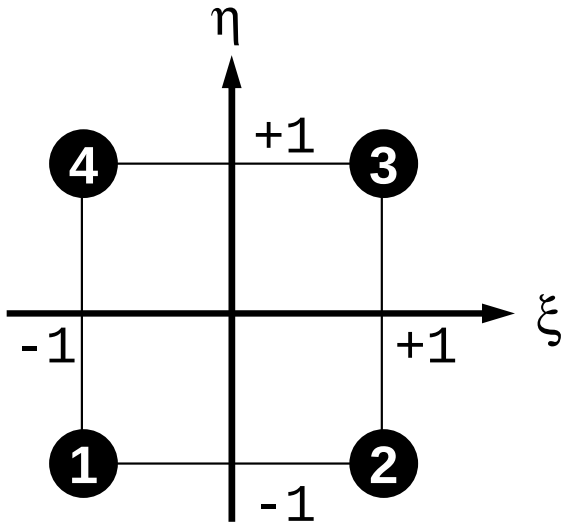
$$\frac{1}{4}(1+\xi+\eta+\xi\eta)T_3 + \frac{1}{4}(1-\xi+\eta-\xi\eta)T_4$$

N_1 N_2

$$= \frac{1}{4}(1-\xi)(1-\eta)T_1 + \frac{1}{4}(1+\xi)(1-\eta)T_2 +$$

$$\frac{1}{4}(1+\xi)(1+\eta)T_3 + \frac{1}{4}(1-\xi)(1+\eta)T_4$$

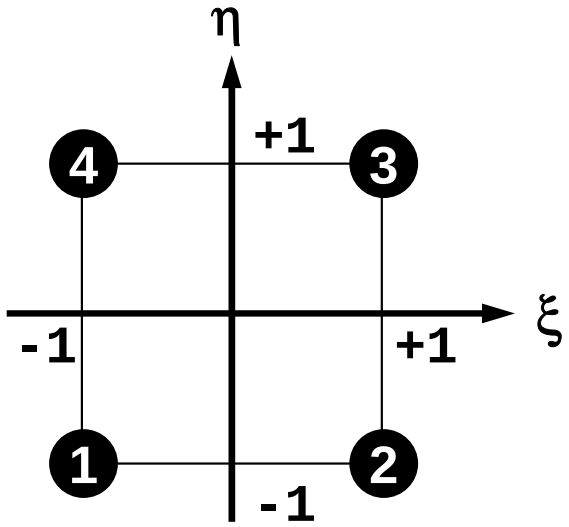
N_3 N_4



Shape Fn's on 2D Natural Coord. (3/3)

- T is defined as follows according to T_i :

$$T = N_1 T_1 + N_2 T_2 + N_3 T_3 + N_4 T_4$$



- Shape functions N_i :

$$N_1(\xi,\eta) = \frac{1}{4}(1-\xi)(1-\eta), \quad N_2(\xi,\eta) = \frac{1}{4}(1+\xi)(1-\eta),$$

$$N_3(\xi,\eta) = \frac{1}{4}(1+\xi)(1+\eta), \quad N_4(\xi,\eta) = \frac{1}{4}(1-\xi)(1+\eta)$$

- Also known as "bi-linear" interpolation
- Calculate N_i at each node

Extension to 3D Problems

- Tetrahedron/Tetrahedra（四面体）: Triangles in 2D
  - can handle arbitrary shape objects
  - Linear elements are generally less accurate, not practical
  - Higher-order tetrahedral elements are widely used.

- In this class, “tri-linear” hexahedral elements (isoparametric) are used（六面体要素）

Shape Fn's: 3D Natural/Local Coord.

$$N_1(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1-\eta)(1-\zeta) \qquad N_5(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1-\eta)(1+\zeta)$$

$$N_2(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1-\eta)(1-\zeta) \qquad N_6(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1-\eta)(1+\zeta)$$

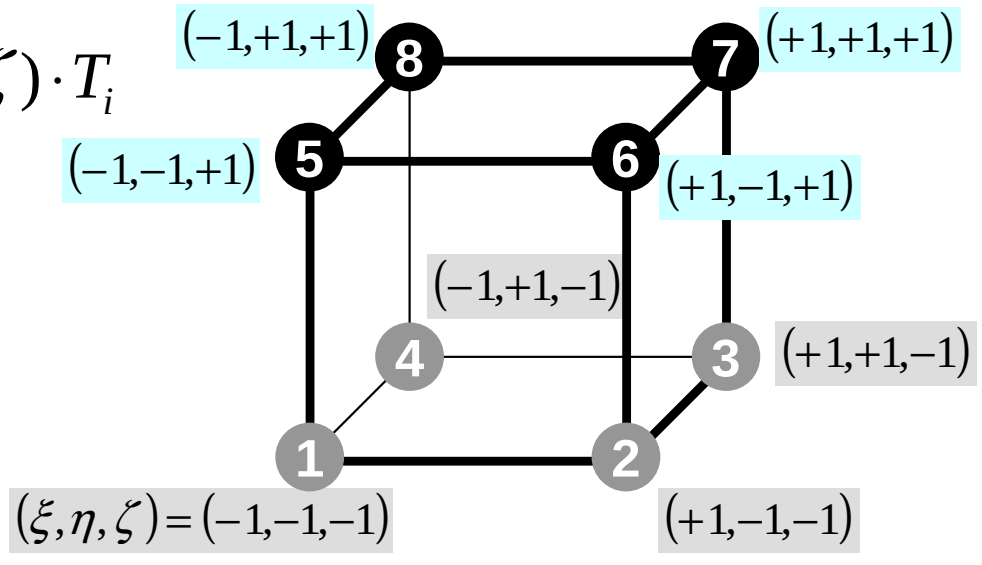
$$N_3(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1+\eta)(1-\zeta) \qquad N_7(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1+\eta)(1+\zeta)$$

$$N_4(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1+\eta)(1-\zeta) \qquad N_8(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1+\eta)(1+\zeta)$$

$$x=\sum_{i=1}^{8}N_i(\xi,\eta,\zeta)\cdot x_i, \quad T=\sum_{i=1}^{8}N_i(\xi,\eta,\zeta)\cdot T_i$$

$$y=\sum_{i=1}^{8}N_i(\xi,\eta,\zeta)\cdot y_i$$

$$z=\sum_{i=1}^{8}N_i(\xi,\eta,\zeta)\cdot z_i$$



- Formulation of 3D Element
- **3D Heat Equations**
  - **Galerkin Method**
  - **Element Matrices**
- Running the Code
- Data Structure
- Overview of the Program

Galerkin Method (1/3)

- Governing Equation for 3D Steady State Heat Conduction Problems (uniform λ):

$$\left(\lambda\frac{\partial^2 T}{\partial x^2}\right)+\left(\lambda\frac{\partial^2 T}{\partial y^2}\right)+\left(\lambda\frac{\partial^2 T}{\partial z^2}\right)+\dot{Q}=0$$

$T=[N]\{\phi\}$ Distribution of temperature in each element (matrix form), ϕ: Temperature at each node

- Following integral equation is obtained at each element by Galerkin method, where $[N]$'s are also weighting functions:

$$\int_V [N]^T\left\{\lambda\left(\frac{\partial^2 T}{\partial x^2}\right)+\lambda\left(\frac{\partial^2 T}{\partial y^2}\right)+\lambda\left(\frac{\partial^2 T}{\partial z^2}\right)+\dot{Q}\right\}dV=0$$

Galerkin Method (2/3)

- Green's Theorem (3D)

$$\int_V A\left(\frac{\partial^2 B}{\partial x^2}+\frac{\partial^2 B}{\partial y^2}+\frac{\partial^2 B}{\partial z^2}\right)dV=\int_S A\frac{\partial B}{\partial n}\,dS-\int_V\left(\frac{\partial A}{\partial x}\frac{\partial B}{\partial x}+\frac{\partial A}{\partial y}\frac{\partial B}{\partial y}+\frac{\partial A}{\partial z}\frac{\partial B}{\partial z}\right)dV$$

- Apply this to the 1st 3-parts of the equation with 2nd-order diff. (surface integration terms are ignored):

$$\int_V [N]^T\left\{\lambda\left(T_{,xx}\right)+\lambda\left(T_{,yy}\right)+\lambda\left(T_{,zz}\right)\right\}dV$$

$$=-\int_V\left\{\lambda\left(\left[N_{,x}\right]^T T_{,x}\right)+\lambda\left(\left[N_{,y}\right]^T T_{,y}\right)+\lambda\left(\left[N_{,z}\right]^T T_{,z}\right)\right\}dV$$

- Consider the following terms:

$$T=[N]\{\phi\},\quad T_{,x}=\left[N_{,x}\right]\{\phi\},\quad T_{,y}=\left[N_{,y}\right]\{\phi\},\quad T_{,z}=\left[N_{,z}\right]\{\phi\}$$

Galerkin Method (3/3)

- Finally, following equation is obtained by considering heat generation term $\dot{Q}$:

$$-\int_V \left\{\lambda\left([N_{,x}]^T[N_{,x}]\right)+\lambda\left([N_{,y}]^T[N_{,y}]\right)+\lambda\left([N_{,z}]^T[N_{,z}]\right)\right\}dV\cdot\{\phi\}+\int_V \dot{Q}[N]dV=0$$

- This is called “weak form（弱形式）”. Original PDE consists of terms with 2nd-order diff., but this “weak form” only includes 1st-order diff by Green’s theorem.
  - Requirements for shape functions are “weaker” in “weak form”. Linear functions can describe effects of 2nd-order differentiation.
  - Same as 1D problem

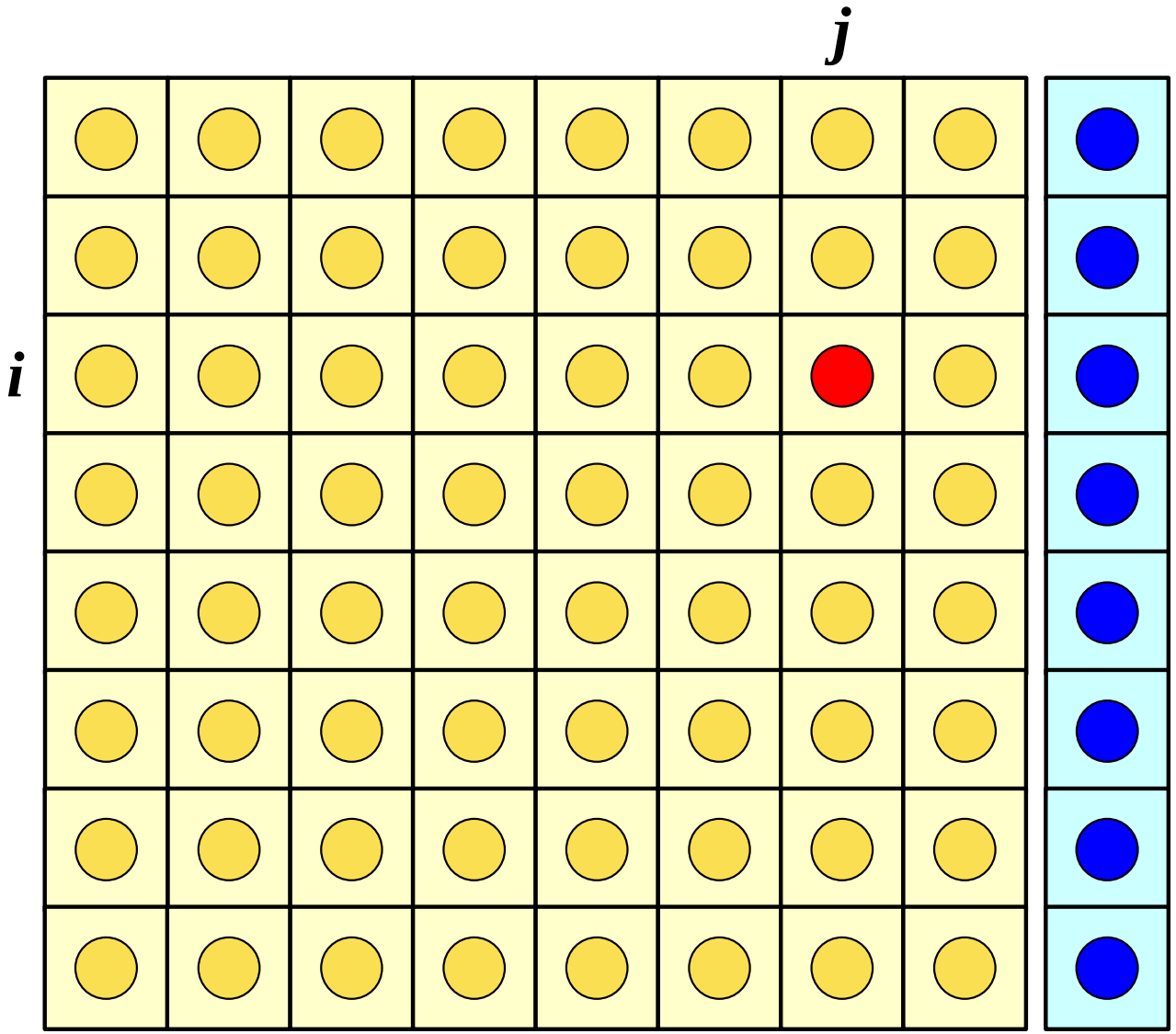
Weak Form with B.C.: on each elem.

$$[k]^{(e)}\{\phi\}^{(e)} = \{f\}^{(e)}$$

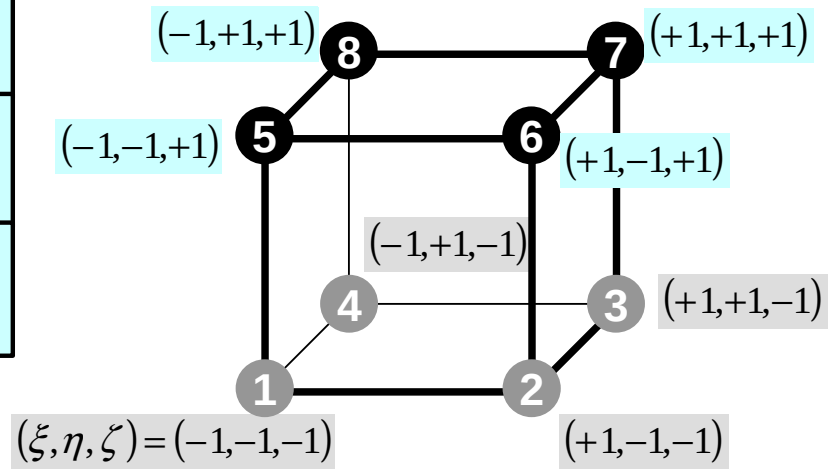
$$[k]^{(e)} = \int_V \lambda\left([N_{,x}]^T[N_{,x}]\right)dV + \int_V \lambda\left([N_{,y}]^T[N_{,y}]\right)dV + \int_V \lambda\left([N_{,z}]^T[N_{,z}]\right)dV$$

$$[f]^{(e)} = \int_V \dot{Q}[N]^T dV$$

Element Matrix: 8x8

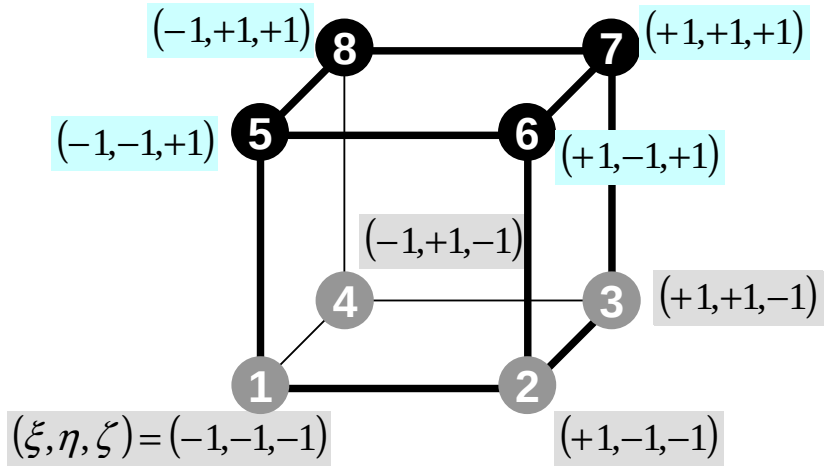


$$\lfloor k_{ij} \rfloor \quad (i, j = 1 \ldots 8)$$



Element Matrix: k_{ij}

$$\lfloor k_{ij} \rfloor \quad (i, j = 1 \ldots 8)$$



$$[k]^{(e)} = \int_V \lambda\left([N_{,x}]^T [N_{,x}]\right) dV + \int_V \lambda\left([N_{,y}]^T [N_{,y}]\right) dV + \int_V \lambda\left([N_{,z}]^T [N_{,z}]\right) dV$$

$$k_{ij} = -\int_V \left\{ \lambda \cdot N_{i,x} \cdot N_{j,x} \right\} dV$$

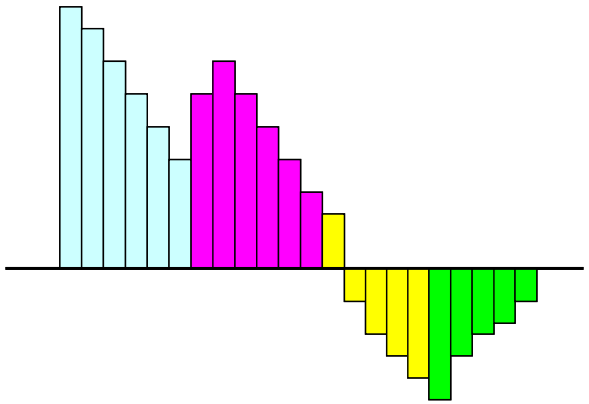
$$k_{ij} = -\int_V \left\{ \lambda \cdot N_{i,x} \cdot N_{j,x} + \lambda \cdot N_{i,y} \cdot N_{j,y} + \lambda \cdot N_{i,z} \cdot N_{j,z} \right\} dV$$

Methods for Numerical Integration

- Trapezoidal Rule
- Simpson's Rule
- Gaussian Quadrature (or Gauss-Legendre)
  - accurate

- Values of functions at finite numbers of sample points are utilized:

$$\int_{X_1}^{X_2} f(x)dx \Rightarrow \sum_{k=1}^{m} [w_k \cdot f(x_k)]$$



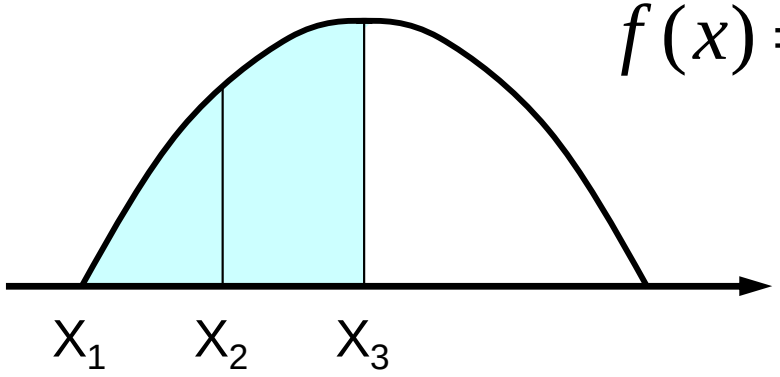
Gaussian Quadrature in 1D

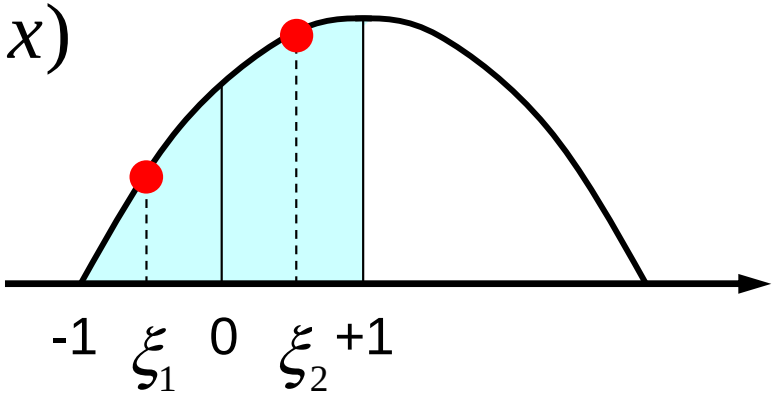
more accurate than Simpson's rule

Simpson's

Gauss

$$f(x) = \sin(x)$$





$$X_1 = 0, \quad X_2 = \frac{\pi}{4}, \quad X_3 = \frac{\pi}{2}$$

$$\xi_1, \xi_2 = \pm 0.5773502692$$

$$h = X_2 - X_1 = X_3 - X_1 = \frac{\pi}{4}$$

$$S = \int_0^{\pi/2} f(x)dx = \int_{-1}^{+1} f(\xi)\, h\, d\xi$$

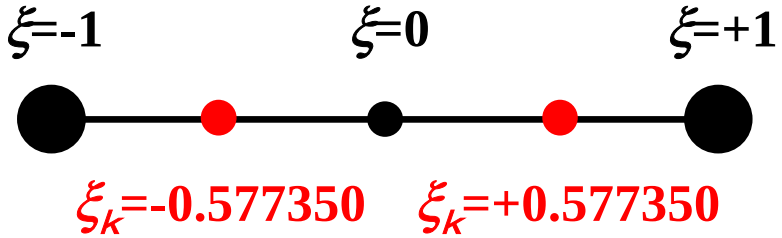
$$S = \frac{h}{3}\left[f(X_1) + 4f(X_2) + f(X_3)\right] = 1.0023$$

$$\cong h\sum_{k=1}^{2} W_k \cdot f(\xi_k) = 0.99847$$

Gaussian Quadrature
ガウスの積分公式

- On normalized “natural (or local)” coordinate system [-1,+1]（自然座標系，局所座標系）
- Can approximate up to (*2m-1*)-th order of functions by *m* quadrature points (*m*=2 is enough for quadratic shape functions).

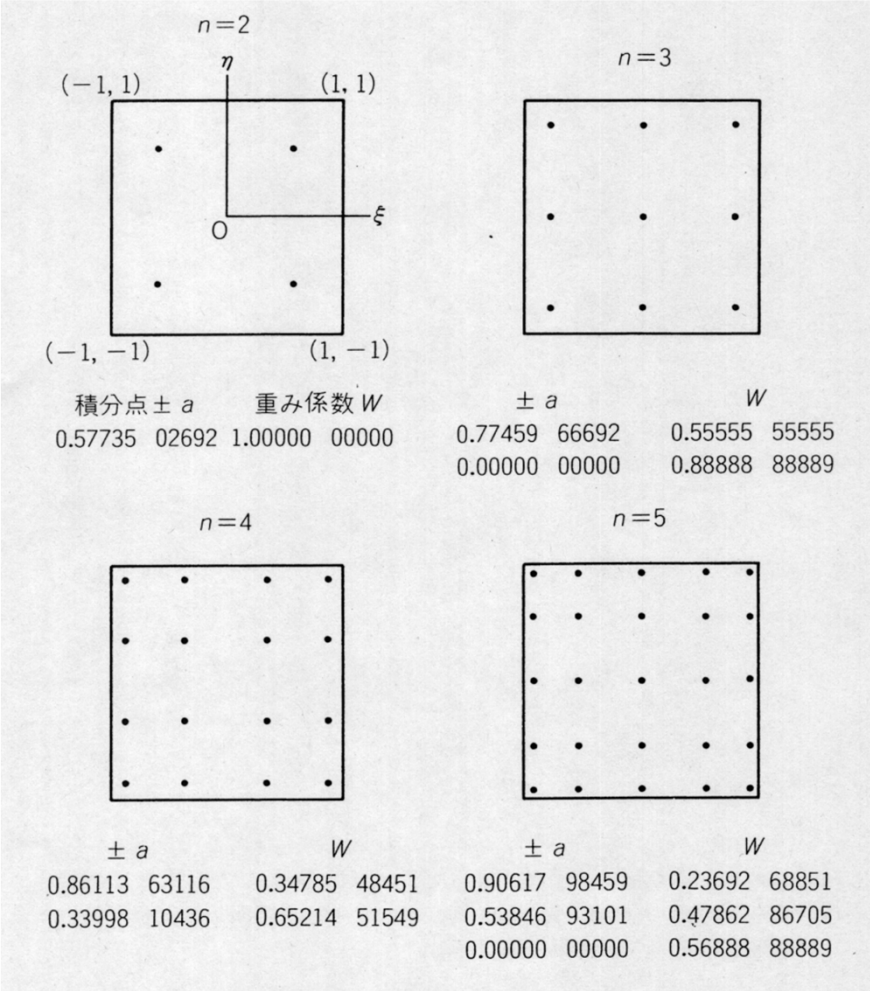
$$\int_{-1}^{+1} f(\xi)d\xi = \sum_{k=1}^{m}[w_k \cdot f(\xi_k)]$$



$$m=1 \quad \xi_k = 0.00,\ w_k = 2.00$$
$$m=2 \quad \xi_k = \pm 0.577350,\ w_k = 1.00$$
$$m=3 \quad \xi_k = 0.00,\ w_k = 8/9$$
$$\xi_k = \pm 0.774597,\ w_k = 5/9$$

Gaussian Quadrature

can be easily extended to 2D & 3D



$$I = \int_{-1}^{+1} \int_{-1}^{+1} f(\xi,\eta)\, d\xi d\eta$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{n} \left[W_i \cdot W_j \cdot f(\xi_i,\eta_j) \right]$$

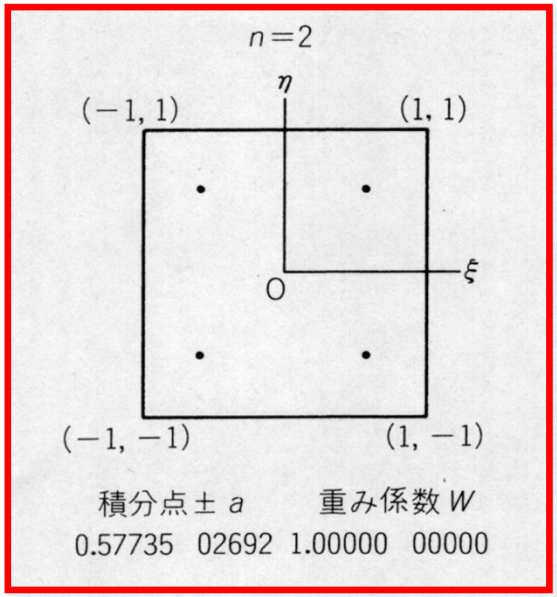
m,n: number of quadrature points in ξ,η-direction

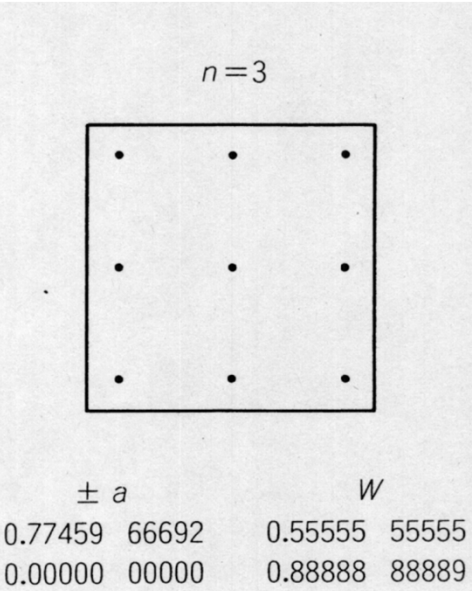
(ξ_i,η_j): Coordinates of Quad's

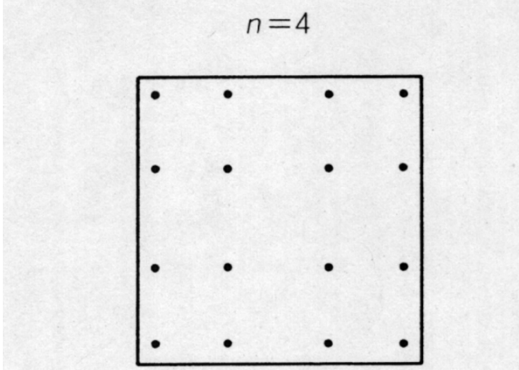
W_i, W_j: Weighting Factor

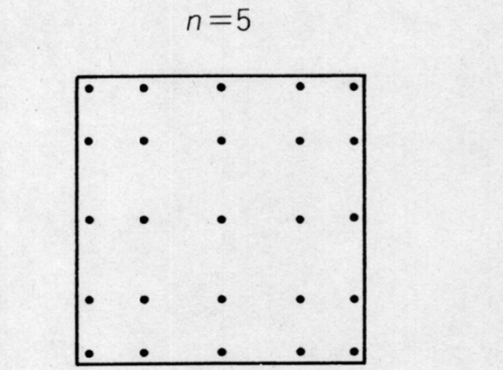
Gaussian Quadrature
ガウスの積分公式

This configuration is widely used. In 2D problem, integration is done using values of “f” at 4 quad. points.



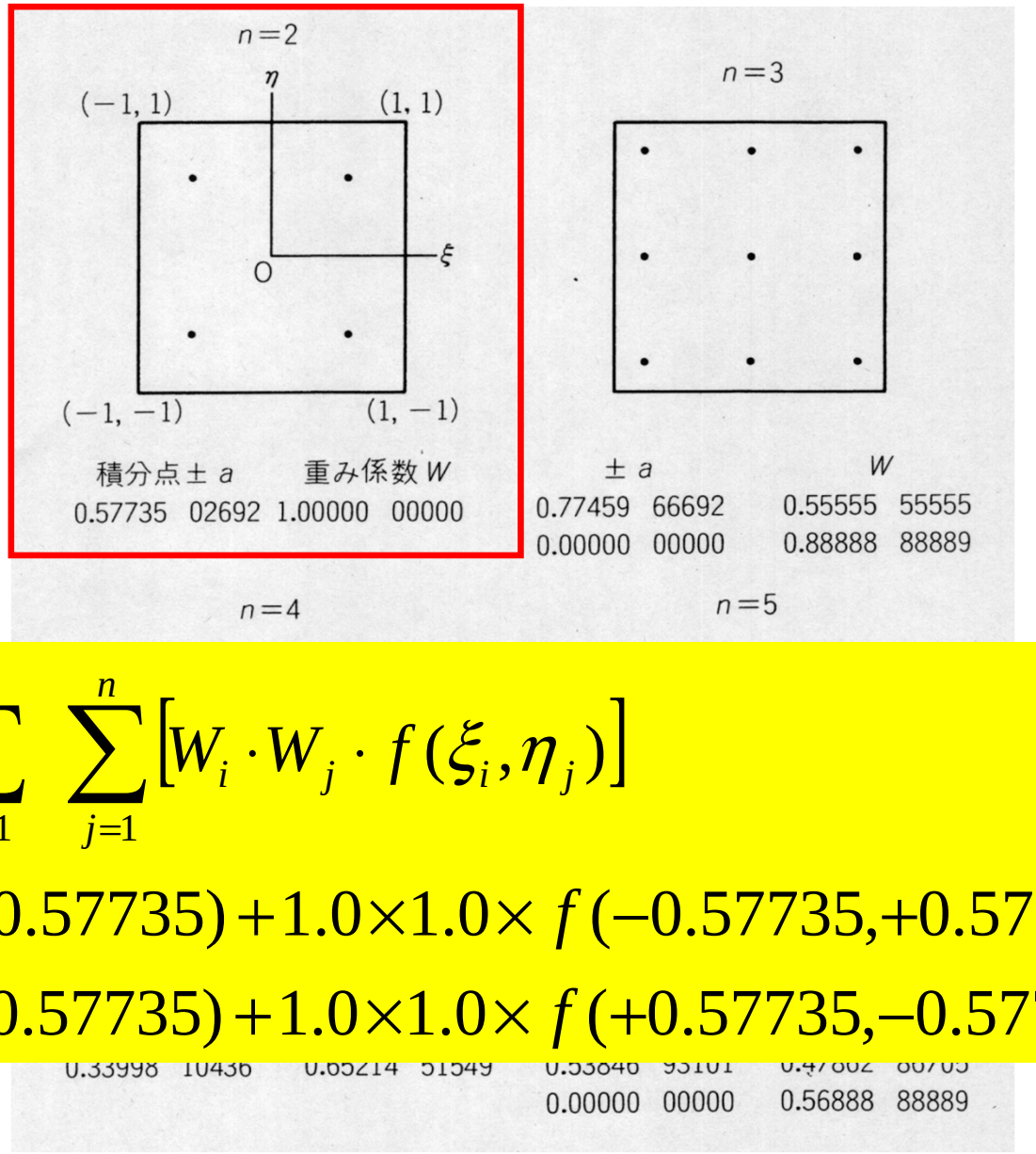






Gaussian Quadrature
ガウスの積分公式

This configuration is widely used. In 2D problem, integration is done using values of “f” at 4 quad. points.



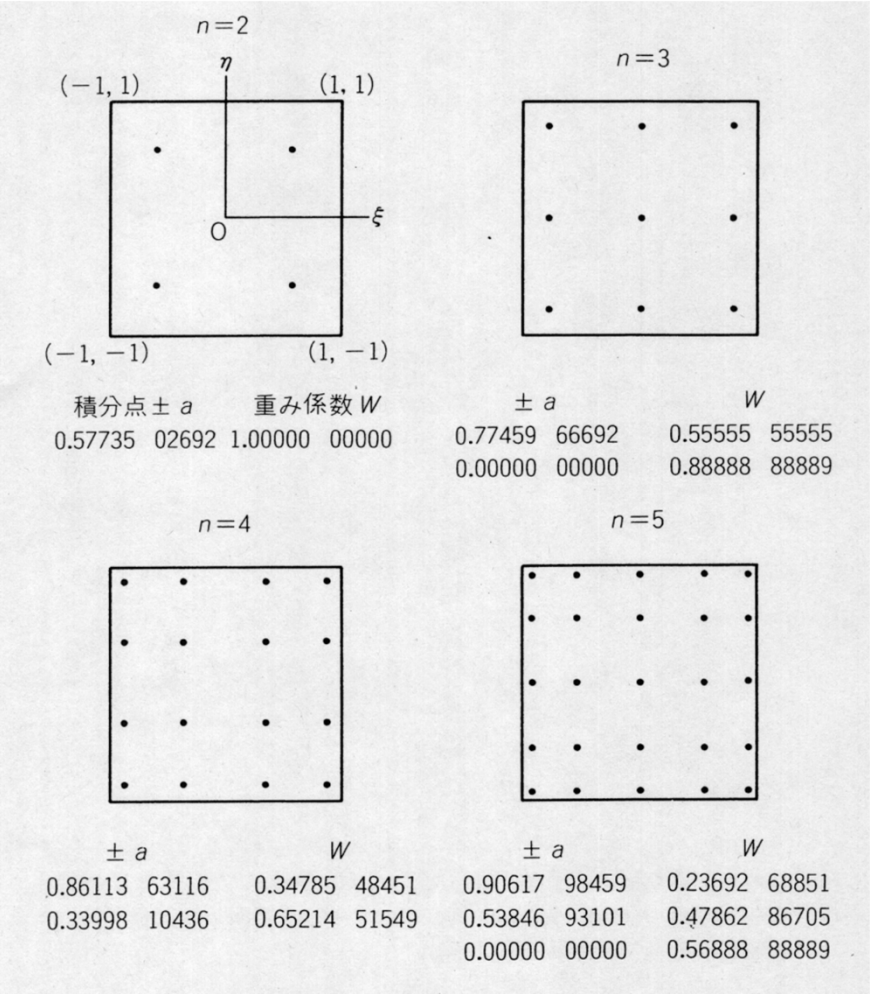
$$I = \int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta)\,d\xi d\eta = \sum_{i=1}^{m}\sum_{j=1}^{n}\left[W_i \cdot W_j \cdot f(\xi_i,\eta_j)\right]$$

$$= 1.0\times 1.0\times f(-0.57735,-0.57735) + 1.0\times 1.0\times f(-0.57735,+0.57735)$$

$$+ 1.0\times 1.0\times f(+0.57735,+0.57735) + 1.0\times 1.0\times f(+0.57735,-0.57735)$$

Next Stage: Integration

- 3D Natural/Local Coordinate (ξ,η,ζ):
  - Gaussian Quadrature



$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta$$

$$= \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N}\left[W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)\right]$$

L,M,N: number of quadrature points in ξ,η,ζ-direction

(ξ_i,η_j,ζ_k) : Coordinates of Quad's

W_i,W_j,W_k : Weighting Factor

Partial Diff. on Natural Coord. (1/4)

- According to formulae:

$$\frac{\partial N_i(\xi,\eta,\zeta)}{\partial \xi} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \xi} + \frac{\partial N_i}{\partial z}\frac{\partial z}{\partial \xi}$$

$$\frac{\partial N_i(\xi,\eta,\zeta)}{\partial \eta} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \eta} + \frac{\partial N_i}{\partial z}\frac{\partial z}{\partial \eta}$$

$$\frac{\partial N_i(\xi,\eta,\zeta)}{\partial \zeta} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \zeta} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \zeta} + \frac{\partial N_i}{\partial z}\frac{\partial z}{\partial \zeta}$$

$\left[\frac{\partial N_i}{\partial \xi}, \frac{\partial N_i}{\partial \eta}, \frac{\partial N_i}{\partial \zeta}\right]$ can be easily derived according to definitions.

$\left[\frac{\partial N_i}{\partial x}, \frac{\partial N_i}{\partial y}, \frac{\partial N_i}{\partial z}\right]$ are required for computations.

Partial Diff. on Natural Coord. (2/4)

- In matrix form:

$$\begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = [J] \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix}$$

$[J]$: Jacobi matrix, Jacobian

Partial Diff. on Natural Coord. (3/4)

- Components of Jacobian:

$$J_{11}=\frac{\partial x}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{8}N_i x_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \xi}x_i,\quad J_{12}=\frac{\partial y}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{8}N_i y_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \xi}y_i,$$

$$J_{13}=\frac{\partial z}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{8}N_i z_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \xi}z_i$$

$$J_{21}=\frac{\partial x}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{8}N_i x_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \eta}x_i,\quad J_{22}=\frac{\partial y}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{8}N_i y_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \eta}y_i,$$

$$J_{23}=\frac{\partial z}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{8}N_i z_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \eta}z_i$$

$$J_{31}=\frac{\partial x}{\partial \zeta}=\frac{\partial}{\partial \zeta}\left(\sum_{i=1}^{8}N_i x_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \zeta}x_i,\quad J_{32}=\frac{\partial y}{\partial \zeta}=\frac{\partial}{\partial \zeta}\left(\sum_{i=1}^{8}N_i y_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \zeta}y_i,$$

$$J_{33}=\frac{\partial z}{\partial \zeta}=\frac{\partial}{\partial \zeta}\left(\sum_{i=1}^{8}N_i z_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \zeta}z_i$$

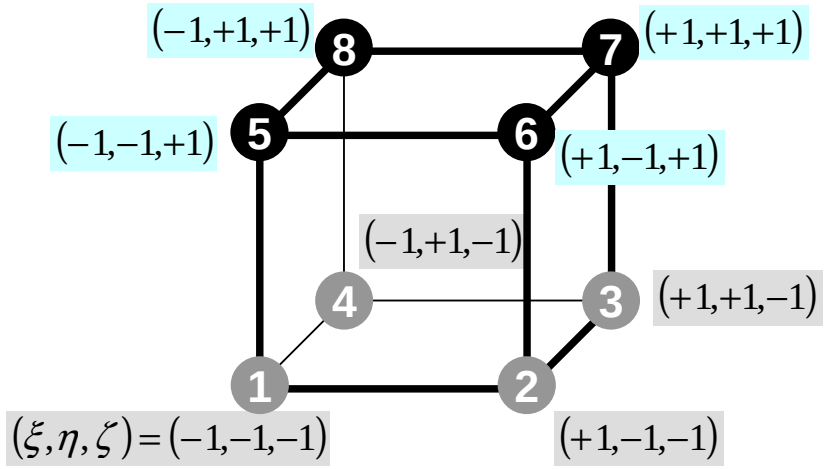
Partial Diff. on Natural Coord. (4/4)

- Partial differentiation on global coordinate system is introduced as follows (with inverse of Jacobian matrix (3×3))

$$\begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix}^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = \left[J \right]^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix}$$

Integration on Element

$$\lfloor k_{ij} \rfloor \quad (i, j = 1 \ldots 8)$$

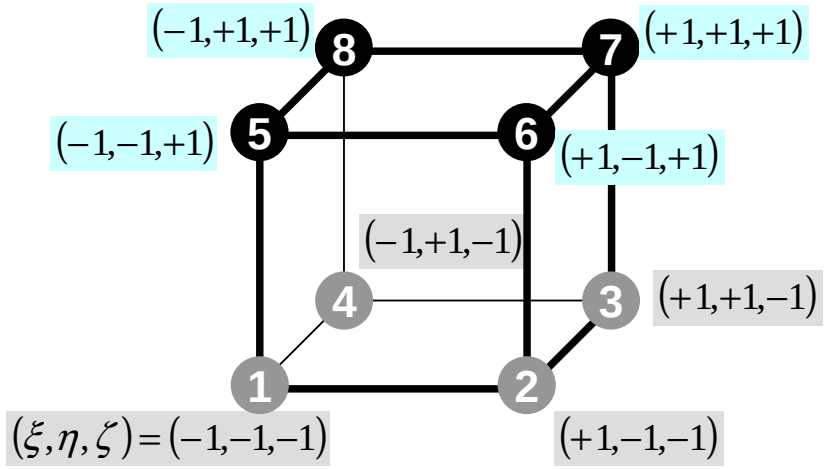


$$k_{ij} = -\int_V \left\{ \lambda \cdot N_{i,x} \cdot N_{j,x} + \lambda \cdot N_{i,y} \cdot N_{j,y} + \lambda \cdot N_{i,z} \cdot N_{j,z} \right\} dV$$

$$= -\int_V \left\{ \lambda \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right\} dV$$

Integration on Natural Coord.

$$\lfloor k_{ij} \rfloor \quad (i, j = 1 \ldots 8)$$



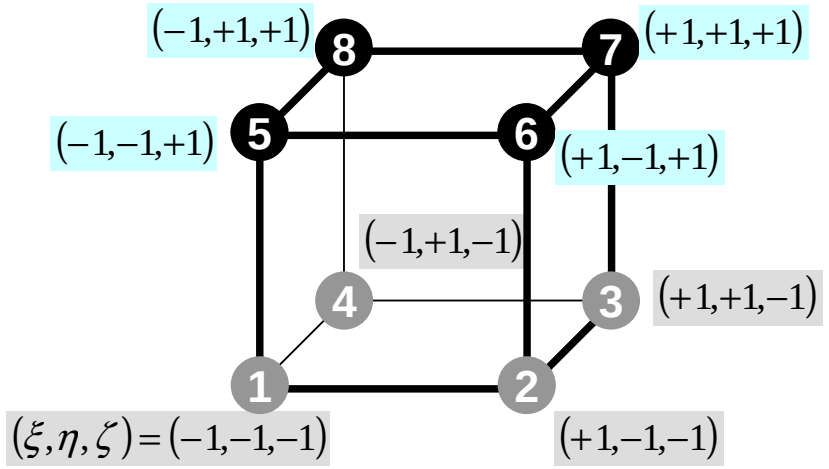
$$-\int_V \left\{ \lambda \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} dV =$$

$$-\int\int\int \left\{ \lambda \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} dxdydz =$$

$$-\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} \left\{ \lambda \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} \det|J| \, d\xi d\eta d\zeta$$

Gaussian Quadrature

$$\left[k_{ij}\right] \quad (i, j = 1 \ldots 8)$$



$$-\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1}\left\{\lambda\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\lambda\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}+\lambda\frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}\right\}\det\left|J\right|\,d\xi d\eta d\zeta$$

$$I=\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\,d\xi d\eta d\zeta$$

$$=\sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N}\left[W_i\cdot W_j\cdot W_k\cdot f(\xi_i,\eta_j,\zeta_k)\right]$$

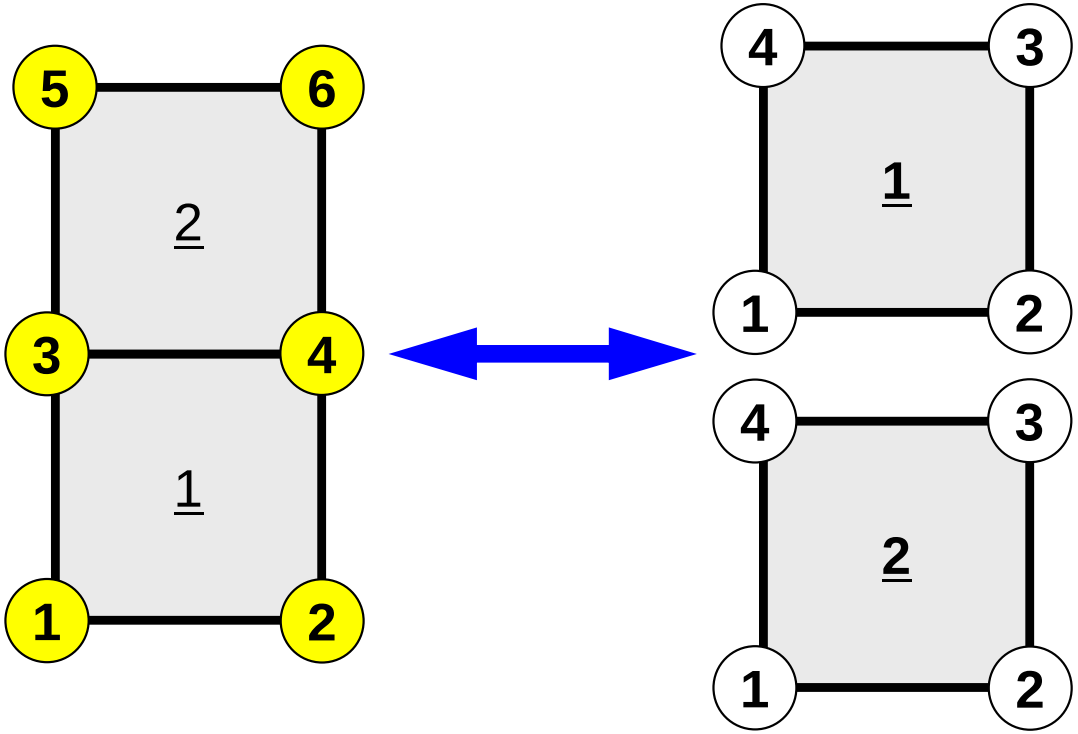
Remaining Procedures

- Element matrices have been formed.

- Accumulation to Global Matrix
- Implementation of Boundary Conditions
- Solving Linear Equations

- Details of implementation will be discussed in classes later than next week through explanation of programs

Accumulation: Local -> Global Matrices



$$[k^{(2)}]\{\phi^{(2)}\} = \{f^{(2)}\}$$

$$\begin{bmatrix} k_{11}^{(2)} & k_{12}^{(2)} & k_{13}^{(2)} & k_{14}^{(2)} \\ k_{21}^{(2)} & k_{22}^{(2)} & k_{23}^{(2)} & k_{24}^{(2)} \\ k_{31}^{(2)} & k_{32}^{(2)} & k_{33}^{(2)} & k_{34}^{(2)} \\ k_{41}^{(2)} & k_{42}^{(2)} & k_{43}^{(2)} & k_{44}^{(2)} \end{bmatrix} \begin{Bmatrix} \phi_1^{(2)} \\ \phi_2^{(2)} \\ \phi_3^{(2)} \\ \phi_4^{(2)} \end{Bmatrix} = \begin{Bmatrix} f_1^{(2)} \\ f_2^{(2)} \\ f_3^{(2)} \\ f_4^{(2)} \end{Bmatrix}$$

$$[k^{(1)}]\{\phi^{(1)}\} = \{f^{(1)}\}$$

$$\begin{bmatrix} k_{11}^{(1)} & k_{12}^{(1)} & k_{13}^{(1)} & k_{14}^{(1)} \\ k_{21}^{(1)} & k_{22}^{(1)} & k_{23}^{(1)} & k_{24}^{(1)} \\ k_{31}^{(1)} & k_{32}^{(1)} & k_{33}^{(1)} & k_{34}^{(1)} \\ k_{41}^{(1)} & k_{42}^{(1)} & k_{43}^{(1)} & k_{44}^{(1)} \end{bmatrix} \begin{Bmatrix} \phi_1^{(1)} \\ \phi_2^{(1)} \\ \phi_3^{(1)} \\ \phi_4^{(1)} \end{Bmatrix} = \begin{Bmatrix} f_1^{(1)} \\ f_2^{(1)} \\ f_3^{(1)} \\ f_4^{(1)} \end{Bmatrix}$$

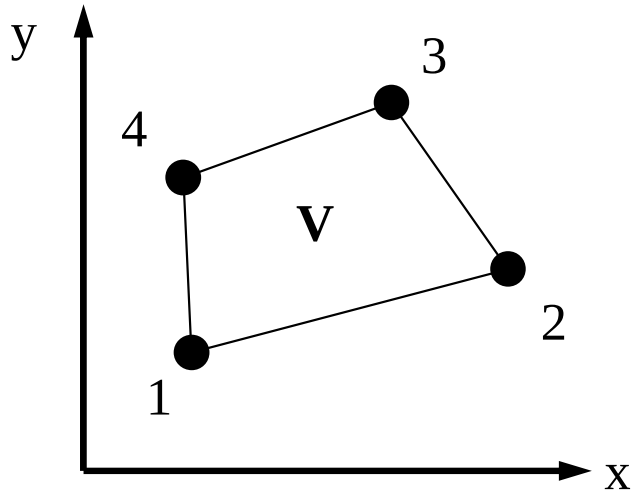
$$[K]\{\Phi\} = \{F\}$$

$$\begin{bmatrix} D_1 & X & X & X & & \\ X & D_2 & X & X & & \\ X & X & D_3 & X & X & X \\ X & X & X & D_4 & X & X \\ & & X & X & D_5 & X \\ & & X & X & X & D_6 \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \end{Bmatrix} = \begin{Bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \\ B_6 \end{Bmatrix}$$

- Formulation of 3D Element
- 3D Heat Equations
  - Galerkin Method
  - Element Matrices
  - **Exercise**
- Running the Code
- Data Structure
- Overview of the Program

Exercise

- Develop a program and calculate area of the following quadrilateral using Gaussian Quadrature.



1 : (1.0, 1.0)
2 : (4.0, 2.0)
3 : (3.0, 5.0)
4 : (2.0, 4.0)

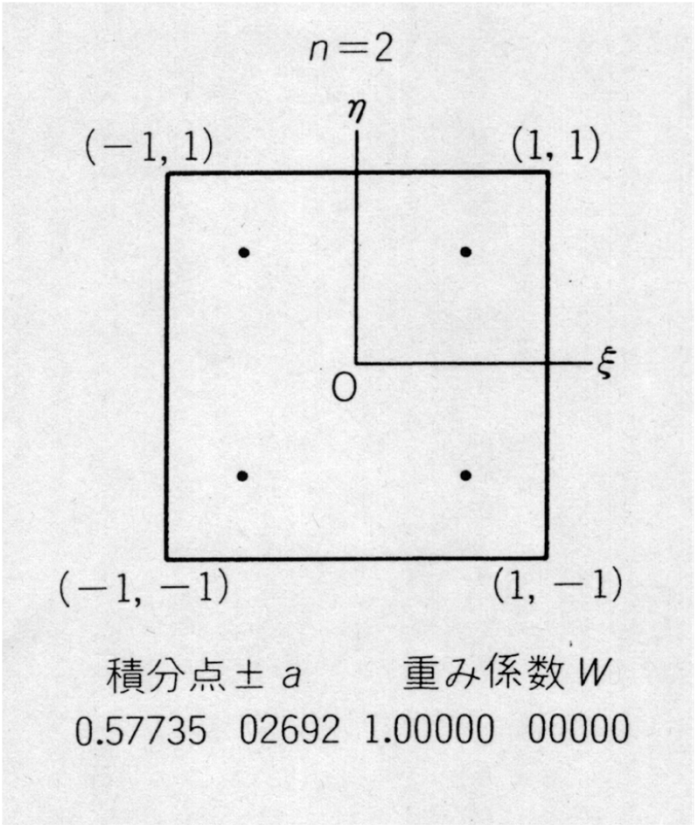
$$I = \int_V dV = \int_{-1}^{+1}\int_{-1}^{+1} \det|J|\, d\xi d\zeta$$

Tips (1/2)

- Calculate Jacobian
- Apply Gaussian Quadrature (n=2)

$$I = \int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta)\,d\xi d\eta = \sum_{i=1}^{m}\sum_{j=1}^{n}\left[W_i \cdot W_j \cdot f(\xi_i,\eta_j)\right]$$

```
implicit REAL*8 (A-H,O-Z)
real*8 W(2)
real*8 POI(2)

W(1)= 1.0d0
W(2)= 1.0d0
POI(1)= -0.5773502692d0
POI(2)= +0.5773502692d0

SUM= 0.d0
do jp= 1, 2
do ip= 1, 2
  FC = F(POI(ip),POI(jp))
  SUM= SUM + W (ip)*W (jp)*FC
enddo
enddo
```



Tips (2/2)

$$[J]=\begin{bmatrix}\dfrac{\partial x}{\partial \xi} & \dfrac{\partial y}{\partial \xi}\\ \dfrac{\partial x}{\partial \eta} & \dfrac{\partial y}{\partial \eta}\end{bmatrix},\quad \det|J|=\frac{\partial x}{\partial \xi}\cdot\frac{\partial y}{\partial \eta}-\frac{\partial y}{\partial \xi}\cdot\frac{\partial x}{\partial \eta}$$

$$\frac{\partial x}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{4}N_i x_i\right)=\sum_{i=1}^{4}\frac{\partial N_i}{\partial \xi}x_i,\quad \frac{\partial y}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{4}N_i y_i\right)=\sum_{i=1}^{4}\frac{\partial N_i}{\partial \xi}y_i,$$

$$\frac{\partial x}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{4}N_i x_i\right)=\sum_{i=1}^{4}\frac{\partial N_i}{\partial \eta}x_i,\quad \frac{\partial y}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{4}N_i y_i\right)=\sum_{i=1}^{4}\frac{\partial N_i}{\partial \eta}y_i$$

$$N_1(\xi,\eta)=\frac{1}{4}(1-\xi)(1-\eta),\quad N_2(\xi,\eta)=\frac{1}{4}(1+\xi)(1-\eta),$$

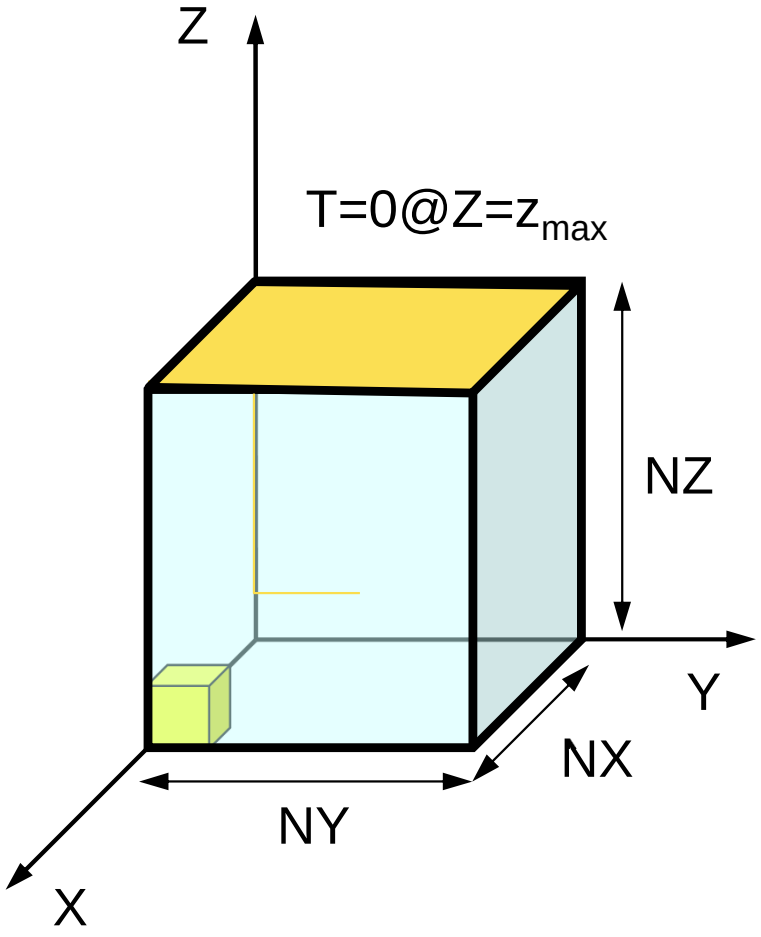
$$N_3(\xi,\eta)=\frac{1}{4}(1+\xi)(1+\eta),\quad N_4(\xi,\eta)=\frac{1}{4}(1-\xi)(1+\eta)$$

- Formulation of 3D Element
- 3D Heat Equations
  - Galerkin Method
  - Element Matrices

- **Running the Code**
- Data Structure
- Overview of the Program

3D Steady-State Heat Conduction

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



- Heat Generation
- Uniform thermal conductivity λ
- HEX meshes
  - 1x1x1 cubes
  - NX, NY, NZ cubes in each direction
- Boundary Conditions
  - T=0@Z=z_{max}
- Heat Gen. Rate is a function of location (cell center: x_c,y_c)
  - $\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$

Copy/Installation

Install

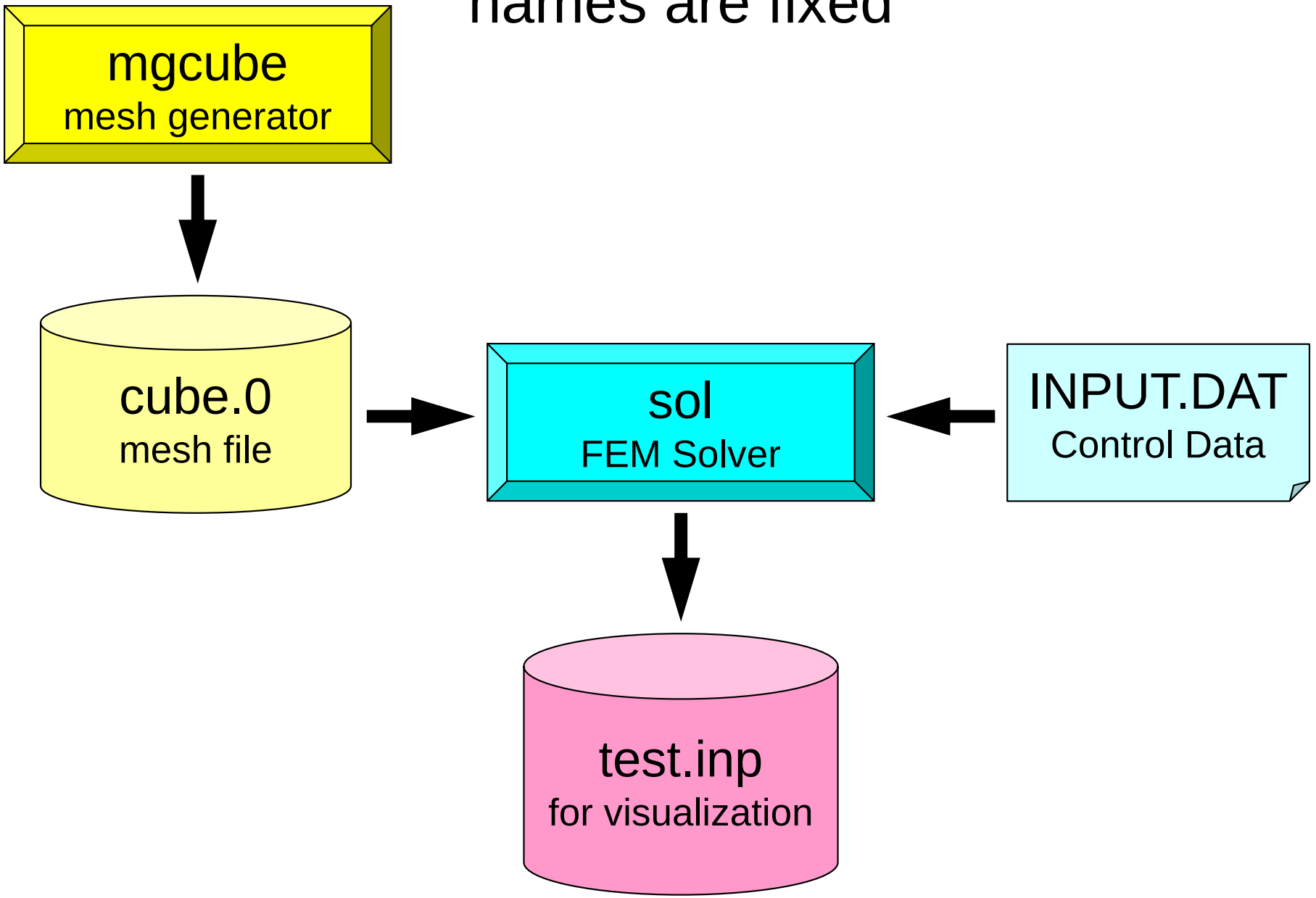
```
>$ cd
>$ cd fem-c/fem3d/src
>$ make
>$ ls ../run/sol
   sol
```

Install of Mesh Generator

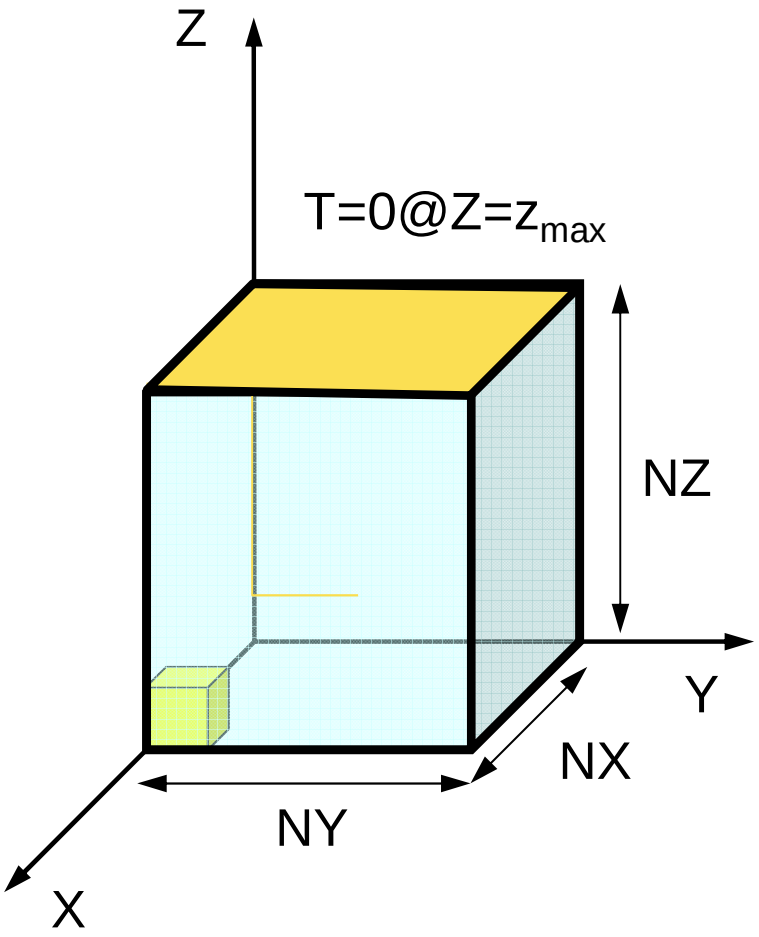
```
>$ cd
>$ cd fem-c/fem3d/run
>$ gcc -O3 mgcube.c -o mgcube
```

Operations

Starting from Grid Generation to Computation, File-names are fixed



Mesh Generation




```
>$ cd
>$ cd fem-c/fem3d/run
>$ ./mgcube.exe (or ./mgcube)

   NX, NY, NZ          ←  Number of
                          Elem's in each
                          direction
   20 20 20            ←  example


>$ ls cube.0               confirmation

    cube.0
```

Control File: INPUT.DAT

```
INPUT.DAT

cube.0          fname
2000            ITER
1.0 1.0         COND, QVOL
1.0e-08         RESID
```

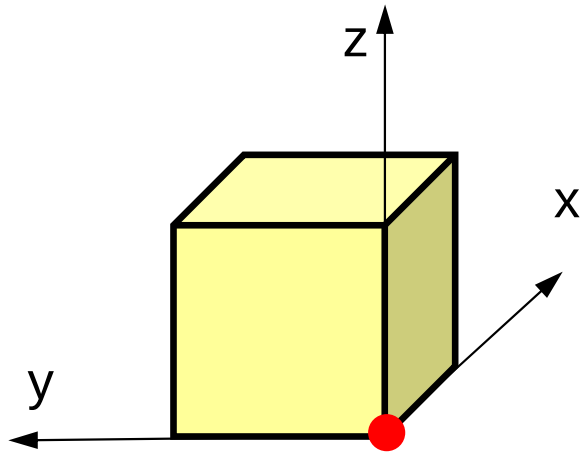
- fname : Name of Mesh File
- ITER : Max. Iterations for CG
- COND : Thermal Conductivity
- QVOL : Heat Generation Rate
- RESID : Criteria for Convergence of CG

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

$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

Running

```
>$ cd
>$ cd fem-c/fem3d/run
>$ ./sol.exe (or ./sol)

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




```
1 4.025833e+00
2 3.628020e+00
3 3.319234e+00
4 3.073771e+00
(…)
55 9.238550e-07
56 3.876258e-07
57 1.854812e-07
58 1.062119e-07
59 3.541404e-08
60 1.284087e-08
61 6.073277e-09          Total Number of Itreations

1  3.391200e+03          Temperature at Origin (0,0,0)
```

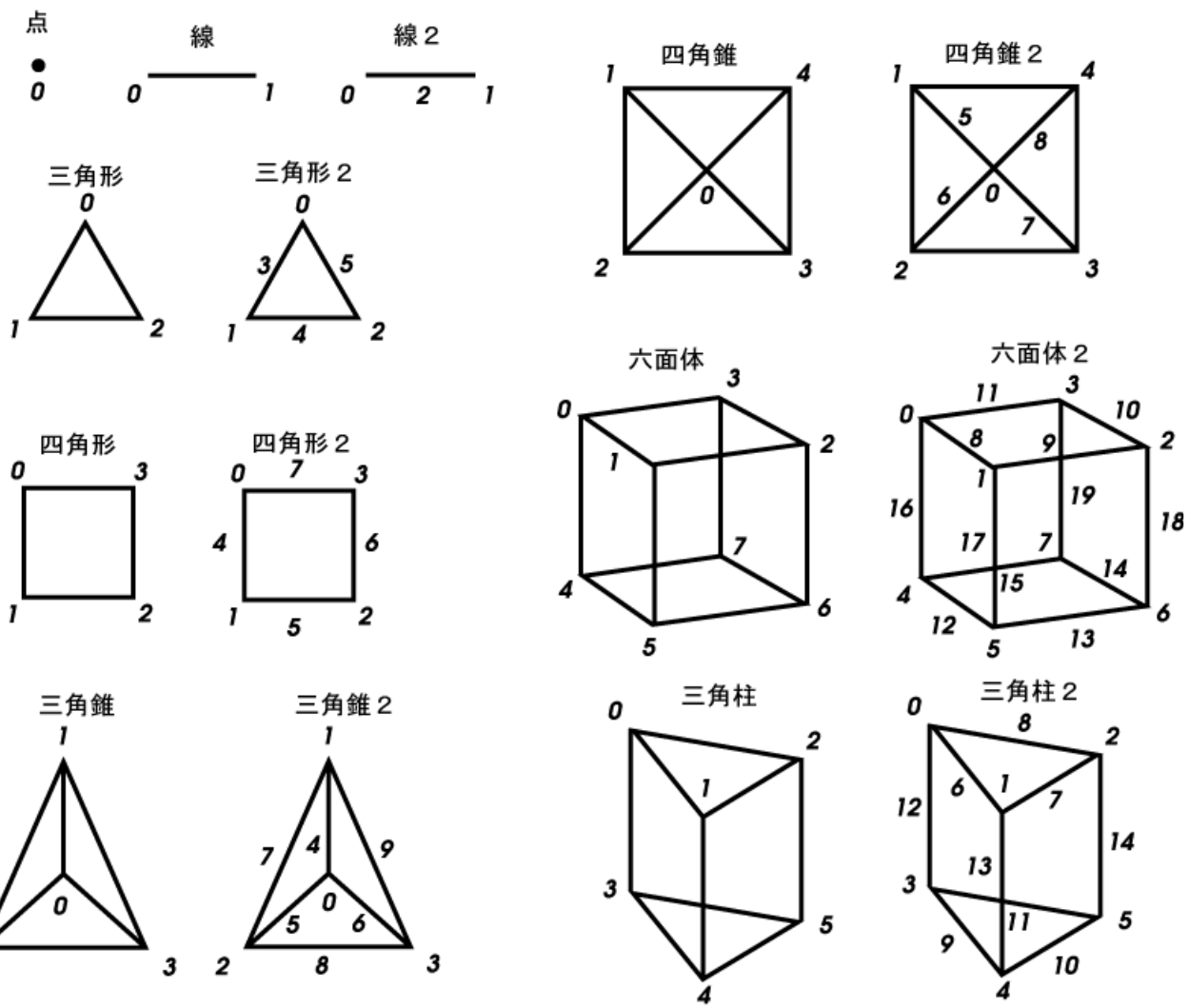
ParaView

- http://www.paraview.org/

- Opening files
- Displaying figures
- Saving image files
  - http://nkl.cc.u-tokyo.ac.jp/20w/ParaView.pdf

UCD Format (1/3)
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 (2/3)

- 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.

UCD Format (3/3): Old Format

(全節点数) (全要素数) (各節点のデータ数) (各要素のデータ数) (モデルのデータ数)
(節点番号1) (X座標) (Y座標) (Z座標)
(節点番号2) (X座標) (Y座標) (Z座標)

.
.
.

(要素番号1) (材料番号) (要素の種類) (要素を構成する節点のつながり)
(要素番号2) (材料番号) (要素の種類) (要素を構成する節点のつながり)

.
.
.

(節点のデータ成分数) (成分1の構成数) (成分2の構成数) ・・・(各成分の構成数)
(節点データ成分1のラベル), (単位)
(節点データ成分2のラベル), (単位)

.
.
.

(各節点データ成分のラベル), (単位)
(節点番号1) (節点データ1) (節点データ2) ・・・・・
(節点番号2) (節点データ1) (節点データ2) ・・・・・

.
.
.

(要素のデータ成分数) (成分1の構成数) (成分2の構成数) ・・・(各成分の構成数)
(要素データ成分1のラベル), (単位)
(要素データ成分2のラベル), (単位)

.
.
.

(各要素データ成分のラベル), (単位)
(要素番号1) (要素データ1) (要素データ2) ・・・・・
(要素番号2) (要素データ1) (要素データ2) ・・・・・

.
.
.

- Formulation of 3D Element
- 3D Heat Equations
  - Galerkin Method
  - Element Matrices

- Running the Code
- **Data Structure**
- Overview of the Program

Overview of Mesh File: cube.0

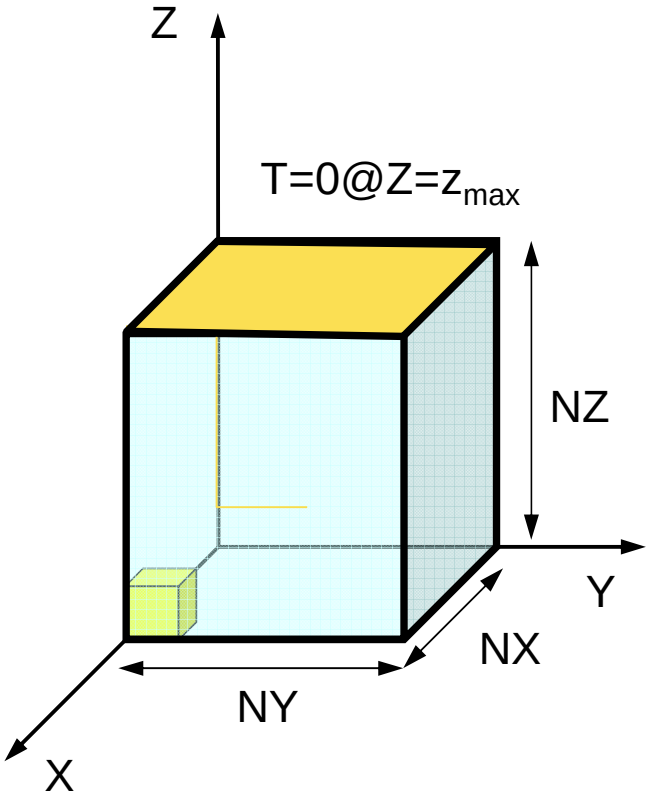
numbering starts from “1”

- Nodes
  - Node # (How many nodes ?)
  - Node ID, Coordinates
- Elements
  - Element #
  - Element Type
  - Element ID, Material ID, Connectivity
- Node Groups
  - Group #
  - Node # in each group
  - Group Name
  - Nodes in each group

Example of “cube.0” (NX=NY=NZ=4)

Node

```
  125                                    =5*5*5 (Node #)
    1      0.00      0.00      0.00
    2      1.00      0.00      0.00
    3      2.00      0.00      0.00
    4      3.00      0.00      0.00
    5      4.00      0.00      0.00
    6      0.00      1.00      0.00
    7      1.00      1.00      0.00
    8      2.00      1.00      0.00
    9      3.00      1.00      0.00

...

  121      0.00      4.00      4.00
  122      1.00      4.00      4.00
  123      2.00      4.00      4.00
  124      3.00      4.00      4.00
  125      4.00      4.00      4.00

Node  ID X-coord.   Y         Z
```



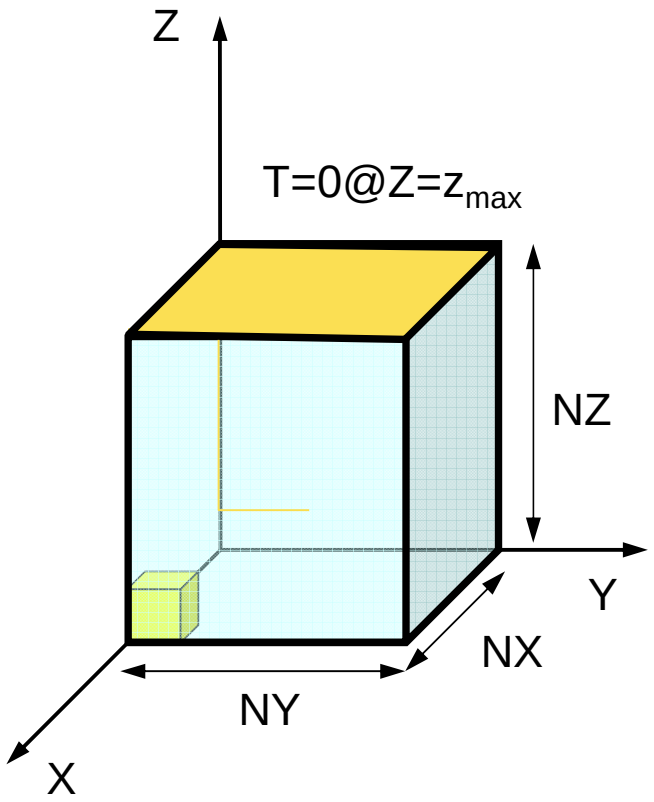
movie

Example of “cube.0” (NX=NY=NZ=4) Element (1/2)

```
  64                                        =4*4*4 (Element #)
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361
```

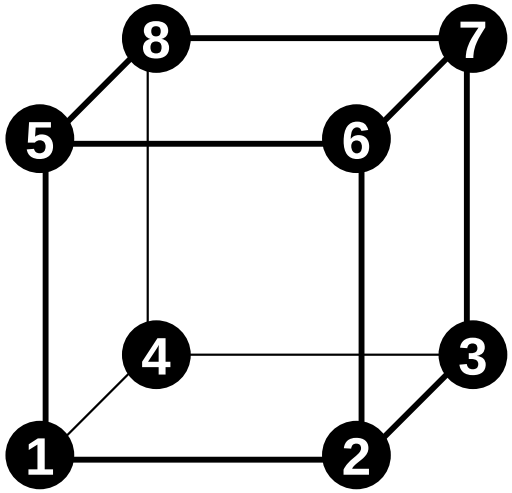
Element Type: 361

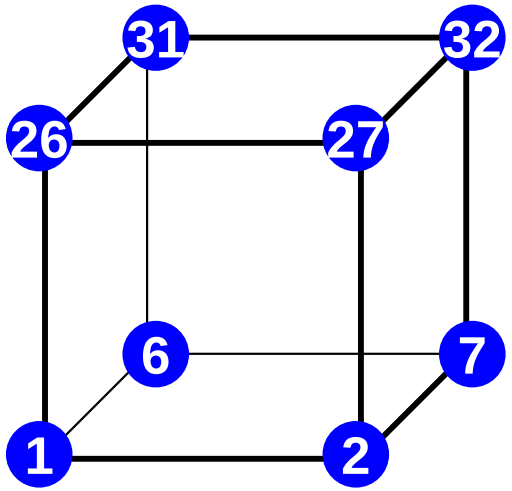
3D, Hexahedron, Linear (1st order)



Example of “cube.0” Element (2/2)

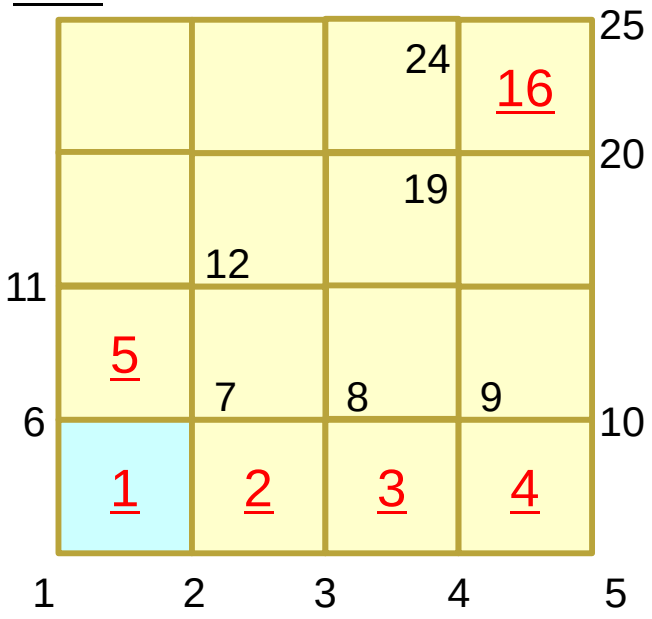
```
      1    1      1    2    7    6   26   27   32   31
      2    1      2    3    8    7   27   28   33   32
      3    1      3    4    9    8   28   29   34   33
      4    1      4    5   10    9   29   30   35   34
      5    1      6    7   12   11   31   32   37   36
      6    1      7    8   13   12   32   33   38   37
      7    1      8    9   14   13   33   34   39   38
      8    1      9   10   15   14   34   35   40   39
      9    1     11   12   17   16   36   37   42   41
     10    1     12   13   18   17   37   38   43   42
     11    1     13   14   19   18   38   39   44   43
     12    1     14   15   20   19   39   40   45   44
     13    1     16   17   22   21   41   42   47   46
...
     53    1     81   82   87   86  106  107  112  111
     54    1     82   83   88   87  107  108  113  112
     55    1     83   84   89   88  108  109  114  113
     56    1     84   85   90   89  109  110  115  114
     57    1     86   87   92   91  111  112  117  116
     58    1     87   88   93   92  112  113  118  117
     59    1     88   89   94   93  113  114  119  118
     60    1     89   90   95   94  114  115  120  119
     61    1     91   92   97   96  116  117  122  121
     62    1     92   93   98   97  117  118  123  122
     63    1     93   94   99   98  118  119  124  123
     64    1     94   95  100   99  119  120  125  124

Elem ID  MAT-ID          ID of 8 nodes
```



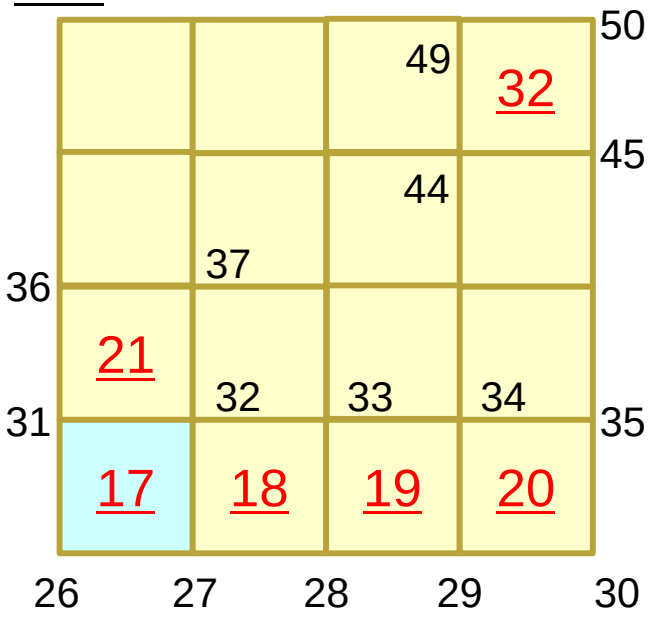


NX=NY=NZ=4, NXP1=NYP1=NZP1=5
ICELTOT= 64, INODTOT= 125, IBNODTOT= 25

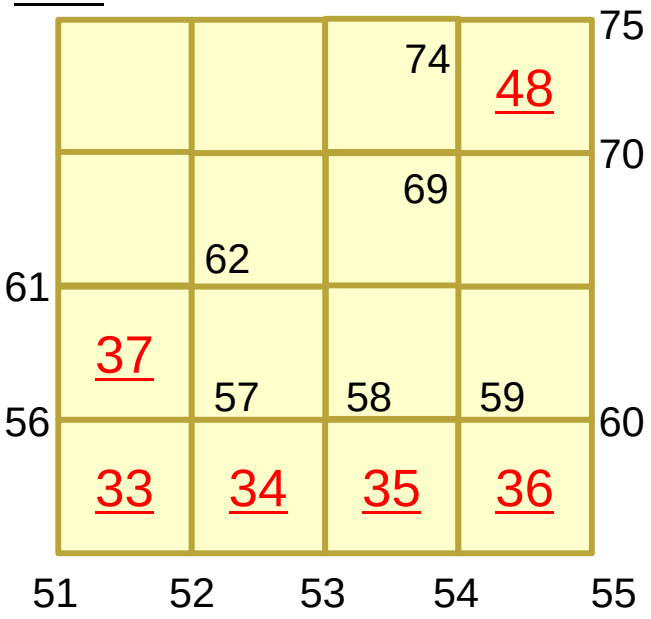
k=1

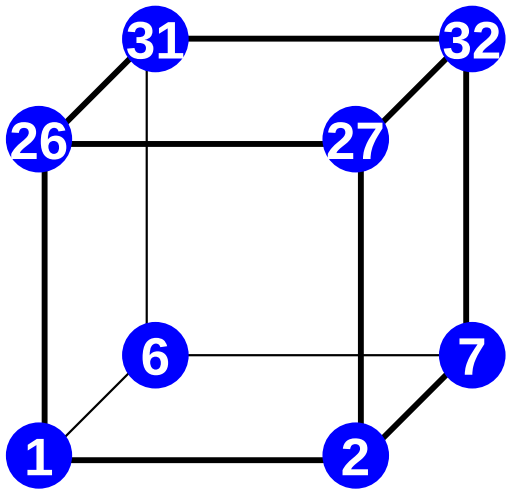


k=2

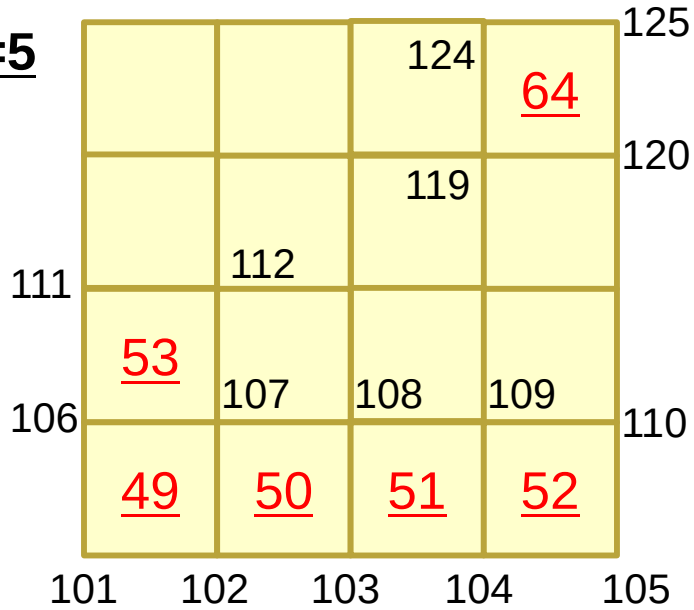


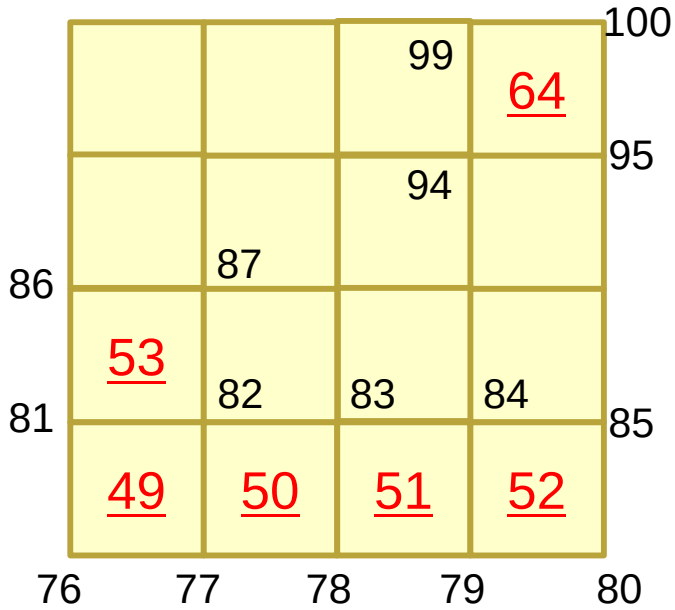
k=3





k=5

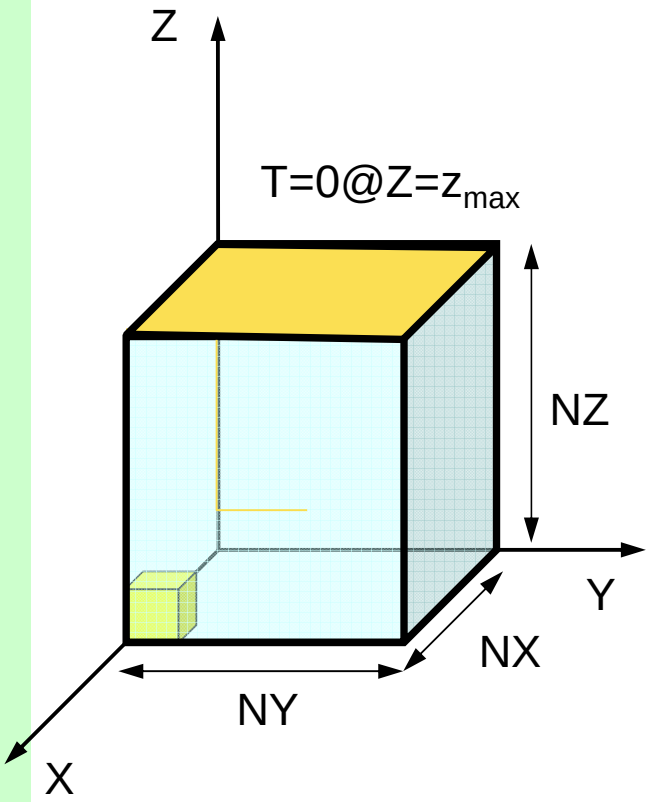




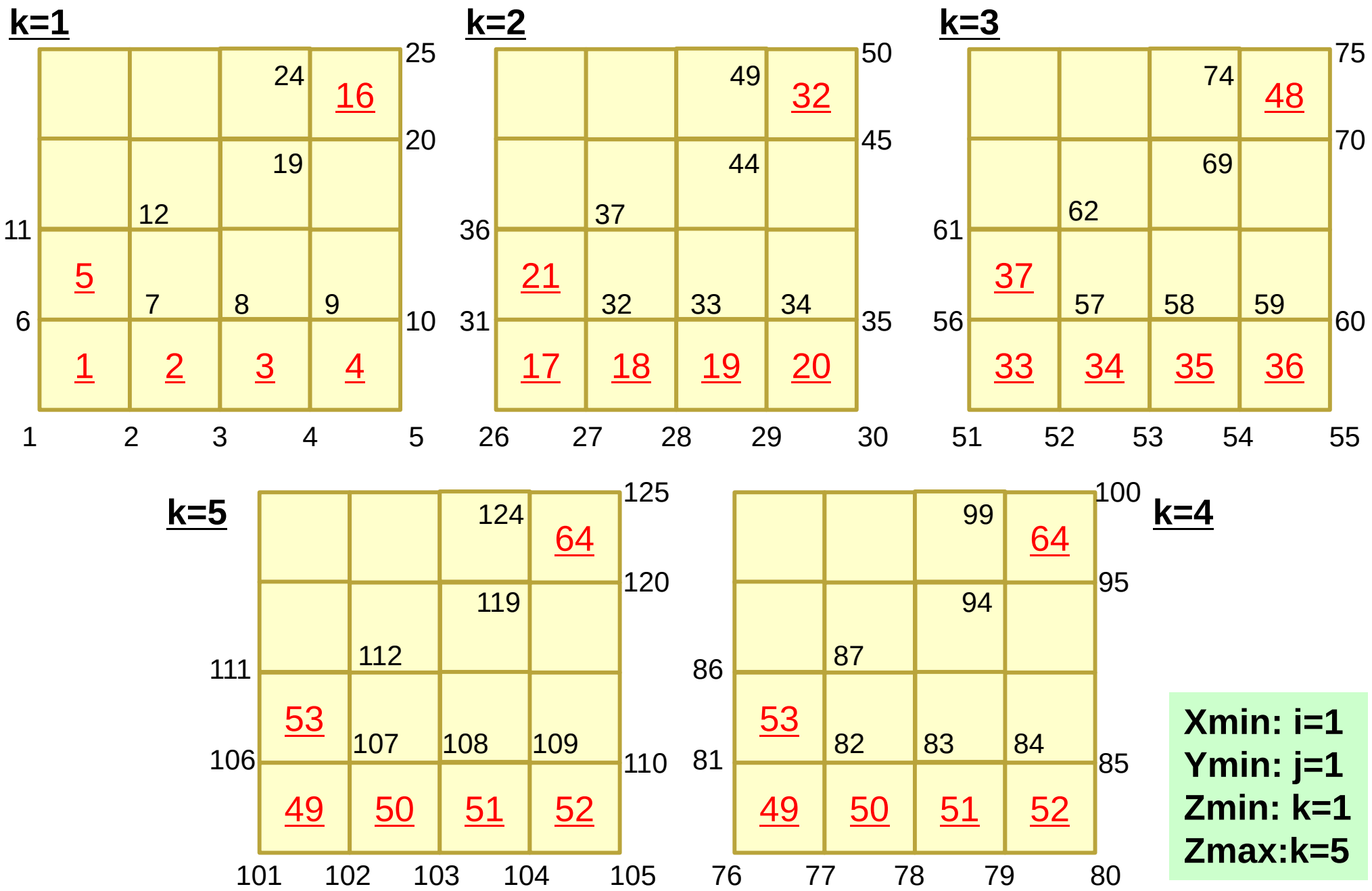
k=4

Example of “cube.0” Node Grp. Info.

```
   4                          Number of Groups
  25   50   75 100            Number of Nodes (ea. grp.)

Xmin
    1    6   11   16   21   26   31   36   41   46
   51   56   61   66   71   76   81   86   91   96
  101 106 111 116 121

Ymin
    1    2    3    4    5   26   27   28   29   30
   51   52   53   54   55   76   77   78   79   80
  101 102 103 104 105

Zmin
    1    2    3    4    5    6    7    8    9   10
   11   12   13   14   15   16   17   18   19   20
   21   22   23   24   25

Zmax
  101 102 103 104 105 106 107 108 109 110
  111 112 113 114 115 116 117 118 119 120
  121 122 123 124 125

no use after this line
```



NX=NY=NZ=4, NXP1=NYP1=NZP1=5
ICELTOT= 64, INODTOT= 125, IBNODTOT= 25



Mesh Generation

- Big Technical & Research Issue
  - Complicated Geometry
  - Large Scale
- Parallelization is difficult

- Commercial Mesh Generator
  - FEMAP
    - Interface to CAD Data Format

movie

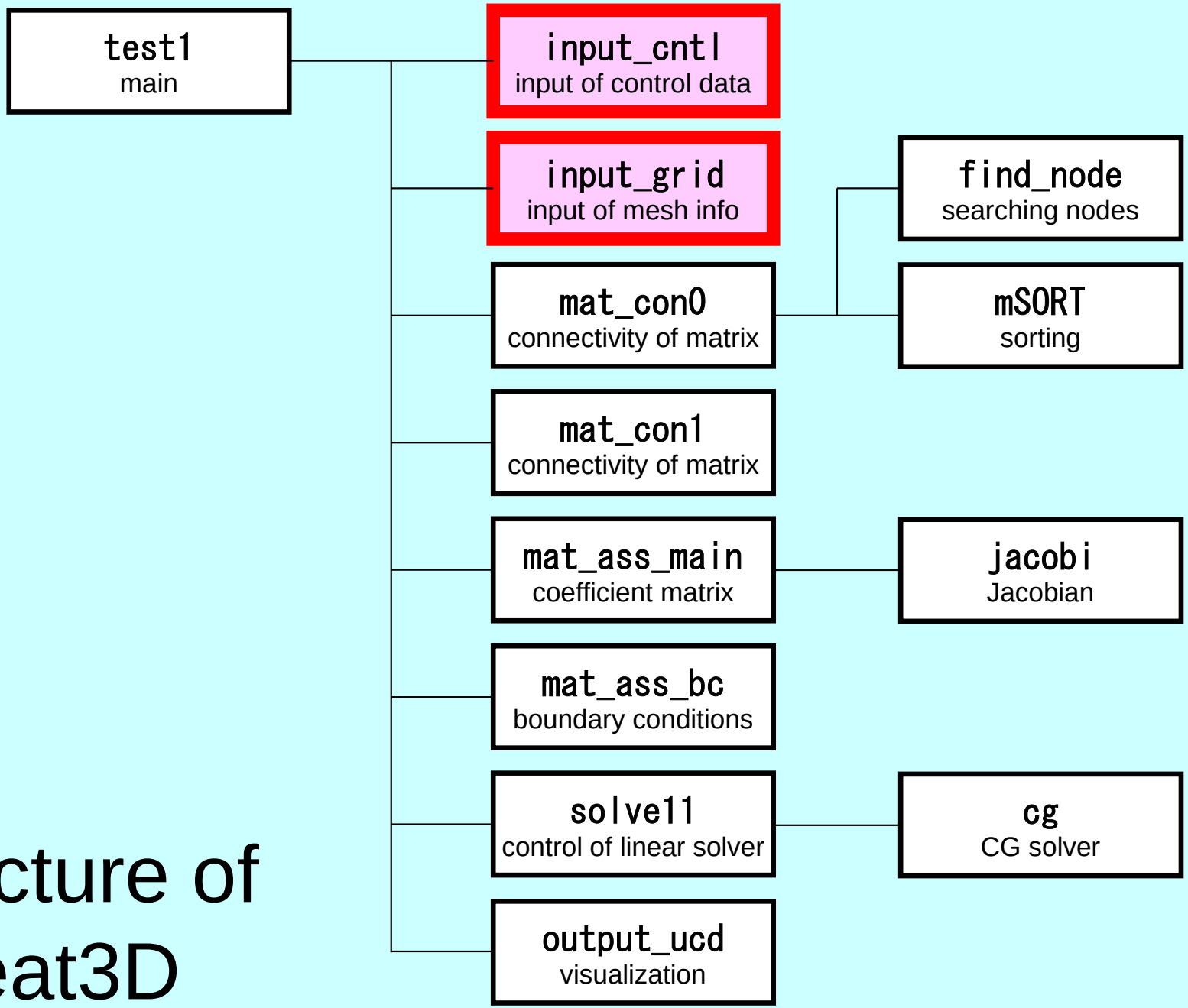
- Formulation of 3D Element
- 3D Heat Equations
  - Galerkin Method
  - Element Matrices

- Running the Code
- Data Structure
- **Overview of the Program**

FEM Procedures: Program

- Initialization
  - Control Data
  - Node, Connectivity of Elements (N: Node#, NE: Elem#)
  - Initialization of Arrays (Global/Element Matrices)
  - Element-Global Matrix Mapping (Index, Item)
- Generation of Matrix
  - Element-by-Element Operations (do icel= 1, NE)
    - Element matrices
    - Accumulation to global matrix
  - Boundary Conditions
- Linear Solver
  - Conjugate Gradient Method

Structure of heat3D



Main Part

```
int main()
{
  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()  ;

  SOLVE11();

  OUTPUT_UCD()    ;
  for(i=0;i<N;i++){
    if (XYZ[i][0]==0.e0) {
    if (XYZ[i][1]==0.e0) {
    if (XYZ[i][2]==0.e0) {
      printf("%8d%16.6e¥n¥n¥n", i+1, X[i]);}
    }}}
}
```

Global Variables: pfem_util.h (1/3)

Name	Type	Size	I/O	Definition
fname	C	[80]	I	Name of mesh file
N,NP	I		I	# Node
ICELTOT	I		I	# Element
NODGRPtot	I		I	# Node Group
XYZ	R	[N][3]	I	Node Coordinates
ICELNOD	I	[ICELTOT][8]	I	Element Connectivity
NODGRP_INDEX	I	[NODGRPtot+1]	I	# Node in each Node Group
NODGRP_ITEM	I	[NODGRP_INDEX[NODGRPTOT+1]]	I	Node ID in each Node Group
NODGRP_NAME	C80	[NODGRP_INDEX[NODGRPTOT+1]]	I	Name of NodeGroup
NLU	I		O	# Non-Zero Off-Diagonals at each node
NPLU	I		O	# Non-Zero Off-Diagonals
D	R	[N]	O	Diagonal Block of Global Matrix
B,X	R	[N]	O	RHS, Unknown Vector

Global Variables: pfem_util.h (2/3)

Name	Type	Size	I/O	Definition
AMAT	R	[NPLU]	O	Non-Zero Off-Diagonal Components of Global Matrix
indexLU	I	[N+1]	O	# Non-Zero Off-Diagonal Components
itemLU	I	[NPLU]	O	Column ID of Non-Zero Off-Diagonal Components
INLU	I	[N]	O	Number of Non-Zero Off-Diagonal Components at Each Node
IALU	I	[N][NLU]	O	Column ID of Non-Zero Off-Diagonal Components at Each Node
IWKX	I	[N][2]	O	Work Arrays
ITER, ITERactual	I		I	Number of CG Iterations (MAX, Actual)
RESID	R		I	Convergence Criteria (fixed as 1.e-8)
pfemIarray	I	[100]	O	Integer Parameter Array
pfemRarray	R	[100]	O	Real Parameter Array

Global Variables: pfem_util.h (3/3)

Name	Type	Size	I/O	Definition
O8th	R		I	= 0.125
PNQ, PNE, PNT	R	[2][2][8]	O	$\frac{\partial N_i}{\partial \xi}, \frac{\partial N_i}{\partial \eta}, \frac{\partial N_i}{\partial \zeta} (i = 1 \sim 8)$ at each Gaussian Quad. Point
POS, WEI	R	[2]	O	Coordinates, Weighting Factor at each Gaussian Quad. Point
NCOL1, NCOL2	I	[100]	O	Work arrays for sorting
SHAPE	R	[2][2][2][8]	O	N_i (i=1~8) at each Gaussian Quad Point
PNX, PNY, PNZ	R	[2][2][2][8]	O	$\frac{\partial N_i}{\partial x}, \frac{\partial N_i}{\partial y}, \frac{\partial N_i}{\partial z} (i = 1 \sim 8)$ at each Gaussian Quad. Point
DETJ	R	[2][2][2]	O	Determinant of Jacobian Matrix at each Gaussian Quad. Point
COND, QVOL	R		I	Thermal Conductivity, Heat Generation Rate

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

$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

INPUT_CNTL: Control Data

```
/**
 ** INPUT_CNTL
 **/
#include <stdio.h>
#include <stdlib.h>
#include "pfem_util.h"
/** **/
void INPUT_CNTL()
{
        FILE *fp;

        if( (fp=fopen("INPUT.DAT","r")) == NULL){
                fprintf(stdout,"input file cannot be opened!¥n");
                exit(1);
        }
        fscanf(fp,"%s",fname);
        fscanf(fp,"%d",&ITER);
        fscanf(fp, "%lf %lf", &COND, &QVOL);
        fscanf(fp, "%lf",     &RESID);
        fclose(fp);

        pfemRarray[0]= RESID;
        pfemIarray[0]= ITER;
}
```

INPUT.DAT

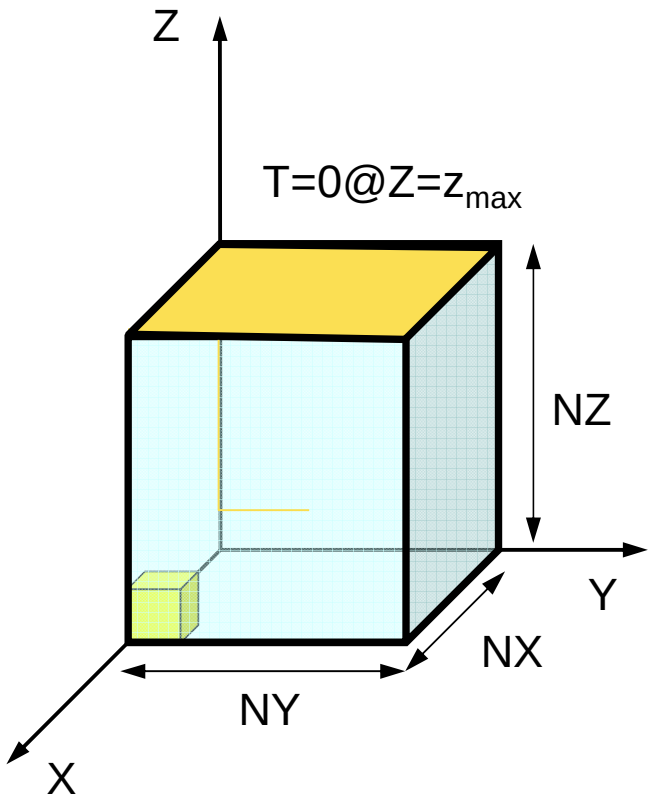
```
cube.0          fname
2000            ITER
1.0 1.0         COND, QVOL
1.0e-08         RESID
```

INPUT_GRID (1/3)

```
#include <stdio.h>
#include <stdlib.h>
#include "pfem_util.h"
#include "allocate.h"
void INPUT_GRID()
{
        FILE *fp;
        int i,j,k,ii,kk,nn,icel,iS,iE;
        int NTYPE,IMAT;

        if( (fp=fopen(fname,"r")) == NULL){
                fprintf(stdout,"input file cannot be opened!¥n");
                exit(1);
        }
/**
        NODE
**/
        fscanf(fp,"%d",&N);

        NP=N;
        XYZ=(KREAL**)allocate_matrix(sizeof(KREAL),N,3);

        for(i=0;i<N;i++){
                for(j=0;j<3;j++){
                        XYZ[i][j]=0.0;
                }
        }

        for(i=0;i<N;i++){
                fscanf(fp,"%d %lf %lf %lf",&ii,&XYZ[i][0],&XYZ[i][1],&XYZ[i][2]);
        }
```

Example of “cube.0” Node

```
  125                                        = N
    1      0.00      0.00      0.00
    2      1.00      0.00      0.00
    3      2.00      0.00      0.00
    4      3.00      0.00      0.00
    5      4.00      0.00      0.00
    6      0.00      1.00      0.00
    7      1.00      1.00      0.00
    8      2.00      1.00      0.00
    9      3.00      1.00      0.00

...

  121      0.00      4.00      4.00
  122      1.00      4.00      4.00
  123      2.00      4.00      4.00
  124      3.00      4.00      4.00
  125      4.00      4.00      4.00

                  XYZ[i][3]
```



allocate, deallocate (1/2)

Same interface with FORTRAN

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

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;
}

void deallocate_vector(void *a)
{
  free( a );
}
```

```
INDEX=(KINT*  )allocate_vector(sizeof(KINT),NGtot+1);  INDEX[Ngtot+1]
NAME =(CHAR80*)allocate_vector(sizeof(CHAR80),NGtot); NAME[NGtot]
WW=(KREAL**) allocate_matrix(sizeof(KREAL),4,N);      WW[4][N]
```

allocate, deallocate (2/2)

Same interface with FORTRAN

```
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;
}

void deallocate_matrix(void **aa)
{
        free( aa );
}
```

```
INDEX=(KINT*  )allocate_vector(sizeof(KINT),NGtot+1);  INDEX[Ngtot+1]
NAME =(CHAR80*)allocate_vector(sizeof(CHAR80),NGtot); NAME[NGtot]
WW=(KREAL**) allocate_matrix(sizeof(KREAL),4,N);      WW[4][N]
```

INPUT_GRID (2/3)

```
/**
        ELEMENT
**/
        fscanf(fp,"%d",&ICELTOT);

        ICELNOD=(KINT**)allocate_matrix(sizeof(KINT),ICELTOT,8);
        for(i=0;i<ICELTOT;i++) fscanf(fp,"%d",&NTYPE);


        for(icel=0;icel<ICELTOT;icel++){
                fscanf(fp,"%d %d %d %d %d %d %d %d %d %d",&ii,&IMAT,
                &ICELNOD[icel][0],&ICELNOD[icel][1],&ICELNOD[icel][2],&ICELNOD[icel][3],
                &ICELNOD[icel][4],&ICELNOD[icel][5],&ICELNOD[icel][6],&ICELNOD[icel][7]);
        }
```

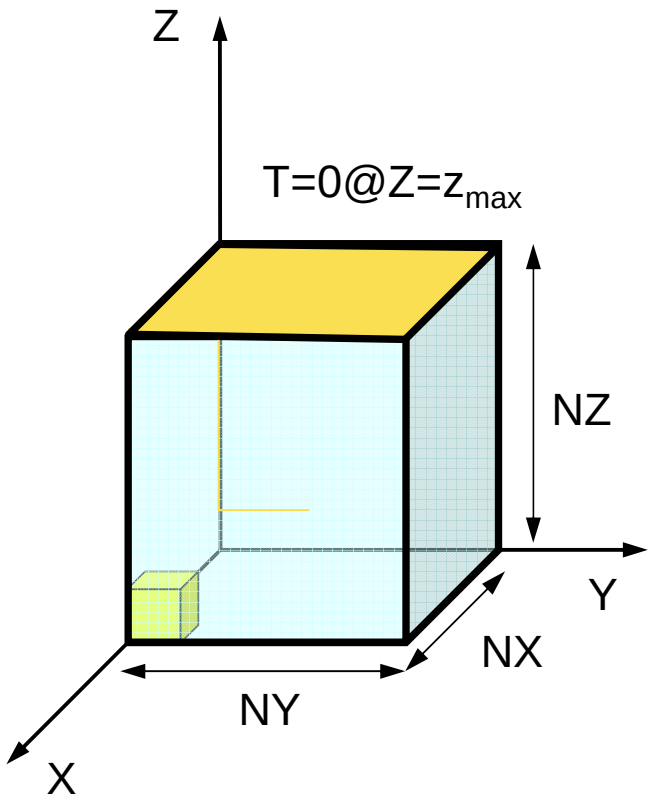
ICELNOD[i][j]:
Node ID starting from “1”.
Element ID starts from “0”.

Example of “cube.0” Element (1/2)

```
  64                                    = ICELTOT

 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361 361 361 361 361 361 361
 361 361 361 361
```

Element Type: 361

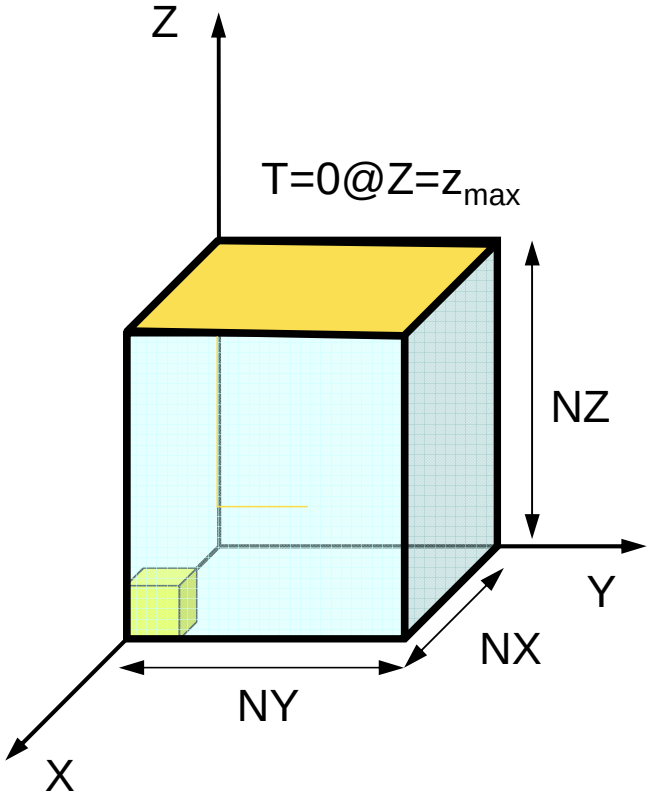
3D, Hexahedron, Linear (1st order)

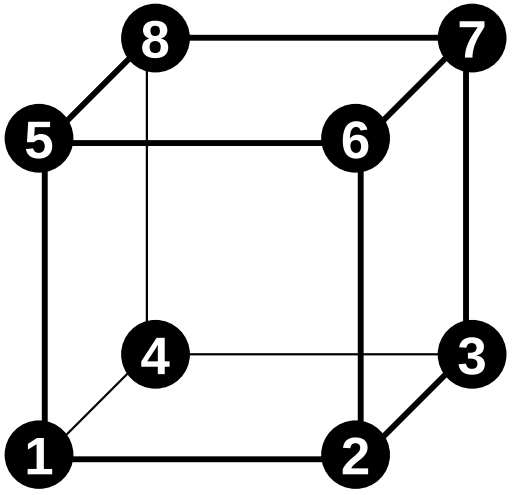


Example of “cube.0” Element (2/2)

1	1	1	2	7	6	26	27	32	31
2	1	2	3	8	7	27	28	33	32
3	1	3	4	9	8	28	29	34	33
4	1	4	5	10	9	29	30	35	34
5	1	6	7	12	11	31	32	37	36
6	1	7	8	13	12	32	33	38	37
7	1	8	9	14	13	33	34	39	38
8	1	9	10	15	14	34	35	40	39
9	1	11	12	17	16	36	37	42	41
10	1	12	13	18	17	37	38	43	42
11	1	13	14	19	18	38	39	44	43
12	1	14	15	20	19	39	40	45	44
13	1	16	17	22	21	41	42	47	46
...									
53	1	81	82	87	86	106	107	112	111
54	1	82	83	88	87	107	108	113	112
55	1	83	84	89	88	108	109	114	113
56	1	84	85	90	89	109	110	115	114
57	1	86	87	92	91	111	112	117	116
58	1	87	88	93	92	112	113	118	117
59	1	88	89	94	93	113	114	119	118
60	1	89	90	95	94	114	115	120	119
61	1	91	92	97	96	116	117	122	121
62	1	92	93	98	97	117	118	123	122
63	1	93	94	99	98	118	119	124	123
64	1	94	95	100	99	119	120	125	124

iMAT ICELNOD[icel][8]





INPUT_GRID (3/3)

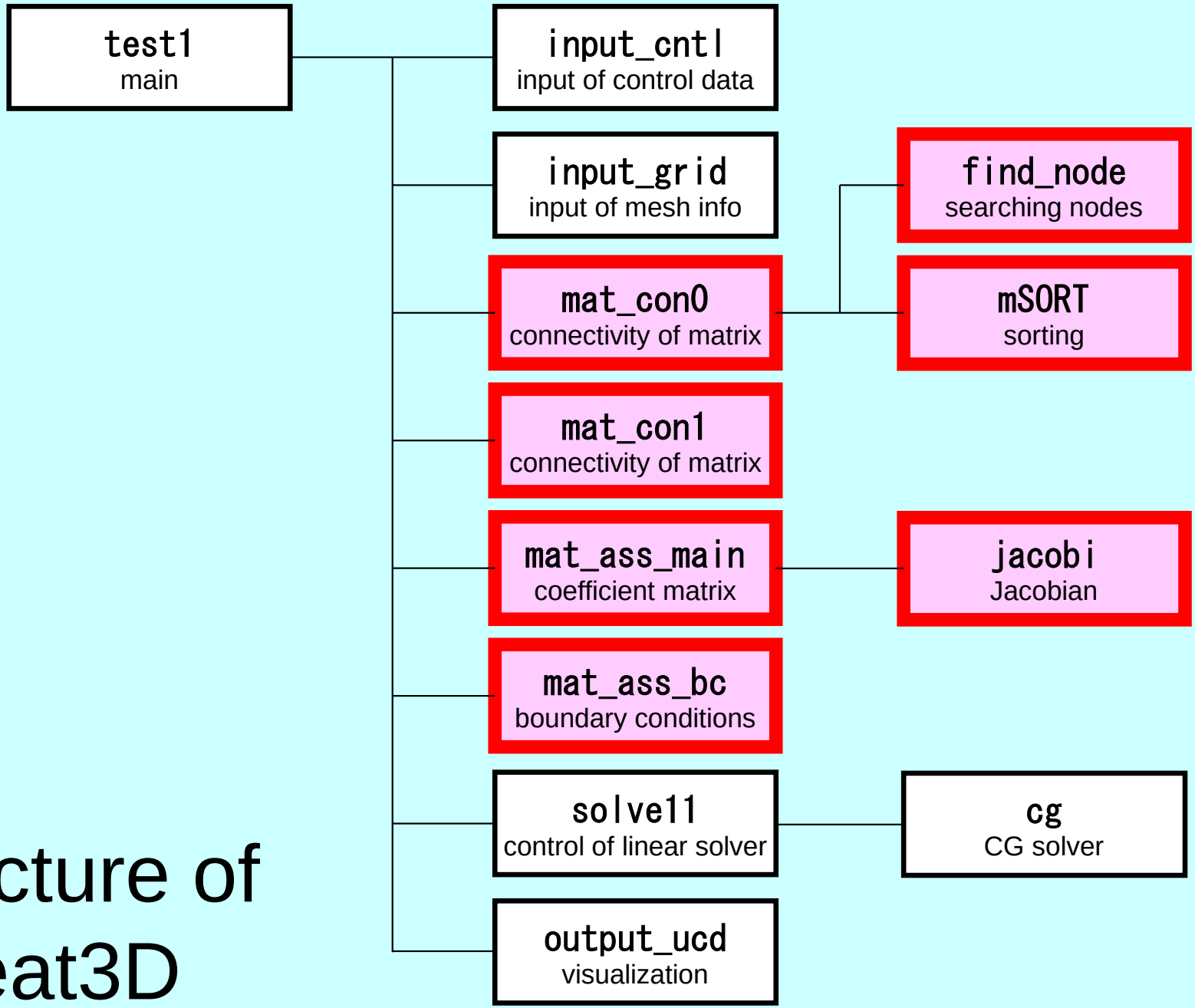
```
/**
        NODE grp.  info.
**/
        fscanf(fp,"%d",&NODGRPtot);

        NODGRP_INDEX=(KINT*  )allocate_vector(sizeof(KINT),NODGRPtot+1);
        NODGRP_NAME =(CHAR80*)allocate_vector(sizeof(CHAR80),NODGRPtot);
        for(i=0;i<NODGRPtot+1;i++) NODGRP_INDEX[i]=0;

        for(i=0;i<NODGRPtot;i++) fscanf(fp,"%d",&NODGRP_INDEX[i+1]);
        nn=NODGRP_INDEX[NODGRPtot];
        NODGRP_ITEM=(KINT*)allocate_vector(sizeof(KINT),nn);

        for(k=0;k<NODGRPtot;k++){
                iS= NODGRP_INDEX[k];
                iE= NODGRP_INDEX[k+1];
                fscanf(fp,"%s",NODGRP_NAME[k].name);
                nn= iE - iS;
                if( nn != 0 ){
                        for(kk=iS;kk<iE;kk++) fscanf(fp,"%d",&NODGRP_ITEM[kk]);
                }
        }

        fclose(fp);
}
```

Node Group:
Node ID's start from "1"

Example of “cube.0” Node Grp. Info.

```
   4                                                        NODGRPtot
  25  50  75 100                                           NODGRP_INDEX[1-4]

Xmin                                                       NODGRP_NAME[0]
   1   6  11  16  21  26  31  36  41  46                   NODGRP_ITEM[0-24]
  51  56  61  66  71  76  81  86  91  96
 101 106 111 116 121

Ymin                                                       NODGRP_NAME[1]
   1   2   3   4   5  26  27  28  29  30                   NODGRP_ITEM[25-49]
  51  52  53  54  55  76  77  78  79  80
 101 102 103 104 105

Zmin                                                       NODGRP_NAME[2]
   1   2   3   4   5   6   7   8   9  10                   NODGRP_ITEM[50-74]
  11  12  13  14  15  16  17  18  19  20
  21  22  23  24  25

Zmax                                                       NODGRP_NAME[3]
 101 102 103 104 105 106 107 108 109 110                   NODGRP_ITEM[75-99]
 111 112 113 114 115 116 117 118 119 120
 121 122 123 124 125
```

Structure of heat3D



Global Variables: pfem_util.h (1/3)

Name	Type	Size	I/O	Definition
fname	C	[80]	I	Name of mesh file
N,NP	I		I	# Node
ICELTOT	I		I	# Element
NODGRPtot	I		I	# Node Group
XYZ	R	[N][3]	I	Node Coordinates
ICELNOD	I	[ICELTOT][8]	I	Element Connectivity
NODGRP_INDEX	I	[NODGRPtot+1]	I	# Node in each Node Group
NODGRP_ITEM	I	[NODGRP_INDEX[NODGRPTOT+1]]	I	Node ID in each Node Group
NODGRP_NAME	C80	[NODGRP_INDEX[NODGRPTOT+1]]	I	Name of NodeGroup
NLU	I		O	# Non-Zero Off-Diagonals at each node
NPLU	I		O	# Non-Zero Off-Diagonals
D	R	[N]	O	Diagonal Block of Global Matrix
B,X	R	[N]	O	RHS, Unknown Vector

Global Variables: pfem_util.h (2/3)

Name	Type	Size	I/O	Definition
AMAT	R	[NPLU]	O	Non-Zero Off-Diagonal Components of Global Matrix
indexLU	I	[N+1]	O	# Non-Zero Off-Diagonal Components
itemLU	I	[NPLU]	O	Column ID of Non-Zero Off-Diagonal Components
INLU	I	[N]	O	Number of Non-Zero Off-Diagonal Components at Each Node
IALU	I	[N][NLU]	O	Column ID of Non-Zero Off-Diagonal Components at Each Node
IWKX	I	[N][2]	O	Work Arrays
ITER, ITERactual	I		I	Number of CG Iterations (MAX, Actual)
RESID	R		I	Convergence Criteria (fixed as 1.e-8)
pfemIarray	I	[100]	O	Integer Parameter Array
pfemRarray	R	[100]	O	Real Parameter Array

Global Variables: pfem_util.h (3/3)

Name	Type	Size	I/O	Definition
O8th	R		I	= 0.125
PNQ, PNE, PNT	R	[2][2][8]	O	$\frac{\partial N_i}{\partial \xi}, \frac{\partial N_i}{\partial \eta}, \frac{\partial N_i}{\partial \zeta} (i = 1 \sim 8)$ at each Gaussian Quad. Point
POS, WEI	R	[2]	O	Coordinates, Weighting Factor at each Gaussian Quad. Point
NCOL1, NCOL2	I	[100]	O	Work arrays for sorting
SHAPE	R	[2][2][2][8]	O	N_i (i=1~8) at each Gaussian Quad Point
PNX, PNY, PNZ	R	[2][2][2][8]	O	$\frac{\partial N_i}{\partial x}, \frac{\partial N_i}{\partial y}, \frac{\partial N_i}{\partial z} (i = 1 \sim 8)$ at each Gaussian Quad. Point
DETJ	R	[2][2][2]	O	Determinant of Jacobian Matrix at each Gaussian Quad. Point
COND, QVOL	R		I	Thermal Conductivity, Heat Generation Rate

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

$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

Towards Matrix Assembling

- In 1D, it was easy to obtain information related to index and item.
  - 2 non-zero off-diagonals for each node
  - ID of non-zero off-diagonal : i+1, i-1, where “i” is node ID
- In 3D, situation is more complicated:
  - Number of non-zero off-diagonal components is between 7 and 26 for the current target problem
  - More complicated for real problems.
  - Generally, there are no information related to number of non-zero off-diagonal components beforehand.

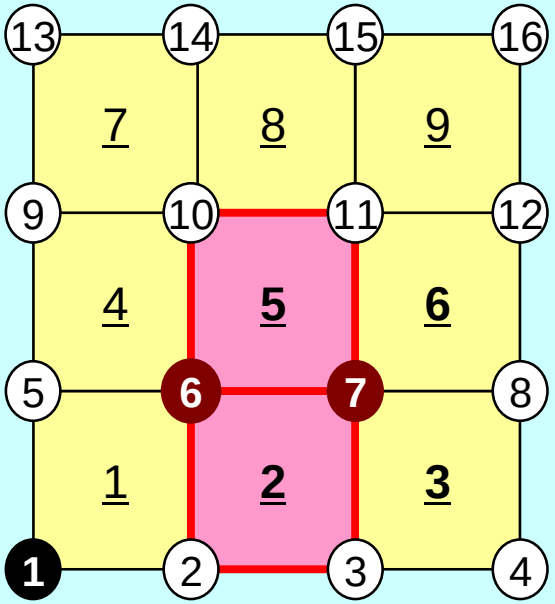
movie

Towards Matrix Assembling

- In 1D, it was easy to obtain information related to index and item.
  - 2 non-zero off-diagonals for each node
  - ID of non-zero off-diagonal : i+1, i-1, where “i” is node ID
- In 3D, situation is more complicated:
  - Number of non-zero off-diagonal components is between 7 and 26 for the current target problem
  - More complicated for real problems.
  - Generally, there are no information related to number of non-zero off-diagonal components beforehand.
- Count number of non-zero off-diagonals using arrays: INLU[N], IALU[N][NLU]

Main Part

```
/**
        program heat3D
**/
#include <stdio.h>
#include <stdlib.h>
FILE* fp_log;
#define GLOBAL_VALUE_DEFINE
#include "pfem_util.h"
//#include "solver11.h"
extern void INPUT_CNTL();
extern void INPUT_GRID();
extern void MAT_CON0();
extern void MAT_CON1();
extern void MAT_ASS_MAIN();
extern void MAT_ASS_BC();
extern void SOLVE11();
extern void OUTPUT_UCD();
int main()
{

  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()   ;

  SOLVE11();

  OUTPUT_UCD()     ;
}
```

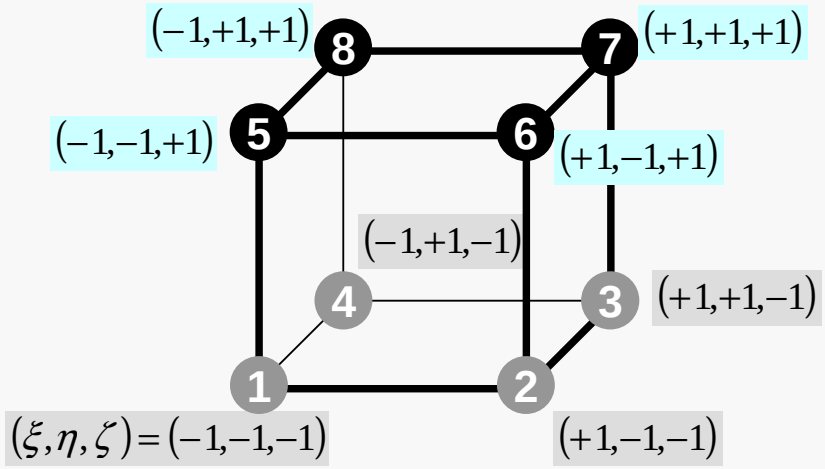


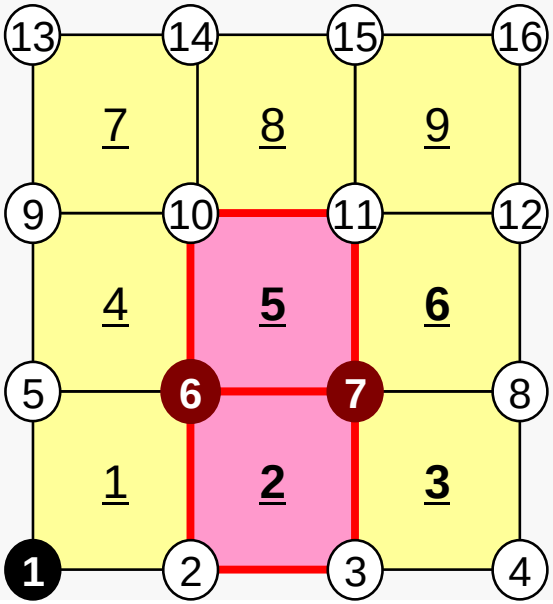
MAT_CON0: generates INU, IALU
MAT_CON1: generates index, item

Node ID starting from “1”

MAT_CON0: Overview

```
do icel= 1, ICELTOT
   generate INLU, IALU
   according to 8 nodes of hex. elements
   (FIND_NODE)
enddo
```





Generating Connectivity of Matrix MAT_CON0 (1/4)

```
/**
 ** MAT_CON0
 **/

#include <stdio.h>
#include "pfem_util.h"
#include "allocate.h "

extern FILE *fp_log;
/*** external functions ***/
extern void mSORT(int*, int*, int);
/*** static functuons ***/
static void FIND_TS_NODE (int,int);

void MAT_CON0()
{
  int i,j,k,icel,in;
  int in1,in2,in3,in4,in5,in6,in7,in8;
  int NN;

  NLU= 26;

  INLU=(KINT* )allocate_vector(sizeof(KINT),N);
  IALU=(KINT**)allocate_matrix(sizeof(KINT),N,NLU);

  for(i=0;i<N;i++) INLU[i]=0;
  for(i=0;i<N;i++) for(j=0;j<NLU;j++) IALU[i][j]=0;
```

NLU:
Number of maximum number of connected nodes to each node (number of upper/lower non-zero off-diagonal nodes)

In the current problem, geometry is rather simple. Therefore we can specify NLU in this way.

If it's not clear ->
Try more flexible implementation

Why NLU=26 ?

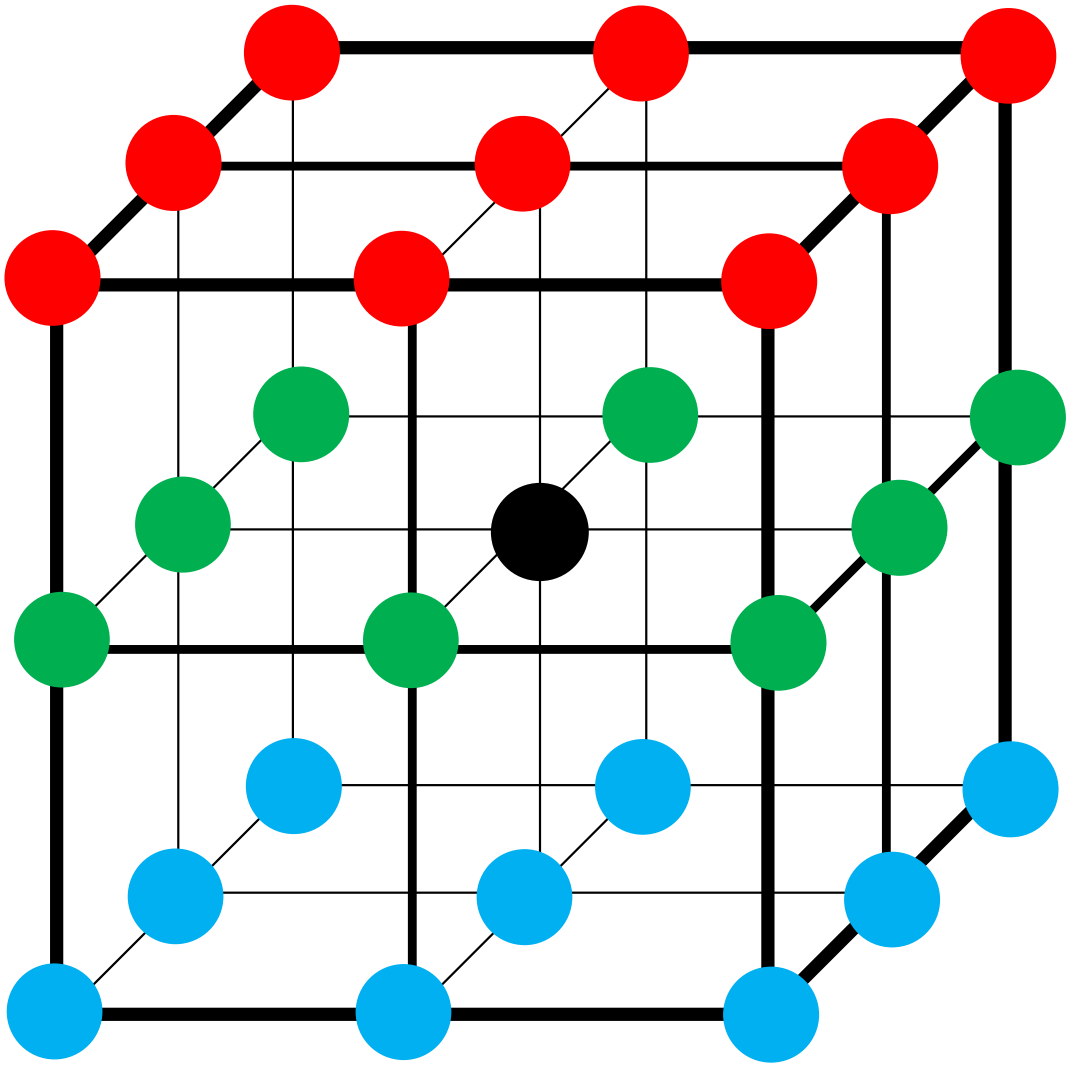
Max Number of Neighboring Nodes

9+8+9= 26

NLU:
Number of maximum number of connected nodes to each node (number of upper/lower non-zero off-diagonal nodes)

In the current problem, geometry is rather simple. Therefore we can specify NLU in this way.

If it's not clear ->
Try more flexible implementation



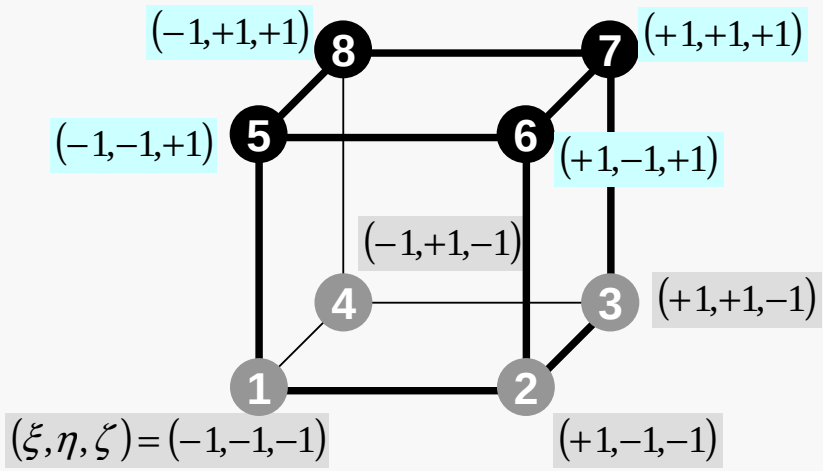
Generating Connectivity of Matrix MAT_CON0 (1/4)

```
/**
 ** MAT_CON0
 **/

#include <stdio.h>
#include "pfem_util.h"
#include "allocate.h "

extern FILE *fp_log;
/*** external functions ***/
extern void mSORT(int*, int*, int);
/*** static functuons ***/
static void FIND_TS_NODE (int,int);

void MAT_CON0()
{
  int i,j,k,icel,in;
  int in1,in2,in3,in4,in5,in6,in7,in8;
  int NN;

  NLU= 26;

  INLU=(KINT* )allocate_vector(sizeof(KINT),N);
  IALU=(KINT**)allocate_matrix(sizeof(KINT),N,NLU);

  for(i=0;i<N;i++) INLU[i]=0;
  for(i=0;i<N;i++) for(j=0;j<NLU;j++) IALU[i][j]=0;
```

Array	Size	Description
INLU	[N]	Number of connected nodes to each node (lower/upper)
IALU	[N][NLU]	Corresponding connected node ID (column ID)

Generating Connectivity of Matrix MAT_CON0 (2/4): Starting from 1

```
for( icel=0;icel< ICELTOT;icel++){
   in1=ICELNOD[icel][0];
   in2=ICELNOD[icel][1];
   in3=ICELNOD[icel][2];
   in4=ICELNOD[icel][3];
   in5=ICELNOD[icel][4];
   in6=ICELNOD[icel][5];
   in7=ICELNOD[icel][6];
   in8=ICELNOD[icel][7];

   FIND_TS_NODE (in1,in2);
   FIND_TS_NODE (in1,in3);
   FIND_TS_NODE (in1,in4);
   FIND_TS_NODE (in1,in5);
   FIND_TS_NODE (in1,in6);
   FIND_TS_NODE (in1,in7);
   FIND_TS_NODE (in1,in8);

   FIND_TS_NODE (in2,in1);
   FIND_TS_NODE (in2,in3);
   FIND_TS_NODE (in2,in4);
   FIND_TS_NODE (in2,in5);
   FIND_TS_NODE (in2,in6);
   FIND_TS_NODE (in2,in7);
   FIND_TS_NODE (in2,in8);

   FIND_TS_NODE (in3,in1);
   FIND_TS_NODE (in3,in2);
   FIND_TS_NODE (in3,in4);
   FIND_TS_NODE (in3,in5);
   FIND_TS_NODE (in3,in6);
   FIND_TS_NODE (in3,in7);
   FIND_TS_NODE (in3,in8);
```



FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search

```
/***
 *** FIND_TS_NODE
 **/

static void FIND_TS_NODE (int ip1,int ip2)
{
  int kk,icou;

  for(kk=1;kk<=INLU[ip1-1];kk++){
    if(ip2 == IALU[ip1-1][kk-1]) return;
  }

  icou=INLU[ip1-1]+1;
  IALU[ip1-1][icou-1]=ip2;
  INLU[ip1-1]=icou;

  return;
}
```

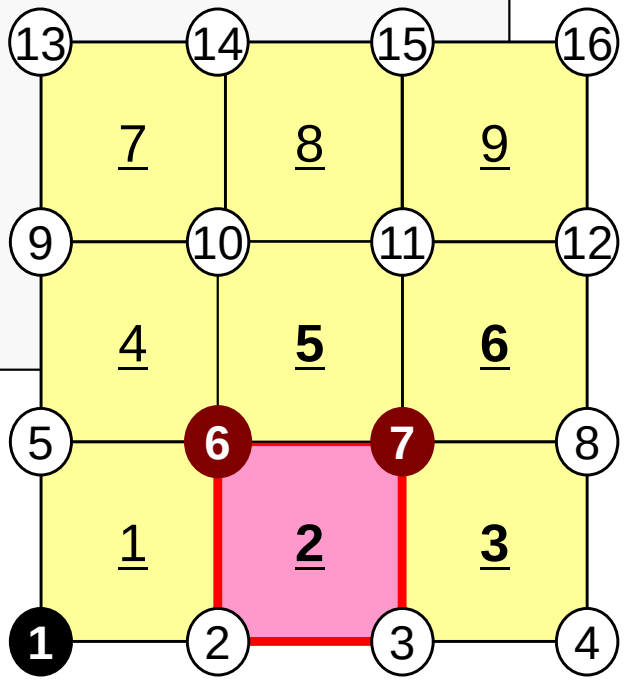
Array	Size	Description
INLU	[N]	Number of connected nodes to each node (lower/upper)
IALU	[N][NLU]	Corresponding connected node ID (column ID)

FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search, **#2 Element**

```
/***
 *** FIND_TS_NODE
 **/

static void FIND_TS_NODE (int ip1,int ip2)
{
  int kk,icou;

  for(kk=1;kk<=INLU[ip1-1];kk++){
    if(ip2 == IALU[ip1-1][kk-1]) return;
  }

  icou=INLU[ip1-1]+1;
  IALU[ip1-1][icou-1]=ip2;
  INLU[ip1-1]=icou;

  return;
}
```

Checking whether “ip2” is already included in IALU[ip1-1][kk], or not



ip1: No.6 node
ip2: No.7 node

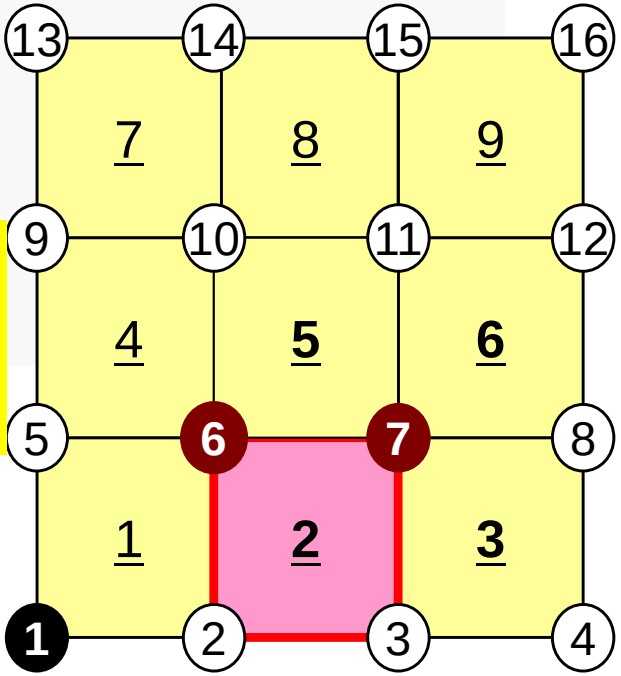
FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search, **#2 Element**

```
/***
 *** FIND_TS_NODE
 **/

static void FIND_TS_NODE (int ip1,int ip2)
{
  int kk,icou;

  for(kk=1;kk<=INLU[ip1-1];kk++){
    if(ip2 == IALU[ip1-1][kk-1]) return;
  }

  icou=INLU[ip1-1]+1;
  IALU[ip1-1][icou-1]=ip2;
  INLU[ip1-1]=icou;

  return;
}
```

If the target node is NOT included in IALU, store the node in IALU, and add 1 to INLU.

ip1: No.6 node
ip2: No.7 node

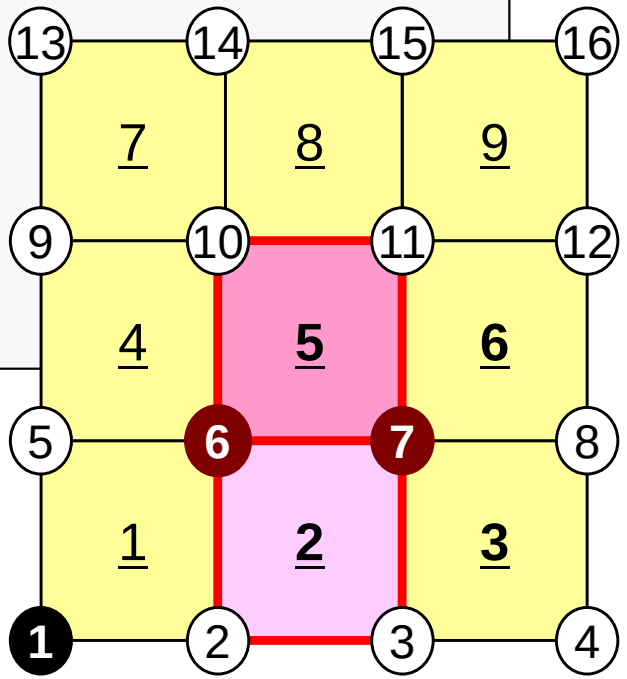


FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search, **#5 Element**

```
/***
 *** FIND_TS_NODE
 **/

static void FIND_TS_NODE (int ip1,int ip2)
{
  int kk,icou;

  for(kk=1;kk<=INLU[ip1-1];kk++){
    if(ip2 == IALU[ip1-1][kk-1]) return;
  }

  icou=INLU[ip1-1]+1;
  IALU[ip1-1][icou-1]=ip2;
  INLU[ip1-1]=icou;

  return;
}
```

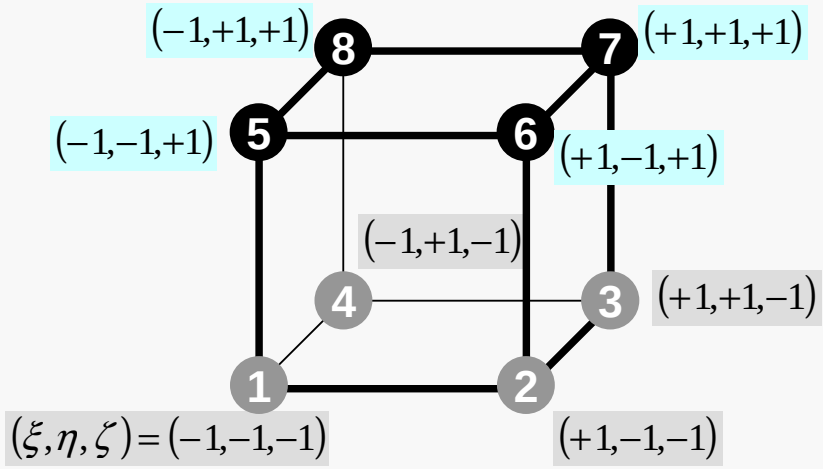
If the target node is already included in IALU, proceed to next pair of nodes



ip1: No.6 node
ip2: No.7 node

Generating Connectivity of Matrix MAT_CON0 (3/4)

```
    FIND_TS_NODE (in4,in1);
    FIND_TS_NODE (in4,in2);
    FIND_TS_NODE (in4,in3);
    FIND_TS_NODE (in4,in5);
    FIND_TS_NODE (in4,in6);
    FIND_TS_NODE (in4,in7);
    FIND_TS_NODE (in4,in8);

    FIND_TS_NODE (in5,in1);
    FIND_TS_NODE (in5,in2);
    FIND_TS_NODE (in5,in3);
    FIND_TS_NODE (in5,in4);
    FIND_TS_NODE (in5,in6);
    FIND_TS_NODE (in5,in7);
    FIND_TS_NODE (in5,in8);

    FIND_TS_NODE (in6,in1);
    FIND_TS_NODE (in6,in2);
    FIND_TS_NODE (in6,in3);
    FIND_TS_NODE (in6,in4);
    FIND_TS_NODE (in6,in5);
    FIND_TS_NODE (in6,in7);
    FIND_TS_NODE (in6,in8);

    FIND_TS_NODE (in7,in1);
    FIND_TS_NODE (in7,in2);
    FIND_TS_NODE (in7,in3);
    FIND_TS_NODE (in7,in4);
    FIND_TS_NODE (in7,in5);
    FIND_TS_NODE (in7,in6);
    FIND_TS_NODE (in7,in8);
```



Generating Connectivity of Matrix MAT_CON0 (4/4)

```
    FIND_TS_NODE (in8,in1);
    FIND_TS_NODE (in8,in2);
    FIND_TS_NODE (in8,in3);
    FIND_TS_NODE (in8,in4);
    FIND_TS_NODE (in8,in5);
    FIND_TS_NODE (in8,in6);
    FIND_TS_NODE (in8,in7);
  }

  for(in=0;in<N;in++){

    NN=INLU[in];
    for (k=0;k<NN;k++){
      NCOL1[k]=IALU[in][k];
    }

    mSORT(NCOL1,NCOL2,NN);

    for(k=NN;k>0;k--){
      IALU[in][NN-k]= NCOL1[NCOL2[k-1]-1];
    }
  }
```

Sort IALU[i][k] in ascending order by “bubble” sorting for less than 100 components.

MAT_CON1: CRS format

```
#include <stdio.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE* fp_log;
void MAT_CON1()
{
  int i,k,kk;

  indexLU=(KINT*)allocate_vector(sizeof(KINT),N+1);
  for(i=0;i<N+1;i++) indexLU[i]=0;

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

  NPLU=indexLU[N];
  itemLU=(KINT*)allocate_vector(sizeof(KINT),NPLU);

  for(i=0;i<N;i++){
    for(k=0;k<INLU[i];k++){
      kk=k+indexLU[i];
      itemLU[kk]=IALU[i][k]-1;
    }
  }
  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

C

$$\mathrm{index}[i+1]=\sum_{k=0}^{i}\mathrm{INLU}[k]$$

$$\mathrm{index}[0]=0$$

FORTRAN

$$\mathrm{index}(i)=\sum_{k=1}^{i}\mathrm{INLU}(k)$$

$$\mathrm{index}(0)=0$$

MAT_CON1: CRS format

```
#include <stdio.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE* fp_log;
void MAT_CON1()
{
  int i,k,kk;

  indexLU=(KINT*)allocate_vector(sizeof(KINT),N+1);
  for(i=0;i<N+1;i++) indexLU[i]=0;

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

  NPLU=indexLU[N];
  itemLU=(KINT*)allocate_vector(sizeof(KINT),NPLU);

  for(i=0;i<N;i++){
    for(k=0;k<INLU[i];k++){
      kk=k+indexLU[i];
      itemLU[kk]=IALU[i][k]-1;
    }
  }
  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

NPLU=indexLU[N]
Size of array: itemLU
Total number of non-zero off-diagonal blocks

MAT_CON1: CRS format

```
#include <stdio.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE* fp_log;
void MAT_CON1()
{
  int i,k,kk;

  indexLU=(KINT*)allocate_vector(sizeof(KINT),N+1);
  for(i=0;i<N+1;i++) indexLU[i]=0;

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

  NPLU=indexLU[N];
  itemLU=(KINT*)allocate_vector(sizeof(KINT),NPLU);

  for(i=0;i<N;i++){
    for(k=0;k<INLU[i];k++){
      kk=k+indexLU[i];
      itemLU[kk]=IALU[i][k]-1;
    }
  }
  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

itemLU
store node ID starting from 0

MAT_CON1: CRS format

```
#include <stdio.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE* fp_log;
void MAT_CON1()
{
  int i,k,kk;

  indexLU=(KINT*)allocate_vector(sizeof(KINT),N+1);
  for(i=0;i<N+1;i++) indexLU[i]=0;

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

  NPLU=indexLU[N];
  itemLU=(KINT*)allocate_vector(sizeof(KINT),NPLU);

  for(i=0;i<N;i++){
    for(k=0;k<INLU[i];k++){
      kk=k+indexLU[i];
      itemLU[kk]=IALU[i][k]-1;
    }
  }
  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

Not required any more

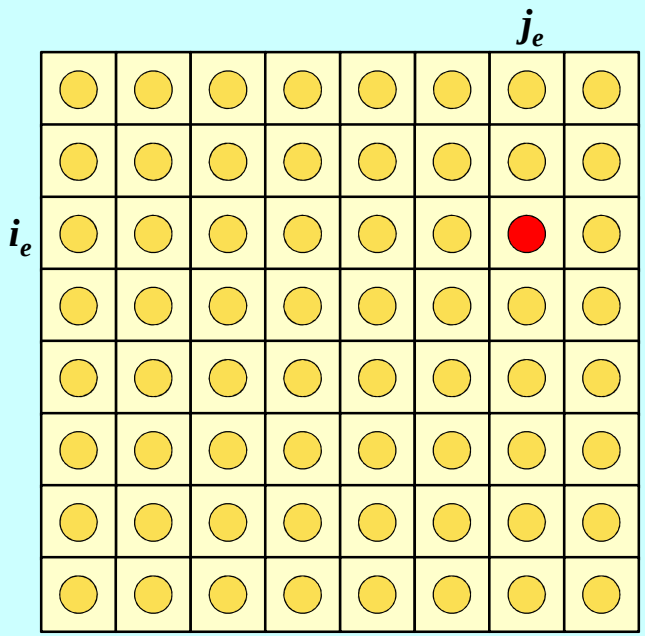
Main Part

```
int main()
{
  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()  ;

  SOLVE11();

  OUTPUT_UCD()    ;
  for(i=0;i<N;i++){
    if (XYZ[i][0]==0.e0) {
    if (XYZ[i][1]==0.e0) {
    if (XYZ[i][2]==0.e0) {
      printf("%8d%16.6e¥n¥n¥n", i+1, X[i]);}
    }}}
}
```

MAT_ASS_MAIN: Overview

```
do kpn= 1, 2          Gaussian Quad. points in ζ-direction
  do jpn= 1, 2        Gaussian Quad. points in η-direction
    do ipn= 1, 2      Gaussian Quad. Pointe in ξ-direction
      Define Shape Function at Gaussian Quad. Points (8-points)
      Its derivative on natural/local coordinate is also defined.
    enddo
  enddo
enddo
```

```
do icel= 1, ICELTOT   Loop for Element
  Jacobian and derivative on global coordinate of shape functions at
  Gaussian Quad. Points are defined according to coordinates of 8 nodes. (JACOBI)

  do ie= 1, 8         Local Node ID
    do je= 1, 8       Local Node ID
      Global Node ID: ip, jp
      Address of A_ip,jp in "itemLU" : kk

      do kpn= 1, 2        Gaussian Quad. points in ζ-direction
        do jpn= 1, 2      Gaussian Quad. points in η-direction
          do ipn= 1, 2    Gaussian Quad. points in ξ-direction
            integration on each element
            coefficients of element matrices
            accumulation to global matrix
          enddo
        enddo
      enddo
    enddo
  enddo
enddo
```

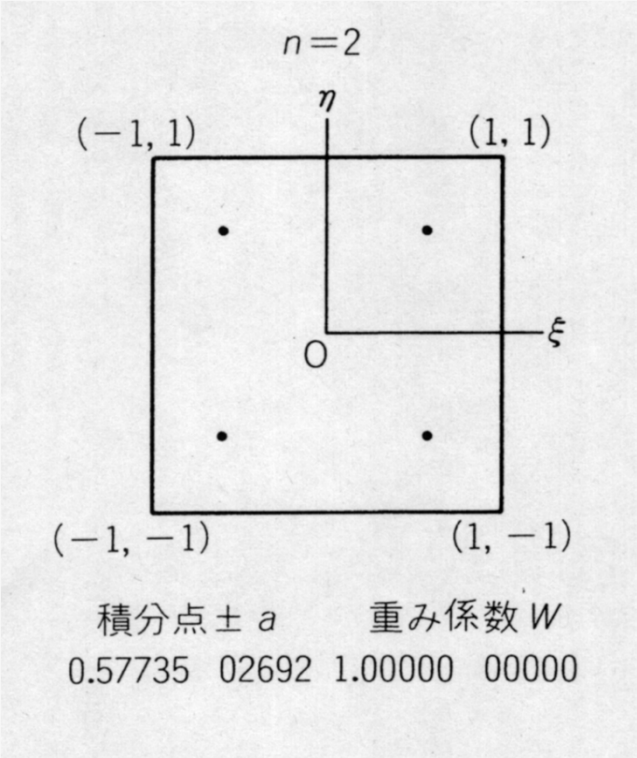


MAT_ASS_MAIN (1/6)

```
#include <stdio.h>
#include <math.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE *fp_log;
extern void JACOBI();
void MAT_ASS_MAIN()
{
  int i,k,kk;
  int ip,jp,kp;
  int ipn,jpn,kpn;
  int icel;
  int ie,je;
  int iiS,iiE;
  int in1,in2,in3,in4,in5,in6,in7,in8;
  double SHi;
  double QP1,QM1,EP1,EM1,TP1,TM1;
  double X1,X2,X3,X4,X5,X6,X7,X8;
  double Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8;
  double Z1,Z2,Z3,Z4,Z5,Z6,Z7,Z8;
  double PNXi,PNYi,PNZi,PNXj,PNYj,PNZj;
  double CONDO, QVO, QVC, COEFij;
  double coef;

  KINT nodLOCAL[8];

  AMAT=(KREAL*) allocate_vector(sizeof(KREAL),NPLU);      Non-Zero Off-Diagonal components (coef. matrix)
  B =(KREAL*) allocate_vector(sizeof(KREAL),N );          RHS vector
  D =(KREAL*) allocate_vector(sizeof(KREAL),N);           Diagonal components (coef. matrix)
  X =(KREAL*) allocate_vector(sizeof(KREAL),N);           Unknowns

  for(i=0;i<NPLU;i++) AMAT[i]=0.0;
  for(i=0;i<N ;i++) B[i]=0.0;
  for(i=0;i<N ;i++) D[i]=0.0;
  for(i=0;i<N ;i++) X[i]=0.0;

  WEI[0]= 1.0000000000e0;
  WEI[1]= 1.0000000000e0;
  POS[0]= -0.5773502692e0;
  POS[1]=  0.5773502692e0;
```

MAT_ASS_MAIN (1/6)

```
#include <stdio.h>
#include <math.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE *fp_log;
extern void JACOBI();
void MAT_ASS_MAIN()
{
  int i,k,kk;
  int ip,jp,kp;
  int ipn,jpn,kpn;
  int icel;
  int ie,je;
  int iiS,iiE;
  int in1,in2,in3,in4,in5,in6,in7,in8;
  double SHi;
  double QP1,QM1,EP1,EM1,TP1,TM1;
  double X1,X2,X3,X4,X5,X6,X7,X8;
  double Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8;
  double Z1,Z2,Z3,Z4,Z5,Z6,Z7,Z8;
  double PNXi,PNYi,PNZi,PNXj,PNYj,PNZj;
  double CONDO, QVO, QVC, COEFij;
  double coef;

  KINT nodLOCAL[8];

  AMAT=(KREAL*) allocate_vector(sizeof(KREAL),NPLU);
  B =(KREAL*) allocate_vector(sizeof(KREAL),N );
  D =(KREAL*) allocate_vector(sizeof(KREAL),N);
  X =(KREAL*) allocate_vector(sizeof(KREAL),N);

  for(i=0;i<NPLU;i++) AMAT[i]=0.0;
  for(i=0;i<N ;i++) B[i]=0.0;
  for(i=0;i<N ;i++) D[i]=0.0;
  for(i=0;i<N ;i++) X[i]=0.0;

  WEI[0]= 1.0000000000e0;
  WEI[1]= 1.0000000000e0;
  POS[0]= -0.5773502692e0;
  POS[1]=  0.5773502692e0;
```



POS: Quad. Point

WEI: Weighting Factor

MAT_ASS_MAIN (2/6)

```
/***
    INIT.
    PNQ   - 1st-order derivative of shape function by QSI
    PNE   - 1st-order derivative of shape function by ETA
    PNT   - 1st-order derivative of shape function by ZET
***/

  for(ip=0;ip<2;ip++){
    for(jp=0;jp<2;jp++){
      for(kp=0;kp<2;kp++){

        QP1= 1.e0 + POS[ip];
        QM1= 1.e0 - POS[ip];
        EP1= 1.e0 + POS[jp];
        EM1= 1.e0 - POS[jp];
        TP1= 1.e0 + POS[kp];
        TM1= 1.e0 - POS[kp];

        SHAPE[ip][jp][kp][0]= 0.8th * QM1 * EM1 * TM1;
        SHAPE[ip][jp][kp][1]= 0.8th * QP1 * EM1 * TM1;
        SHAPE[ip][jp][kp][2]= 0.8th * QP1 * EP1 * TM1;
        SHAPE[ip][jp][kp][3]= 0.8th * QM1 * EP1 * TM1;
        SHAPE[ip][jp][kp][4]= 0.8th * QM1 * EM1 * TP1;
        SHAPE[ip][jp][kp][5]= 0.8th * QP1 * EM1 * TP1;
        SHAPE[ip][jp][kp][6]= 0.8th * QP1 * EP1 * TP1;
        SHAPE[ip][jp][kp][7]= 0.8th * QM1 * EP1 * TP1;
```

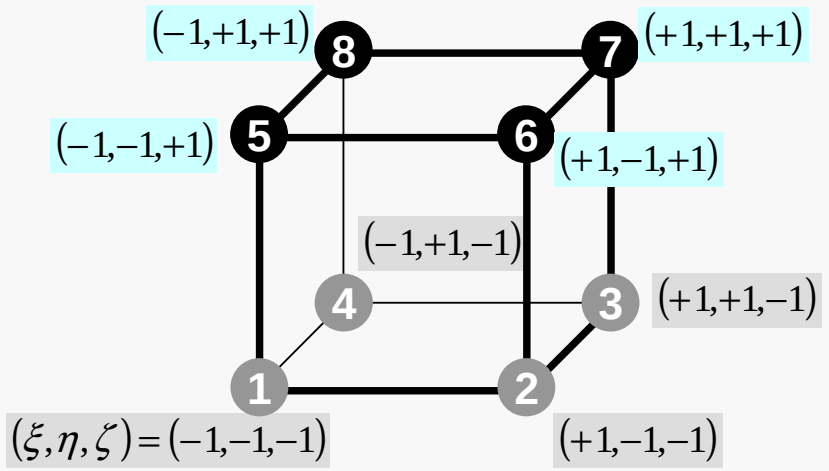
MAT_ASS_MAIN (2/6)

```
/***
    INIT.
    PNQ   - 1st-order derivative of shape function by QSI
    PNE   - 1st-order derivative of shape function by ETA
    PNT   - 1st-order derivative of shape function by ZET
***/

  for(ip=0;ip<2;ip++){
    for(jp=0;jp<2;jp++){
      for(kp=0;kp<2;kp++){

        QP1= 1.e0 + POS[ip];
        QM1= 1.e0 - POS[ip];
        EP1= 1.e0 + POS[jp];
        EM1= 1.e0 - POS[jp];
        TP1= 1.e0 + POS[kp];
        TM1= 1.e0 - POS[kp];

        SHAPE[ip][jp][kp][0]= 08th * QM1 * EM1 * TM1;
        SHAPE[ip][jp][kp][1]= 08th * QP1 * EM1 * TM1;
        SHAPE[ip][jp][kp][2]= 08th * QP1 * EP1 * TM1;
        SHAPE[ip][jp][kp][3]= 08th * QM1 * EP1 * TM1;
        SHAPE[ip][jp][kp][4]= 08th * QM1 * EM1 * TP1;
        SHAPE[ip][jp][kp][5]= 08th * QP1 * EM1 * TP1;
        SHAPE[ip][jp][kp][6]= 08th * QP1 * EP1 * TP1;
        SHAPE[ip][jp][kp][7]= 08th * QM1 * EP1 * TP1;
```

$$\mathrm{QP1(i)} = (1+\xi_i), \quad \mathrm{QM1(i)} = (1-\xi_i)$$
$$\mathrm{EP1(j)} = (1+\eta_j), \quad \mathrm{EM1(j)} = (1-\eta_i)$$
$$\mathrm{TP1(k)} = (1+\zeta_k), \quad \mathrm{TM1(k)} = (1-\zeta_k)$$

MAT_ASS_MAIN (2/6)

```
/***
    INIT.
    PNQ   - 1st-order derivative of shape function by QSI
    PNE   - 1st-order derivative of shape function by ETA
    PNT   - 1st-order derivative of shape function by ZET
***/

  for(ip=0;ip<2;ip++){
    for(jp=0;jp<2;jp++){
      for(kp=0;kp<2;kp++){

        QP1= 1.e0 + POS[ip];
        QM1= 1.e0 - POS[ip];
        EP1= 1.e0 + POS[jp];
        EM1= 1.e0 - POS[jp];
        TP1= 1.e0 + POS[kp];
        TM1= 1.e0 - POS[kp];

        SHAPE[ip][jp][kp][0]= 08th * QM1 * EM1 * TM1;
        SHAPE[ip][jp][kp][1]= 08th * QP1 * EM1 * TM1;
        SHAPE[ip][jp][kp][2]= 08th * QP1 * EP1 * TM1;
        SHAPE[ip][jp][kp][3]= 08th * QM1 * EP1 * TM1;
        SHAPE[ip][jp][kp][4]= 08th * QM1 * EM1 * TP1;
        SHAPE[ip][jp][kp][5]= 08th * QP1 * EM1 * TP1;
        SHAPE[ip][jp][kp][6]= 08th * QP1 * EP1 * TP1;
        SHAPE[ip][jp][kp][7]= 08th * QM1 * EP1 * TP1;
```



MAT_ASS_MAIN (2/6)

```
/***
    INIT.
    PNQ   - 1st-order derivative of shape function by QSI
    PNE   - 1st-order derivative of shape function by ETA
    PNT   - 1st-order derivative of shape function by ZET
***/

  for(ip=0;ip<2;ip++){
    for(jp=0;jp<2;jp++){
      for(kp=0;kp<2;kp++){

        QP1= 1.e0 + POS[ip];
        QM1= 1.e0 - POS[ip];
        EP1= 1.e0 + POS[jp];
        EM1= 1.e0 - POS[jp];
        TP1= 1.e0 + POS[kp];
        TM1= 1.e0 - POS[kp];

        SHAPE[ip][jp][kp][0]= 08th * QM1 * EM1 * TM1;
        SHAPE[ip][jp][kp][1]= 08th * QP1 * EM1 * TM1;
        SHAPE[ip][jp][kp][2]= 08th * QP1 * EP1 * TM1;
        SHAPE[ip][jp][kp][3]= 08th * QM1 * EP1 * TM1;
        SHAPE[ip][jp][kp][4]= 08th * QM1 * EM1 * TP1;
        SHAPE[ip][jp][kp][5]= 08th * QP1 * EM1 * TP1;
        SHAPE[ip][jp][kp][6]= 08th * QP1 * EP1 * TP1;
        SHAPE[ip][jp][kp][7]= 08th * QM1 * EP1 * TP1;
```

$$N_1(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1-\eta)(1-\zeta)$$

$$N_2(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1-\eta)(1-\zeta)$$

$$N_3(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1+\eta)(1-\zeta)$$

$$N_4(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1+\eta)(1-\zeta)$$

$$N_5(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1-\eta)(1+\zeta)$$

$$N_6(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1-\eta)(1+\zeta)$$

$$N_7(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1+\eta)(1+\zeta)$$

$$N_8(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1+\eta)(1+\zeta)$$

MAT_ASS_MAIN (3/6)

```
        PNQ[jp][kp][0]= - 08th * EM1 * TM1;
        PNQ[jp][kp][1]= + 08th * EM1 * TM1;
        PNQ[jp][kp][2]= + 08th * EP1 * TM1;
        PNQ[jp][kp][3]= - 08th * EP1 * TM1;
        PNQ[jp][kp][4]= - 08th * EM1 * TP1;
        PNQ[jp][kp][5]= + 08th * EM1 * TP1;
        PNQ[jp][kp][6]= + 08th * EP1 * TP1;
        PNQ[jp][kp][7]= - 08th * EP1 * TP1;

        PNE[ip][kp][0]= - 08th * QM1 * TM1;
        PNE[ip][kp][1]= - 08th * QP1 * TM1;
        PNE[ip][kp][2]= + 08th * QP1 * TM1;
        PNE[ip][kp][3]= + 08th * QM1 * TM1;
        PNE[ip][kp][4]= - 08th * QM1 * TP1;
        PNE[ip][kp][5]= - 08th * QP1 * TP1;
        PNE[ip][kp][6]= + 08th * QP1 * TP1;
        PNE[ip][kp][7]= + 08th * QM1 * TP1;

        PNT[ip][jp][0]= - 08th * QM1 * EM1;
        PNT[ip][jp][1]= - 08th * QP1 * EM1;
        PNT[ip][jp][2]= - 08th * QP1 * EP1;
        PNT[ip][jp][3]= - 08th * QM1 * EP1;
        PNT[ip][jp][4]= + 08th * QM1 * EM1;
        PNT[ip][jp][5]= + 08th * QP1 * EM1;
        PNT[ip][jp][6]= + 08th * QP1 * EP1;
        PNT[ip][jp][7]= + 08th * QM1 * EP1;
      }
    }
  }

  for( icel=0;icel< ICELTOT;icel++){
    CONDO= COND;

    in1=ICELNOD[icel][0];
    in2=ICELNOD[icel][1];
    in3=ICELNOD[icel][2];
    in4=ICELNOD[icel][3];
    in5=ICELNOD[icel][4];
    in6=ICELNOD[icel][5];
    in7=ICELNOD[icel][6];
    in8=ICELNOD[icel][7];
```

$$PNQ(j,k)=\frac{\partial N_l}{\partial \xi}(\xi=\xi_i,\eta=\eta_j,\zeta=\zeta_k)$$

$$PNE(i,k)=\frac{\partial N_l}{\partial \eta}(\xi=\xi_i,\eta=\eta_j,\zeta=\zeta_k)$$

$$PNT(i,j)=\frac{\partial N_l}{\partial \zeta}(\xi=\xi_i,\eta=\eta_j,\zeta=\zeta_k)$$

$$\frac{\partial N_1}{\partial \xi}(\xi_i,\eta_j,\zeta_k)=-\frac{1}{8}(1-\eta_j)(1-\zeta_k)$$

$$\frac{\partial N_2}{\partial \xi}(\xi_i,\eta_j,\zeta_k)=+\frac{1}{8}(1-\eta_j)(1-\zeta_k)$$

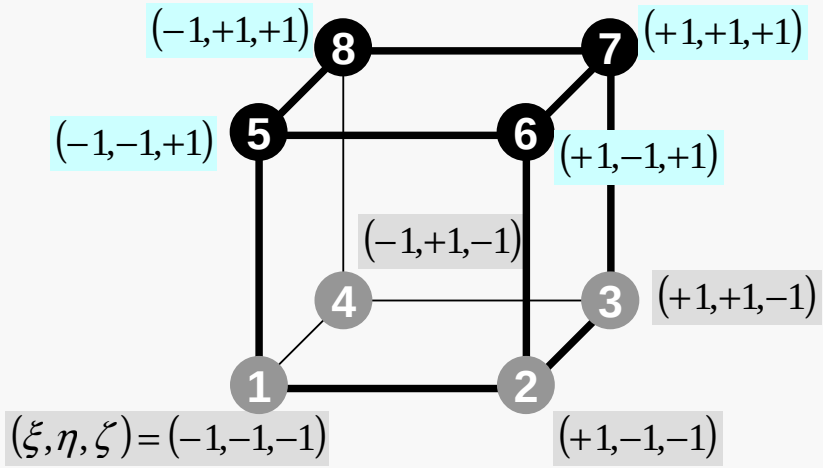
$$\frac{\partial N_3}{\partial \xi}(\xi_i,\eta_j,\zeta_k)=+\frac{1}{8}(1+\eta_j)(1-\zeta_k)$$

$$\frac{\partial N_4}{\partial \xi}(\xi_i,\eta_j,\zeta_k)=-\frac{1}{8}(1+\eta_j)(1+\zeta_k)$$

First Order Derivative of Shape Functions at (ξ_i,η_j,ζ_k)

MAT_ASS_MAIN (3/6)

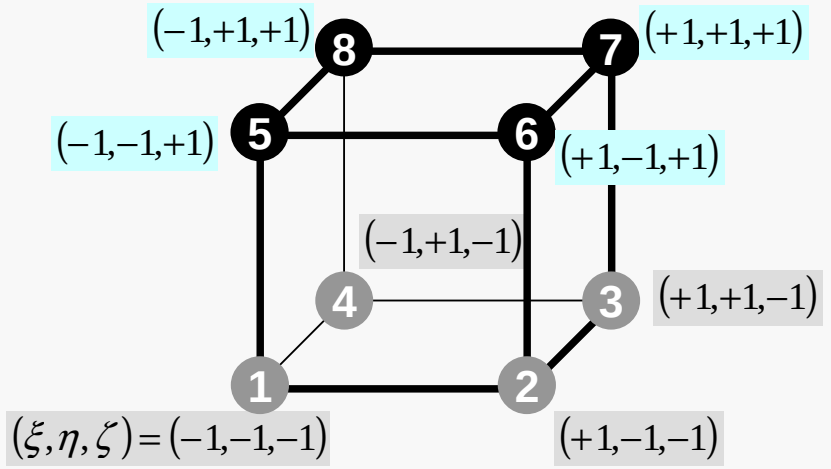
```
        PNQ[jp][kp][0]= - 08th * EM1 * TM1;
        PNQ[jp][kp][1]= + 08th * EM1 * TM1;
        PNQ[jp][kp][2]= + 08th * EP1 * TM1;
        PNQ[jp][kp][3]= - 08th * EP1 * TM1;
        PNQ[jp][kp][4]= - 08th * EM1 * TP1;
        PNQ[jp][kp][5]= + 08th * EM1 * TP1;
        PNQ[jp][kp][6]= + 08th * EP1 * TP1;
        PNQ[jp][kp][7]= - 08th * EP1 * TP1;

        PNE[ip][kp][0]= - 08th * QM1 * TM1;
        PNE[ip][kp][1]= - 08th * QP1 * TM1;
        PNE[ip][kp][2]= + 08th * QP1 * TM1;
        PNE[ip][kp][3]= + 08th * QM1 * TM1;
        PNE[ip][kp][4]= - 08th * QM1 * TP1;
        PNE[ip][kp][5]= - 08th * QP1 * TP1;
        PNE[ip][kp][6]= + 08th * QP1 * TP1;
        PNE[ip][kp][7]= + 08th * QM1 * TP1;

        PNT[ip][jp][0]= - 08th * QM1 * EM1;
        PNT[ip][jp][1]= - 08th * QP1 * EM1;
        PNT[ip][jp][2]= - 08th * QP1 * EP1;
        PNT[ip][jp][3]= - 08th * QM1 * EP1;
        PNT[ip][jp][4]= + 08th * QM1 * EM1;
        PNT[ip][jp][5]= + 08th * QP1 * EM1;
        PNT[ip][jp][6]= + 08th * QP1 * EP1;
        PNT[ip][jp][7]= + 08th * QM1 * EP1;
      }
    }
  }

  for( icel=0;icel< ICELTOT;icel++){
    CONDO= COND;

    in1=ICELNOD[icel][0];
    in2=ICELNOD[icel][1];
    in3=ICELNOD[icel][2];
    in4=ICELNOD[icel][3];
    in5=ICELNOD[icel][4];
    in6=ICELNOD[icel][5];
    in7=ICELNOD[icel][6];
    in8=ICELNOD[icel][7];
```



MAT_ASS_MAIN (4/6)

```
nodLOCAL[0]= in1;
nodLOCAL[1]= in2;
nodLOCAL[2]= in3;
nodLOCAL[3]= in4;
nodLOCAL[4]= in5;
nodLOCAL[5]= in6;
nodLOCAL[6]= in7;
nodLOCAL[7]= in8;

X1=XYZ[in1-1][0];
X2=XYZ[in2-1][0];
X3=XYZ[in3-1][0];
X4=XYZ[in4-1][0];
X5=XYZ[in5-1][0];
X6=XYZ[in6-1][0];
X7=XYZ[in7-1][0];
X8=XYZ[in8-1][0];

Y1=XYZ[in1-1][1];
Y2=XYZ[in2-1][1];
Y3=XYZ[in3-1][1];
Y4=XYZ[in4-1][1];
Y5=XYZ[in5-1][1];
Y6=XYZ[in6-1][1];
Y7=XYZ[in7-1][1];
Y8=XYZ[in8-1][1];

QVC= 08th*(X1+X2+X3+X4+X5+X6+X7+X8+Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8);

Z1=XYZ[in1-1][2];
Z2=XYZ[in2-1][2];
Z3=XYZ[in3-1][2];
Z4=XYZ[in4-1][2];
Z5=XYZ[in5-1][2];
Z6=XYZ[in6-1][2];
Z7=XYZ[in7-1][2];
Z8=XYZ[in8-1][2];

JACOBI(DETJ, PNQ, PNE, PNT, PNX, PNY, PNZ,
       X1, X2, X3, X4, X5, X6, X7, X8,
       Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8, Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8);
```

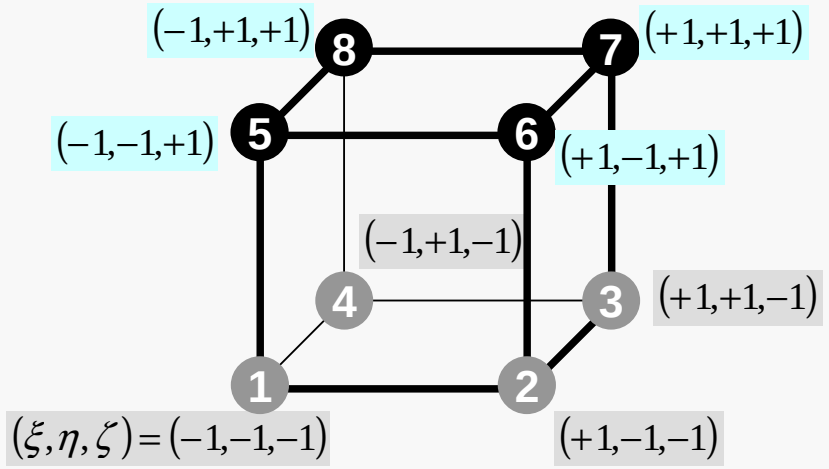
Node ID (Global)



MAT_ASS_MAIN (4/6)

```
nodLOCAL[0]= in1;
nodLOCAL[1]= in2;
nodLOCAL[2]= in3;
nodLOCAL[3]= in4;
nodLOCAL[4]= in5;
nodLOCAL[5]= in6;
nodLOCAL[6]= in7;
nodLOCAL[7]= in8;

X1=XYZ[in1-1][0];
X2=XYZ[in2-1][0];
X3=XYZ[in3-1][0];
X4=XYZ[in4-1][0];
X5=XYZ[in5-1][0];
X6=XYZ[in6-1][0];
X7=XYZ[in7-1][0];
X8=XYZ[in8-1][0];
```

X-Coordinates of 8 nodes




```
Y1=XYZ[in1-1][1];
Y2=XYZ[in2-1][1];
Y3=XYZ[in3-1][1];
Y4=XYZ[in4-1][1];
Y5=XYZ[in5-1][1];
Y6=XYZ[in6-1][1];
Y7=XYZ[in7-1][1];
Y8=XYZ[in8-1][1];
```

Y-Coordinates of 8 nodes

```
QVC= 08th*(X1+X2+X3+X4+X5+X6+X7+X8+Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8);

Z1=XYZ[in1-1][2];
Z2=XYZ[in2-1][2];
Z3=XYZ[in3-1][2];
Z4=XYZ[in4-1][2];
Z5=XYZ[in5-1][2];
Z6=XYZ[in6-1][2];
Z7=XYZ[in7-1][2];
Z8=XYZ[in8-1][2];

JACOBI(DETJ, PNQ, PNE, PNT, PNX, PNY, PNZ,
       X1, X2, X3, X4, X5, X6, X7, X8,
       Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8, Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8);
```

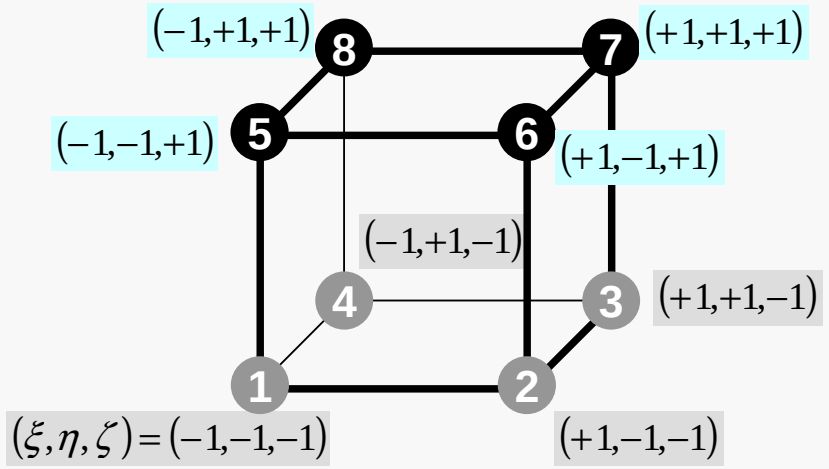
Z-Coordinates of 8 nodes

Coordinates: Node ID - 1

MAT_ASS_MAIN (4/6)

```
nodLOCAL[0]= in1;
nodLOCAL[1]= in2;
nodLOCAL[2]= in3;
nodLOCAL[3]= in4;
nodLOCAL[4]= in5;
nodLOCAL[5]= in6;
nodLOCAL[6]= in7;
nodLOCAL[7]= in8;

X1=XYZ[in1-1][0];
X2=XYZ[in2-1][0];
X3=XYZ[in3-1][0];
X4=XYZ[in4-1][0];
X5=XYZ[in5-1][0];
X6=XYZ[in6-1][0];
X7=XYZ[in7-1][0];
X8=XYZ[in8-1][0];
```

X-Coordinates of 8 nodes




```
Y1=XYZ[in1-1][1];
Y2=XYZ[in2-1][1];
Y3=XYZ[in3-1][1];
Y4=XYZ[in4-1][1];
Y5=XYZ[in5-1][1];
Y6=XYZ[in6-1][1];
Y7=XYZ[in7-1][1];
Y8=XYZ[in8-1][1];
```

Y-Coordinates of 8 nodes

Coordinates: Node ID - 1

```
QVC= 08th*(X1+X2+X3+X4+X5+X6+X7+X8+Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8);

Z1=XYZ[in1-1][2];
Z2=XYZ[in2-1][2];
Z3=XYZ[in3-1][2];
Z4=XYZ[in4-1][2];
Z5=XYZ[in5-1][2];
Z6=XYZ[in6-1][2];
Z7=XYZ[in7-1][2];
Z8=XYZ[in8-1][2];

JACOBI(DETJ, PNQ, PNE, PNT, PNX, PNY, PNZ,
       X1, X2, X3, X4, X5, X6, X7, X8,
       Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8, Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8);
```

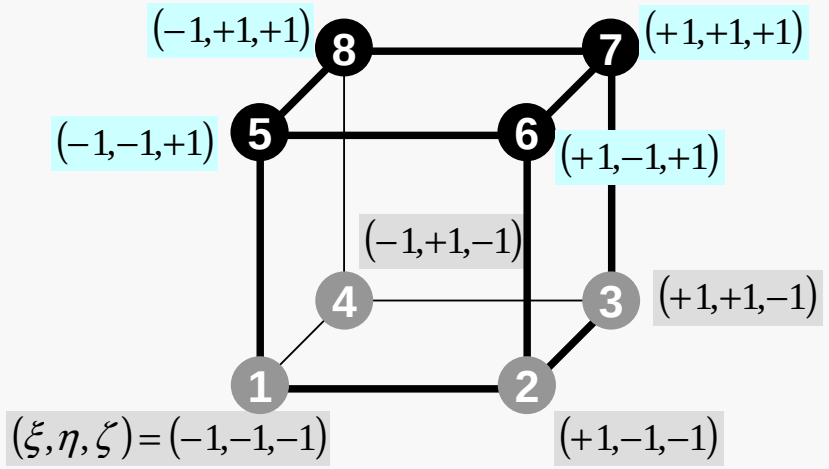
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\dot{Q}(x,y,z)=0$$

$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

Heat Gen. Rate is a function of location (cell center: x_c,y_c)

MAT_ASS_MAIN (4/6)

```
nodLOCAL[0]= in1;
nodLOCAL[1]= in2;
nodLOCAL[2]= in3;
nodLOCAL[3]= in4;
nodLOCAL[4]= in5;
nodLOCAL[5]= in6;
nodLOCAL[6]= in7;
nodLOCAL[7]= in8;

X1=XYZ[in1-1][0];
X2=XYZ[in2-1][0];
X3=XYZ[in3-1][0];
X4=XYZ[in4-1][0];
X5=XYZ[in5-1][0];
X6=XYZ[in6-1][0];
X7=XYZ[in7-1][0];
X8=XYZ[in8-1][0];

Y1=XYZ[in1-1][1];
Y2=XYZ[in2-1][1];
Y3=XYZ[in3-1][1];
Y4=XYZ[in4-1][1];
Y5=XYZ[in5-1][1];
Y6=XYZ[in6-1][1];
Y7=XYZ[in7-1][1];
Y8=XYZ[in8-1][1];

QVC= 08th*(X1+X2+X3+X4+X5+X6+X7+X8+Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8);

Z1=XYZ[in1-1][2];
Z2=XYZ[in2-1][2];
Z3=XYZ[in3-1][2];
Z4=XYZ[in4-1][2];
Z5=XYZ[in5-1][2];
Z6=XYZ[in6-1][2];
Z7=XYZ[in7-1][2];
Z8=XYZ[in8-1][2];

JACOBI(DETJ, PNQ, PNE, PNT, PNX, PNY, PNZ,
       X1, X2, X3, X4, X5, X6, X7, X8,
       Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8, Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8);
```



Coordinates:
Node ID - 1

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

$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

$$QVC=\left|x_C+y_C\right|$$

MAT_ASS_MAIN (4/6)

```
      nodLOCAL[0]= in1;
      nodLOCAL[1]= in2;
      nodLOCAL[2]= in3;
      nodLOCAL[3]= in4;
      nodLOCAL[4]= in5;
      nodLOCAL[5]= in6;
      nodLOCAL[6]= in7;
      nodLOCAL[7]= in8;

      X1=XYZ[in1-1][0];
      X2=XYZ[in2-1][0];
      X3=XYZ[in3-1][0];
      X4=XYZ[in4-1][0];
      X5=XYZ[in5-1][0];
      X6=XYZ[in6-1][0];
      X7=XYZ[in7-1][0];
      X8=XYZ[in8-1][0];

      Y1=XYZ[in1-1][1];
      Y2=XYZ[in2-1][1];
      Y3=XYZ[in3-1][1];
      Y4=XYZ[in4-1][1];
      Y5=XYZ[in5-1][1];
      Y6=XYZ[in6-1][1];
      Y7=XYZ[in7-1][1];
      Y8=XYZ[in8-1][1];

      QVC= O8th*(X1+X2+X3+X4+X5+X6+X7+X8+Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8);

      Z1=XYZ[in1-1][2];
      Z2=XYZ[in2-1][2];
      Z3=XYZ[in3-1][2];
      Z4=XYZ[in4-1][2];
      Z5=XYZ[in5-1][2];
      Z6=XYZ[in6-1][2];
      Z7=XYZ[in7-1][2];
      Z8=XYZ[in8-1][2];

      JACOBI(DETJ, PNQ, PNE, PNT, PNX, PNY, PNZ,
             X1, X2, X3, X4, X5, X6, X7, X8,
             Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8, Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8);
```

JACOBI (1/4)

```
#include <stdio.h>
#include <math.h>
#include "precision.h"
#include "allocate.h"
/***
 *** JACOBI
 ***/
void JACOBI(
            KREAL DETJ[2][2][2],
            KREAL PNQ[2][2][8],KREAL PNE[2][2][8],KREAL PNT[2][2][8],
            KREAL PNX[2][2][2][8],KREAL PNY[2][2][2][8],KREAL PNZ[2][2][2][8],
            KREAL X1,KREAL X2,KREAL X3,KREAL X4,KREAL X5,KREAL X6,KREAL X7,KREAL X8,
            KREAL Y1,KREAL Y2,KREAL Y3,KREAL Y4,KREAL Y5,KREAL Y6,KREAL Y7,KREAL Y8,
            KREAL Z1,KREAL Z2,KREAL Z3,KREAL Z4,KREAL Z5,KREAL Z6,KREAL Z7,KREAL Z8)
{
/**
            calculates JACOBIAN & INVERSE JACOBIAN
                        dNi/dx, dNi/dy & dNi/dz
**/
            int ip,jp,kp;
            double dXdQ,dYdQ,dZdQ,dXdE,dYdE,dZdE,dXdT,dYdT,dZdT;
            double coef;
            double a11,a12,a13,a21,a22,a23,a31,a32,a33;

            for(ip=0;ip<2;ip++){
                for(jp=0;jp<2;jp++){
                    for(kp=0;kp<2;kp++){
                        PNX[ip][jp][kp][0]=0.0;
                        PNX[ip][jp][kp][1]=0.0;
                        PNX[ip][jp][kp][2]=0.0;
                        PNX[ip][jp][kp][3]=0.0;
                        PNX[ip][jp][kp][4]=0.0;
                        PNX[ip][jp][kp][5]=0.0;
                        PNX[ip][jp][kp][6]=0.0;
                        PNX[ip][jp][kp][7]=0.0;
```

Input $\left[\frac{\partial N_l}{\partial \xi},\frac{\partial N_l}{\partial \eta},\frac{\partial N_l}{\partial \zeta}\right],(x_l,y_l,z_l)\,(l=1\sim 8)$

Output $\left[\frac{\partial N_l}{\partial x},\frac{\partial N_l}{\partial y},\frac{\partial N_l}{\partial z}\right],\det|J|$

Values at each Gaussian Quad. Points: [ip][jp][kp]

Partial Diff. on Natural Coord. (1/4)

- According to formulae:

$$\frac{\partial N_i(\xi,\eta,\zeta)}{\partial \xi} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \xi} + \frac{\partial N_i}{\partial z}\frac{\partial z}{\partial \xi}$$

$$\frac{\partial N_i(\xi,\eta,\zeta)}{\partial \eta} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \eta} + \frac{\partial N_i}{\partial z}\frac{\partial z}{\partial \eta}$$

$$\frac{\partial N_i(\xi,\eta,\zeta)}{\partial \zeta} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \zeta} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \zeta} + \frac{\partial N_i}{\partial z}\frac{\partial z}{\partial \zeta}$$

$\left[\frac{\partial N_i}{\partial \xi}, \frac{\partial N_i}{\partial \eta}, \frac{\partial N_i}{\partial \zeta}\right]$ can be easily derived according to definitions.

$\left[\frac{\partial N_i}{\partial x}, \frac{\partial N_i}{\partial y}, \frac{\partial N_i}{\partial z}\right]$ are required for computations.

Partial Diff. on Natural Coord. (2/4)

- In matrix form:

$$\begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = [J] \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix}$$

$$[J] = \begin{bmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{bmatrix}$$

$[J]$: Jacobi matrix, Jacobian

Partial Diff. on Natural Coord. (3/4)

- Components of Jacobian:

$$J_{11}=\frac{\partial x}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{8}N_i x_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \xi}x_i,\quad J_{12}=\frac{\partial y}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{8}N_i y_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \xi}y_i,$$

$$J_{13}=\frac{\partial z}{\partial \xi}=\frac{\partial}{\partial \xi}\left(\sum_{i=1}^{8}N_i z_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \xi}z$$

$$J_{21}=\frac{\partial x}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{8}N_i x_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \eta}x_i,\quad J_{22}=\frac{\partial y}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{8}N_i y_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \eta}y_i,$$

$$J_{23}=\frac{\partial z}{\partial \eta}=\frac{\partial}{\partial \eta}\left(\sum_{i=1}^{8}N_i z_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \eta}z_i$$

$$J_{31}=\frac{\partial x}{\partial \zeta}=\frac{\partial}{\partial \zeta}\left(\sum_{i=1}^{8}N_i x_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \zeta}x_i,\quad J_{32}=\frac{\partial y}{\partial \zeta}=\frac{\partial}{\partial \zeta}\left(\sum_{i=1}^{8}N_i y_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \zeta}y_i,$$

$$J_{33}=\frac{\partial z}{\partial \zeta}=\frac{\partial}{\partial \zeta}\left(\sum_{i=1}^{8}N_i z_i\right)=\sum_{i=1}^{8}\frac{\partial N_i}{\partial \zeta}z_i$$

JACOBI (2/4)

```
                    PNY[ip][jp][kp][0]=0.0;
                    PNY[ip][jp][kp][1]=0.0;
                    PNY[ip][jp][kp][2]=0.0;
                    PNY[ip][jp][kp][3]=0.0;
                    PNY[ip][jp][kp][4]=0.0;
                    PNY[ip][jp][kp][5]=0.0;
                    PNY[ip][jp][kp][6]=0.0;
                    PNY[ip][jp][kp][7]=0.0;

                    PNZ[ip][jp][kp][0]=0.0;
                    PNZ[ip][jp][kp][1]=0.0;
                    PNZ[ip][jp][kp][2]=0.0;
                    PNZ[ip][jp][kp][3]=0.0;
                    PNZ[ip][jp][kp][4]=0.0;
                    PNZ[ip][jp][kp][5]=0.0;
                    PNZ[ip][jp][kp][6]=0.0;
                    PNZ[ip][jp][kp][7]=0.0;

/**
        DETERMINANT of the JACOBIAN
**/
                    dXdQ = PNQ[jp][kp][0]*X1 + PNQ[jp][kp][1]*X2
                         + PNQ[jp][kp][2]*X3 + PNQ[jp][kp][3]*X4
                         + PNQ[jp][kp][4]*X5 + PNQ[jp][kp][5]*X6
                         + PNQ[jp][kp][6]*X7 + PNQ[jp][kp][7]*X8;
                    dYdQ = PNQ[jp][kp][0]*Y1 + PNQ[jp][kp][1]*Y2
                         + PNQ[jp][kp][2]*Y3 + PNQ[jp][kp][3]*Y4
                         + PNQ[jp][kp][4]*Y5 + PNQ[jp][kp][5]*Y6
                         + PNQ[jp][kp][6]*Y7 + PNQ[jp][kp][7]*Y8;
                    dZdQ = PNQ[jp][kp][0]*Z1 + PNQ[jp][kp][1]*Z2
                         + PNQ[jp][kp][2]*Z3 + PNQ[jp][kp][3]*Z4
                         + PNQ[jp][kp][4]*Z5 + PNQ[jp][kp][5]*Z6
                         + PNQ[jp][kp][6]*Z7 + PNQ[jp][kp][7]*Z8;
                    dXdE = PNE[ip][kp][0]*X1 + PNE[ip][kp][1]*X2
                         + PNE[ip][kp][2]*X3 + PNE[ip][kp][3]*X4
                         + PNE[ip][kp][4]*X5 + PNE[ip][kp][5]*X6
                         + PNE[ip][kp][6]*X7 + PNE[ip][kp][7]*X8;
```

$$[J]=\begin{bmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{bmatrix}$$

$$\mathrm{dXdQ}=\frac{\partial x}{\partial \xi}=J_{11}$$

$$\mathrm{dYdQ}=\frac{\partial y}{\partial \xi}=J_{12}$$

$$\mathrm{dZdQ}=\frac{\partial z}{\partial \xi}=J_{13}$$

JACOBI (3/4)

```
                    dYdE = PNE[ip][kp][0]*Y1 + PNE[ip][kp][1]*Y2
                         + PNE[ip][kp][2]*Y3 + PNE[ip][kp][3]*Y4
                         + PNE[ip][kp][4]*Y5 + PNE[ip][kp][5]*Y6
                         + PNE[ip][kp][6]*Y7 + PNE[ip][kp][7]*Y8;
                    dZdE = PNE[ip][kp][0]*Z1 + PNE[ip][kp][1]*Z2
                         + PNE[ip][kp][2]*Z3 + PNE[ip][kp][3]*Z4
                         + PNE[ip][kp][4]*Z5 + PNE[ip][kp][5]*Z6
                         + PNE[ip][kp][6]*Z7 + PNE[ip][kp][7]*Z8;
                    dXdT = PNT[ip][jp][0]*X1 + PNT[ip][jp][1]*X2
                         + PNT[ip][jp][2]*X3 + PNT[ip][jp][3]*X4
                         + PNT[ip][jp][4]*X5 + PNT[ip][jp][5]*X6
                         + PNT[ip][jp][6]*X7 + PNT[ip][jp][7]*X8;
                    dYdT = PNT[ip][jp][0]*Y1 + PNT[ip][jp][1]*Y2
                         + PNT[ip][jp][2]*Y3 + PNT[ip][jp][3]*Y4
                         + PNT[ip][jp][4]*Y5 + PNT[ip][jp][5]*Y6
                         + PNT[ip][jp][6]*Y7 + PNT[ip][jp][7]*Y8;
                    dZdT = PNT[ip][jp][0]*Z1 + PNT[ip][jp][1]*Z2
                         + PNT[ip][jp][2]*Z3 + PNT[ip][jp][3]*Z4
                         + PNT[ip][jp][4]*Z5 + PNT[ip][jp][5]*Z6
                         + PNT[ip][jp][6]*Z7 + PNT[ip][jp][7]*Z8;
                    DETJ[ip][jp][kp]= dXdQ*(dYdE*dZdT-dZdE*dYdT) +
                                      dYdQ*(dZdE*dXdT-dXdE*dZdT) +
                                      dZdQ*(dXdE*dYdT-dYdE*dXdT);
/**
    INVERSE JACOBIAN
**/
                    coef=1.0 / DETJ[ip][jp][kp];

                    a11= coef * ( dYdE*dZdT - dZdE*dYdT );
                    a12= coef * ( dZdQ*dYdT - dYdQ*dZdT );
                    a13= coef * ( dYdQ*dZdE - dZdQ*dYdE );

                    a21= coef * ( dZdE*dXdT - dXdE*dZdT );
                    a22= coef * ( dXdQ*dZdT - dZdQ*dXdT );
                    a23= coef * ( dZdQ*dXdE - dXdQ*dZdE );

                    a31= coef * ( dXdE*dYdT - dYdE*dXdT );
                    a32= coef * ( dYdQ*dXdT - dXdQ*dYdT );
                    a33= coef * ( dXdQ*dYdE - dYdQ*dXdE );

                    DETJ[ip][jp][kp]=fabs(DETJ[ip][jp][kp]);
```

$$[J]=\begin{bmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{bmatrix}$$

Partial Diff. on Natural Coord. (4/4)

- Partial differentiation on global coordinate system is introduced as follows (with inverse of Jacobian matrix (3×3))

$$\begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix}^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = [J]^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix}$$

JACOBI (3/4)

```
                    dYdE = PNE[ip][kp][0]*Y1 + PNE[ip][kp][1]*Y2
                         + PNE[ip][kp][2]*Y3 + PNE[ip][kp][3]*Y4
                         + PNE[ip][kp][4]*Y5 + PNE[ip][kp][5]*Y6
                         + PNE[ip][kp][6]*Y7 + PNE[ip][kp][7]*Y8;
                    dZdE = PNE[ip][kp][0]*Z1 + PNE[ip][kp][1]*Z2
                         + PNE[ip][kp][2]*Z3 + PNE[ip][kp][3]*Z4
                         + PNE[ip][kp][4]*Z5 + PNE[ip][kp][5]*Z6
                         + PNE[ip][kp][6]*Z7 + PNE[ip][kp][7]*Z8;
                    dXdT = PNT[ip][jp][0]*X1 + PNT[ip][jp][1]*X2
                         + PNT[ip][jp][2]*X3 + PNT[ip][jp][3]*X4
                         + PNT[ip][jp][4]*X5 + PNT[ip][jp][5]*X6
                         + PNT[ip][jp][6]*X7 + PNT[ip][jp][7]*X8;
                    dYdT = PNT[ip][jp][0]*Y1 + PNT[ip][jp][1]*Y2
                         + PNT[ip][jp][2]*Y3 + PNT[ip][jp][3]*Y4
                         + PNT[ip][jp][4]*Y5 + PNT[ip][jp][5]*Y6
                         + PNT[ip][jp][6]*Y7 + PNT[ip][jp][7]*Y8;
                    dZdT = PNT[ip][jp][0]*Z1 + PNT[ip][jp][1]*Z2
                         + PNT[ip][jp][2]*Z3 + PNT[ip][jp][3]*Z4
                         + PNT[ip][jp][4]*Z5 + PNT[ip][jp][5]*Z6
                         + PNT[ip][jp][6]*Z7 + PNT[ip][jp][7]*Z8;
                    DETJ[ip][jp][kp]= dXdQ*(dYdE*dZdT-dZdE*dYdT) +
                                      dYdQ*(dZdE*dXdT-dXdE*dZdT) +
                                      dZdQ*(dXdE*dYdT-dYdE*dXdT);
/**
    INVERSE JACOBIAN
**/
                    coef=1.0 / DETJ[ip][jp][kp];

                    a11= coef * ( dYdE*dZdT - dZdE*dYdT );
                    a12= coef * ( dZdQ*dYdT - dYdQ*dZdT );
                    a13= coef * ( dYdQ*dZdE - dZdQ*dYdE );

                    a21= coef * ( dZdE*dXdT - dXdE*dZdT );
                    a22= coef * ( dXdQ*dZdT - dZdQ*dXdT );
                    a23= coef * ( dZdQ*dXdE - dXdQ*dZdE );

                    a31= coef * ( dXdE*dYdT - dYdE*dXdT );
                    a32= coef * ( dYdQ*dXdT - dXdQ*dYdT );
                    a33= coef * ( dXdQ*dYdE - dYdQ*dXdE );

                    DETJ[ip][jp][kp]=fabs(DETJ[ip][jp][kp]);
```

$$[J]^{-1} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

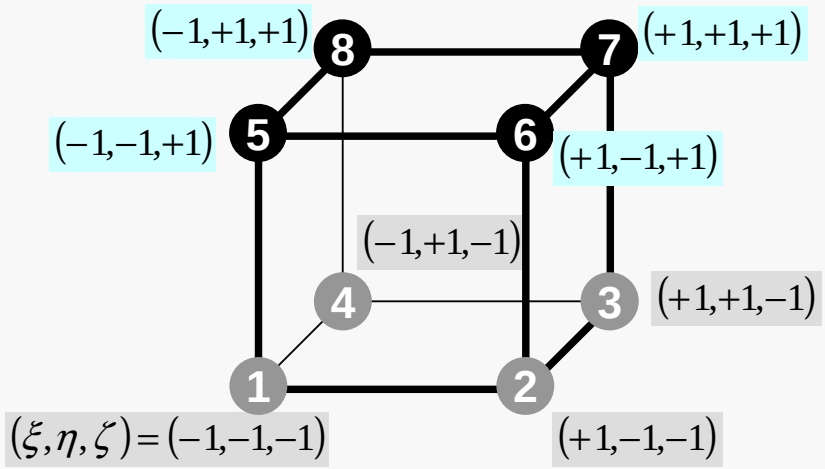
JACOBI (4/4)

```
/**
    set the dNi/dX, dNi/dY & dNi/dZ components
**/
            PNX[ip][jp][kp][0]=a11*PNQ[jp][kp][0]+a12*PNE[ip][kp][0]+a13*PNT[ip][jp][0];
            PNX[ip][jp][kp][1]=a11*PNQ[jp][kp][1]+a12*PNE[ip][kp][1]+a13*PNT[ip][jp][1];
            PNX[ip][jp][kp][2]=a11*PNQ[jp][kp][2]+a12*PNE[ip][kp][2]+a13*PNT[ip][jp][2];
            PNX[ip][jp][kp][3]=a11*PNQ[jp][kp][3]+a12*PNE[ip][kp][3]+a13*PNT[ip][jp][3];
            PNX[ip][jp][kp][4]=a11*PNQ[jp][kp][4]+a12*PNE[ip][kp][4]+a13*PNT[ip][jp][4];
            PNX[ip][jp][kp][5]=a11*PNQ[jp][kp][5]+a12*PNE[ip][kp][5]+a13*PNT[ip][jp][5];
            PNX[ip][jp][kp][6]=a11*PNQ[jp][kp][6]+a12*PNE[ip][kp][6]+a13*PNT[ip][jp][6];
            PNX[ip][jp][kp][7]=a11*PNQ[jp][kp][7]+a12*PNE[ip][kp][7]+a13*PNT[ip][jp][7];
            PNY[ip][jp][kp][0]=a21*PNQ[jp][kp][0]+a22*PNE[ip][kp][0]+a23*PNT[ip][jp][0];
            PNY[ip][jp][kp][1]=a21*PNQ[jp][kp][1]+a22*PNE[ip][kp][1]+a23*PNT[ip][jp][1];
            PNY[ip][jp][kp][2]=a21*PNQ[jp][kp][2]+a22*PNE[ip][kp][2]+a23*PNT[ip][jp][2];
            PNY[ip][jp][kp][3]=a21*PNQ[jp][kp][3]+a22*PNE[ip][kp][3]+a23*PNT[ip][jp][3];
            PNY[ip][jp][kp][4]=a21*PNQ[jp][kp][4]+a22*PNE[ip][kp][4]+a23*PNT[ip][jp][4];
            PNY[ip][jp][kp][5]=a21*PNQ[jp][kp][5]+a22*PNE[ip][kp][5]+a23*PNT[ip][jp][5];
            PNY[ip][jp][kp][6]=a21*PNQ[jp][kp][6]+a22*PNE[ip][kp][6]+a23*PNT[ip][jp][6];
            PNY[ip][jp][kp][7]=a21*PNQ[jp][kp][7]+a22*PNE[ip][kp][7]+a23*PNT[ip][jp][7];
            PNZ[ip][jp][kp][0]=a31*PNQ[jp][kp][0]+a32*PNE[ip][kp][0]+a33*PNT[ip][jp][0];
            PNZ[ip][jp][kp][1]=a31*PNQ[jp][kp][1]+a32*PNE[ip][kp][1]+a33*PNT[ip][jp][1];
            PNZ[ip][jp][kp][2]=a31*PNQ[jp][kp][2]+a32*PNE[ip][kp][2]+a33*PNT[ip][jp][2];
            PNZ[ip][jp][kp][3]=a31*PNQ[jp][kp][3]+a32*PNE[ip][kp][3]+a33*PNT[ip][jp][3];
            PNZ[ip][jp][kp][4]=a31*PNQ[jp][kp][4]+a32*PNE[ip][kp][4]+a33*PNT[ip][jp][4];
            PNZ[ip][jp][kp][5]=a31*PNQ[jp][kp][5]+a32*PNE[ip][kp][5]+a33*PNT[ip][jp][5];
            PNZ[ip][jp][kp][6]=a31*PNQ[jp][kp][6]+a32*PNE[ip][kp][6]+a33*PNT[ip][jp][6];
            PNZ[ip][jp][kp][7]=a31*PNQ[jp][kp][7]+a32*PNE[ip][kp][7]+a33*PNT[ip][jp][7];
                                }
                    }
            }
}
```

$$\begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix}^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix}$$

MAT_ASS_MAIN (5/6)

```
/**
   CONSTRUCT the GLOBAL MATRIX
**/

    for(ie=0;ie<8;ie++){
      ip=nodLOCAL[ie];

      for(je=0;je<8;je++){
        jp=nodLOCAL[je];

        kk=-1;
        if( jp != ip ){
          iiS=indexLU[ip-1];
          iiE=indexLU[ip  ];
          for( k=iiS;k<iiE;k++){
            if( itemLU[k] == jp-1 ){
              kk=k;
              break;
            }
          }
        }
```



Non-Zero Off-Diagonal Block in Global Matix

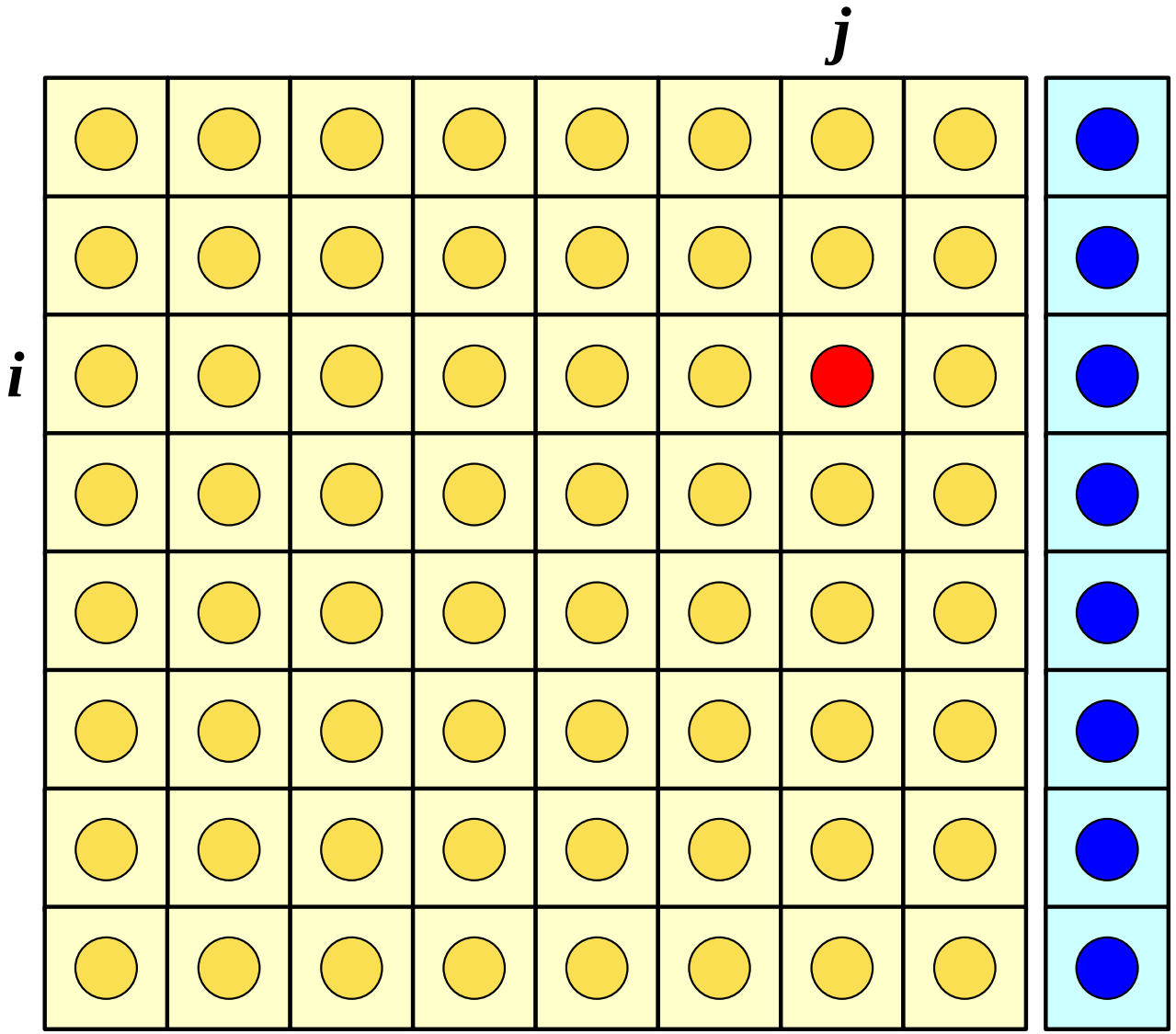
$A_{ip,jp}$

kk: address in “itemLU”

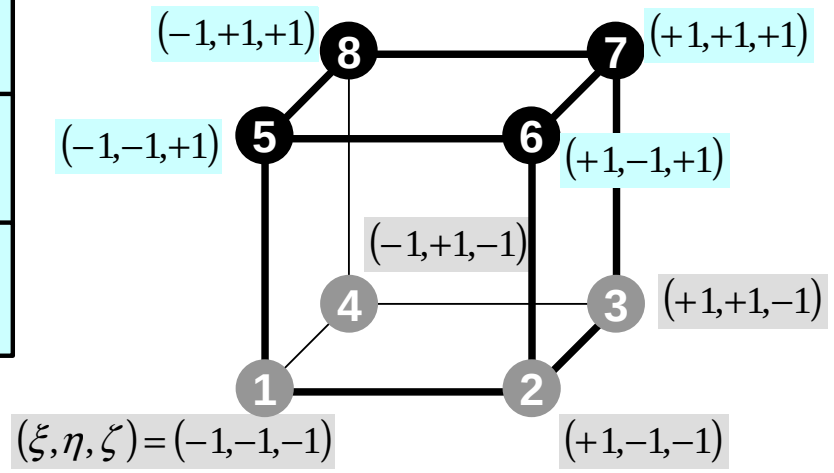
ip= nodLOCAL[ie]
jp= nodLOCAL[je]

Node ID (ip,jp) starting from 1

Element Matrix: 8x8



$$\lfloor k_{ij} \rfloor \quad (i, j = 1 \ldots 8)$$



MAT_ASS_MAIN (5/6)

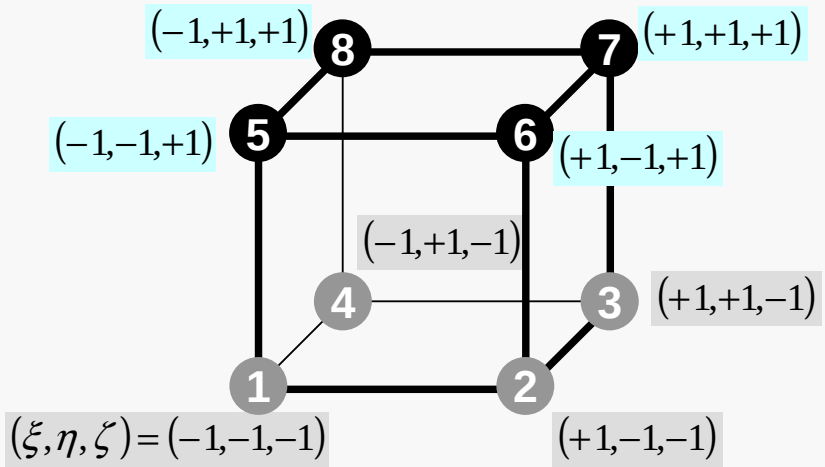
```
/**
   CONSTRUCT the GLOBAL MATRIX
**/

    for(ie=0;ie<8;ie++){
      ip=nodLOCAL[ie];

      for(je=0;je<8;je++){
        jp=nodLOCAL[je];

        kk=-1;
        if( jp != ip ){
          iiS=indexLU[ip-1];
          iiE=indexLU[ip  ];
          for( k=iiS;k<iiE;k++){
            if( itemLU[k] == jp-1 ){
              kk=k;
              break;
            }
          }
        }
```

Element Matrix (i_e~j_e): Local ID
Global Matrix (i_p~j_p): Global ID

kk : address in “itemLU” starting from “0”

k: starting from “0”

ip,jp: starting from “1”



MAT_ASS_MAIN (6/6)

```
        QV0= 0.e0;
        COEFij= 0.e0;

        for(kpn=0;kpn<2;kpn++){
          for(jpn=0;jpn<2;jpn++){
            for(ipn=0;ipn<2;ipn++){
              coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

              PNXi= PNX[ipn][jpn][kpn][ie];
              PNYi= PNY[ipn][jpn][kpn][ie];
              PNZi= PNZ[ipn][jpn][kpn][ie];

              PNXj= PNX[ipn][jpn][kpn][je];
              PNYj= PNY[ipn][jpn][kpn][je];
              PNZj= PNZ[ipn][jpn][kpn][je];

              COEFij+= coef*CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)*DETJ[ipn][jpn][kpn];

              SHi= SHAPE[ipn][jpn][kpn][ie];
              QV0+= SHi * QVOL * coef* DETJ[ipn][jpn][kpn];

            }
          }
        }

        if (jp==ip) {
          D[ip-1]+= COEFij;
          B[ip-1]+= QV0*QVC;
        }
        if (jp != ip) {
          AMAT[kk]+= COEFij;
        }

      }
    }
  }
}
```

$$\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1}\left\{\lambda\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}+\lambda\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}+\lambda\frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}\right\}\det|J|\,d\xi d\eta d\zeta$$

MAT_ASS_MAIN (6/6)

```
        QV0= 0.e0;
        COEFij= 0.e0;

        for(kpn=0;kpn<2;kpn++){
          for(jpn=0;jpn<2;jpn++){
            for(ipn=0;ipn<2;ipn++){
              coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

              PNXi= PNX[ipn][jpn][kpn][ie];
              PNYi= PNY[ipn][jpn][kpn][ie];
              PNZi= PNZ[ipn][jpn][kpn][ie];

              PNXj= PNX[ipn][jpn][kpn][je];
              PNYj= PNY[ipn][jpn][kpn][je];
              PNZj= PNZ[ipn][jpn][kpn][je];

              COEFij+= coef*CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)*DETJ[ipn][jpn][kpn];

              SHi= SHAPE[ipn][jpn][kpn][ie];
              QV0+= SHi * QVOL * coef* DETJ[ipn][jpn][k

            }
          }
        }

        if (jp==ip) {
          D[ip-1]+= COEFij;
          B[ip-1]+= QV0*QVC;
        }
        if (jp != ip) {
          AMAT[kk]+= COEFij;
        }

      }
    }
  }
}
```

$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta$$

$$= \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N} W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)$$

$$\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} \left\{ \lambda \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} \det|J|\, d\xi d\eta d\zeta$$

MAT_ASS_MAIN (6/6)

```
for(kpn=0;kpn<2;kpn++){
  for(jpn=0;jpn<2;jpn++){
    for(ipn=0;ipn<2;ipn++){
      coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

      PNXi= PNX[ipn][jpn][kpn][ie];
      PNYi= PNY[ipn][jpn][kpn][ie];
      PNZi= PNZ[ipn][jpn][kpn][ie];

      PNXj= PNX[ipn][jpn][kpn][je];
      PNYj= PNY[ipn][jpn][kpn][je];
      PNZj= PNZ[ipn][jpn][kpn][je];


      COEFij+= coef* CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)
                          * DETJ[ipn][jpn][kpn];

    }
  }
}
```

$$\text{coef} = W_i \cdot W_j \cdot W_k$$

$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N} W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)$$

$$\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} \left\{ \lambda \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} \det|J|\, d\xi d\eta d\zeta$$

MAT_ASS_MAIN (6/6)

```
for(kpn=0;kpn<2;kpn++){
  for(jpn=0;jpn<2;jpn++){
    for(ipn=0;ipn<2;ipn++){
      coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

      PNXi= PNX[ipn][jpn][kpn][ie];
      PNYi= PNY[ipn][jpn][kpn][ie];
      PNZi= PNZ[ipn][jpn][kpn][ie];

      PNXj= PNX[ipn][jpn][kpn][je];
      PNYj= PNY[ipn][jpn][kpn][je];
      PNZj= PNZ[ipn][jpn][kpn][je];

      COEFij+= coef* CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)
                   * DETJ[ipn][jpn][kpn];

    }
  }
}
```

$$\mathrm{coef} = W_i \cdot W_j \cdot W_k$$

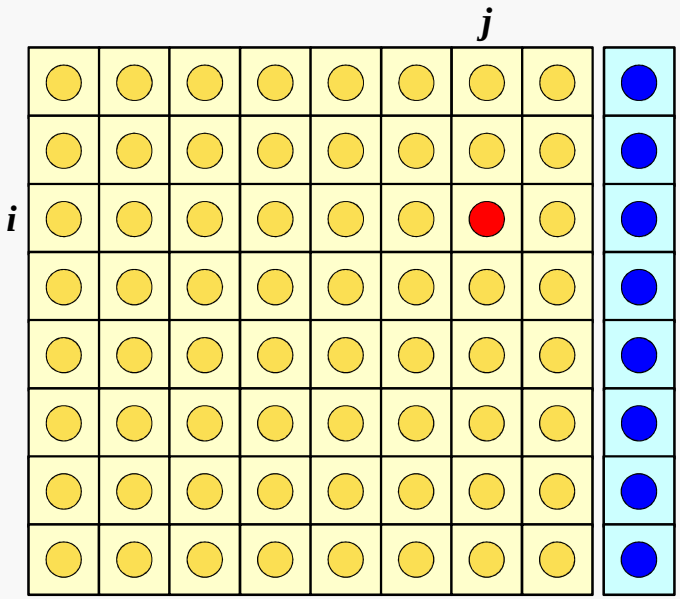
$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N} W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)$$

$$\int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} \left\{ \lambda \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \lambda \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \lambda \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \right\} \det|J|\, d\xi d\eta d\zeta$$

MAT_ASS_MAIN (6/6)

```
        QV0= 0.e0;
        COEFij= 0.e0;

        for(kpn=0;kpn<2;kpn++){
          for(jpn=0;jpn<2;jpn++){
            for(ipn=0;ipn<2;ipn++){
              coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

              PNXi= PNX[ipn][jpn][kpn][ie];
              PNYi= PNY[ipn][jpn][kpn][ie];
              PNZi= PNZ[ipn][jpn][kpn][ie];

              PNXj= PNX[ipn][jpn][kpn][je];
              PNYj= PNY[ipn][jpn][kpn][je];
              PNZj= PNZ[ipn][jpn][kpn][je];

              COEFij+= coef*CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)*DETJ[ipn][jpn][kpn];

              SHi= SHAPE[ipn][jpn][kpn][ie];
              QV0+= SHi * QVOL * coef * DETJ[ipn][jpn][kpn];

            }
          }
        }

        if (jp==ip) {
          D[ip-1]+= COEFij;
          B[ip-1]+= QV0*QVC;
        }
        if (jp != ip) {
          AMAT[kk]+= COEFij;
        }

      }
    }
  }
}
```

$$[k_{ij}] \quad (i, j = 1 \ldots 8)$$



MAT_ASS_MAIN (6/6)

```
        QV0= 0.e0;
        COEFij= 0.e0;

        for(kpn=0;kpn<2;kpn++){
          for(jpn=0;jpn<2;jpn++){
            for(ipn=0;ipn<2;ipn++){
              coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

              PNXi= PNX[ipn][jpn][kpn][ie];
              PNYi= PNY[ipn][jpn][kpn][ie];
              PNZi= PNZ[ipn][jpn][kpn][ie];

              PNXj= PNX[ipn][jpn][kpn][je];
              PNYj= PNY[ipn][jpn][kpn][je];
              PNZj= PNZ[ipn][jpn][kpn][je];

              COEFij+= coef*CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)*DETJ[ipn][jpn][kpn];

              SHi= SHAPE[ipn][jpn][kpn][ie];
              QV0+= SHi * QVOL * coef * DETJ[ipn][jpn][kpn];

            }
          }
        }

        if (jp==ip) {
          D[ip-1]+= COEFij;
          B[ip-1]+= QV0*QVC;
        }
        if (jp != ip) {
          AMAT[kk]+= COEFij;
        }

      }
    }
  }
}
```

$$[k]^{(e)}\{\phi\}^{(e)} = \{f\}^{(e)}$$

$$[f]^{(e)} = \int_V \dot{Q}[N]^T dV$$

$$\dot{Q}(x,y,z) = QVOL\left|x_C + y_C\right|$$

$$QV0 = \int_V QVOL[N]^T dV$$

MAT_ASS_MAIN (6/6)

```
for (kpn=0;kpn<2;kpn++) {
    for (jpn=0;jpn<2;jpn++) {
        for (ipn=0;ipn<2;ipn++) {
            coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

            SHi= SHAPE[ipn][jpn][kpn][ie];
            QVO+= SHi * QVOL * coef * DETJ[ipn][jpn][kpn];

        }
    }
}
```

$$\mathrm{coef} = W_i \cdot W_j \cdot W_k$$

$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N} W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)$$

$$\int_V QVOL[N]^T dV = \iiint QVOL[N] dxdydz = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} \{QVOL\, N_i\} \det|J|\, d\xi d\eta d\zeta$$

MAT_ASS_MAIN (6/6)

```
for (kpn=0;kpn<2;kpn++) {
    for (jpn=0;jpn<2;jpn++) {
        for (ipn=0;ipn<2;ipn++) {
            coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

            SHi= SHAPE[ipn][jpn][kpn][ie];
            QVO+= SHi * QVOL * coef * DETJ[ipn][jpn][kpn];

        }
    }
}
```

$\mathrm{coef} = W_i \cdot W_j \cdot W_k$

$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N} W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)$$

$$\int_V QVOL[N]^T dV = \iiint QVOL[N] dxdydz = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} \{QVOL\, N_i\} \det|J|\, d\xi d\eta d\zeta$$

MAT_ASS_MAIN (6/6)

```
        QV0= 0.e0;
        COEFij= 0.e0;

        for(kpn=0;kpn<2;kpn++){
          for(jpn=0;jpn<2;jpn++){
            for(ipn=0;ipn<2;ipn++){
              coef= WEI[ipn]*WEI[jpn]*WEI[kpn];

              PNXi= PNX[ipn][jpn][kpn][ie];
              PNYi= PNY[ipn][jpn][kpn][ie];
              PNZi= PNZ[ipn][jpn][kpn][ie];

              PNXj= PNX[ipn][jpn][kpn][je];
              PNYj= PNY[ipn][jpn][kpn][je];
              PNZj= PNZ[ipn][jpn][kpn][je];

              COEFij+= coef*CONDO*(PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)*DETJ[ipn][jpn][kpn];

              SHi= SHAPE[ipn][jpn][kpn][ie];
              QV0+= SHi * QVOL * coef * DETJ[ipn][jpn][kpn];

            }
          }
        }

        if (jp==ip) {
          D[ip-1]+= COEFij;
          B[ip-1]+= QV0*QVC;
        }
        if (jp != ip) {
          AMAT[kk]+= COEFij;
        }

      }
    }
  }
}
```

$$[k]^{(e)}\{\phi\}^{(e)} = \{f\}^{(e)}$$

$$[f]^{(e)} = \int_V \dot{Q}[N]^T dV$$

$$\dot{Q}(x,y,z) = QVOL\left|x_C + y_C\right|$$

$$QV0 = \int_V QVOL[N]^T dV$$

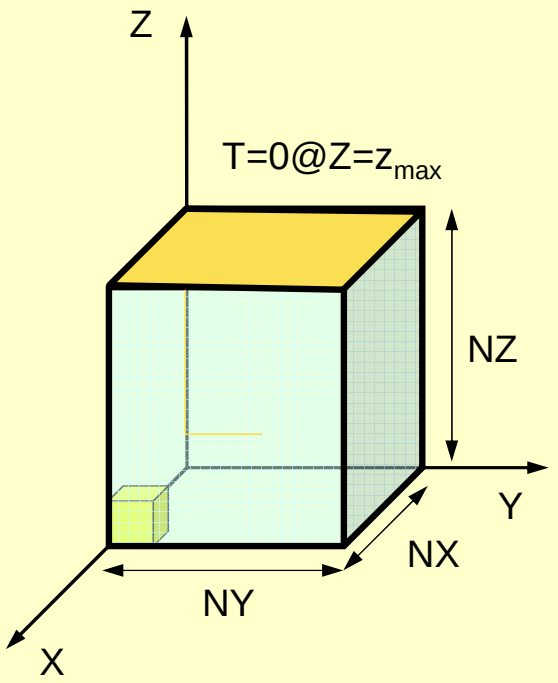
$$QVC = \left|x_C + y_C\right|$$

$$[f]^{(e)} = QV0 \cdot QVC$$

MAT_ASS_BC: Overview

```
do i= 1, N      Loop for Nodes
   “Mark” nodes where Dirichlet B.C. are applied (IWKX)
enddo
```

```
do i= 1, N  Loop for Nodes
  if (IWKX(i,1).eq.1) then  if “marked” nodes
    corresponding components of RHS (B),
    Diagonal (D) are corrected
    do k= indexLU(i-1)+1, indexLU(i)   Non-Zero Off-Diagonal Nodes
       corresponding comp. of non-zero off-diagonal
       components (AMAT) are corrected
    enddo
  endif
enddo

do i= 1, N  Loop for Nodes
  do k= indexLU(i-1)+1, indexLU(i)   Non-Zero Off-Diagonal Nodes
    if (IWKX(itemLU(k),1).eq.1) then  if corresponding non-zero
                                      off-diagonal node is “marked”
      corresponding components of RHS and AMAT are corrected (col.)
    endif
  enddo
enddo
```



MAT_ASS_BC (1/2)

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE *fp_log;
void MAT_ASS_BC()
{
  int i,j,k,in,ib,ib0,icel;
  int in1,in2,in3,in4,in5,in6,in7,in8;
  int iq1,iq2,iq3,iq4,iq5,iq6,iq7,iq8;
  int iS,iE;
  double STRESS,VAL;

  IWKX=(KINT**) allocate_matrix(sizeof(KINT),N,2);
  for(i=0;i<N;i++) for(j=0;j<2;j++) IWKX[i][j]=0;

/**
   Z=Zmax
**/

  for(in=0;in<N;in++) IWKX[in][0]=0;

  ib0=-1;

  for( ib0=0;ib0<NODGRPtot;ib0++){
    if( strcmp(NODGRP_NAME[ib0].name,"Zmax") == 0 ) break;
  }

  for( ib=NODGRP_INDEX[ib0];ib<NODGRP_INDEX[ib0+1];ib++){
    in=NODGRP_ITEM[ib];
    IWKX[in-1][0]=1;
  }
```

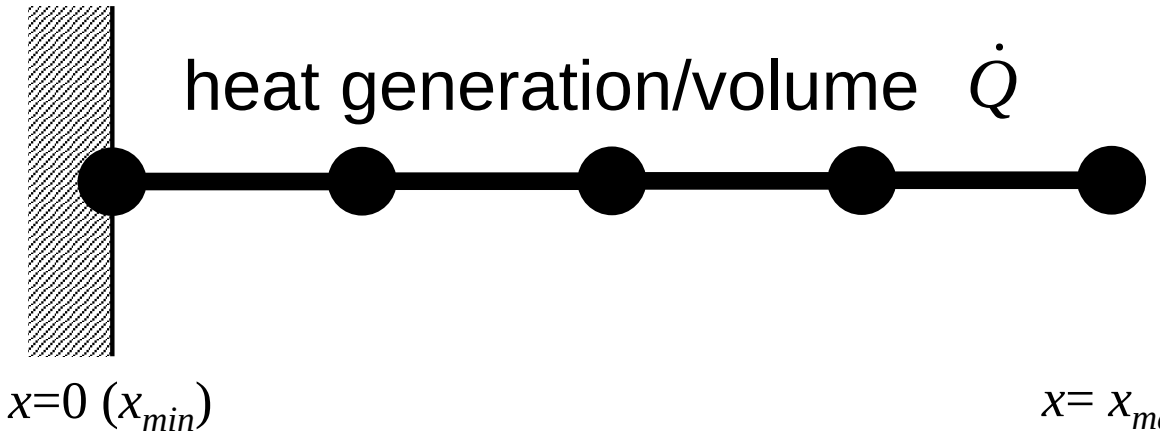
If the node “in” is included in the node group “Zmax”

IWKX[in-1][0]= 1

MAT_ASS_BC (2/2)

```
 for(in=0;in<N;in++){
    if( IWKX[in][0] == 1 ){
      B[in]= 0.e0;
      D[in]= 1.e0;
      for(k=indexLU[in];k<indexLU[in+1];k++){
        AMAT[k]= 0.e0;
      }
    }
  }

  for(in=0;in<N;in++){
    for(k=indexLU[in];k<indexLU[in+1];k++){
      if (IWKX[itemLU[k]][0] == 1 ) {
        AMAT[k]= 0.e0;
      }
    }
  }
}
```

1D Steady State Heat Conduction



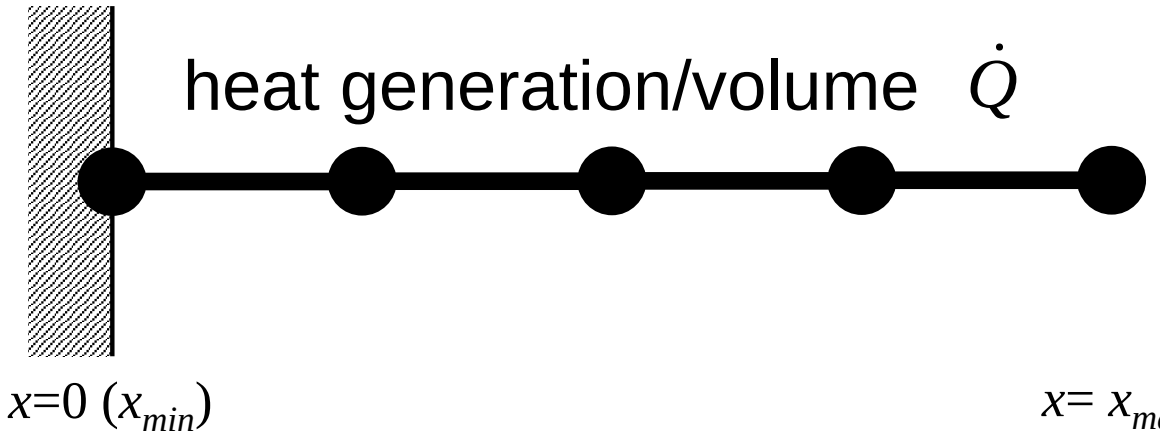
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\dot{Q}=0$$

- Uniform: Sectional Area: A, Thermal Conductivity: λ
- Heat Generation Rate/Volume/Time [$QL^{-3}T^{-1}$] $\dot{Q}$
- Boundary Conditions
  - x=0 : T= 0 (Fixed Temperature)
  - x=x_{max} : $\frac{\partial T}{\partial x}=0$ (Insulated)

1D

(Linear) Equation at x=0

T_1= 0 (or T_0 = 0)



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

- Uniform: Sectional Area: A, Thermal Conductivity: λ
- Heat Generation Rate/Volume/Time [$QL^{-3}T^{-1}$] $\dot{Q}$
- Boundary Conditions
  - x=0 : T= 0 (Fixed Temperature)
  - x=x_{max} : $\dfrac{\partial T}{\partial x}=0$ (Insulated)

1D

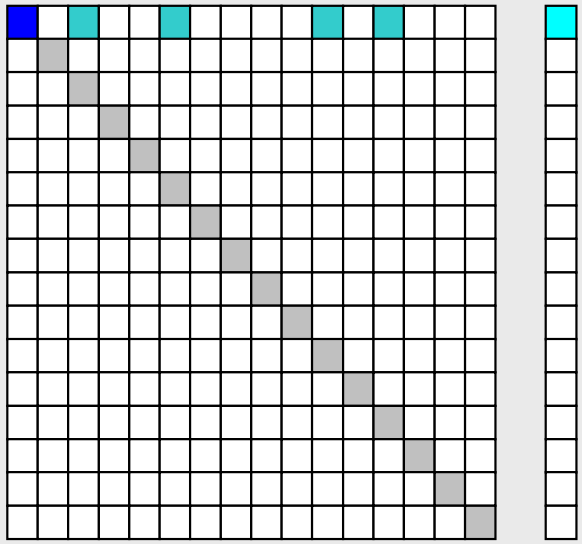
Program: 1d.c (6/6)

Dirichlet B.C. @ X=0

```
/*
// +--------------------+
// | BOUNDARY conditions |
// +--------------------+
*/

/* X=Xmin */
        i=0;
        jS= Index[i];
        AMat[jS]= 0.0;
        Diag[i ]= 1.0;
        Rhs [i ]= 0.0;

        for(k=0;k<NPLU;k++){
          if(Item[k]==0){AMat[k]=0.0;
          }}
```

$T_1=0$

Diagonal Component=1
RHS=0
Off-Diagonal Components= 0.



Program: 1d.c (6/6)

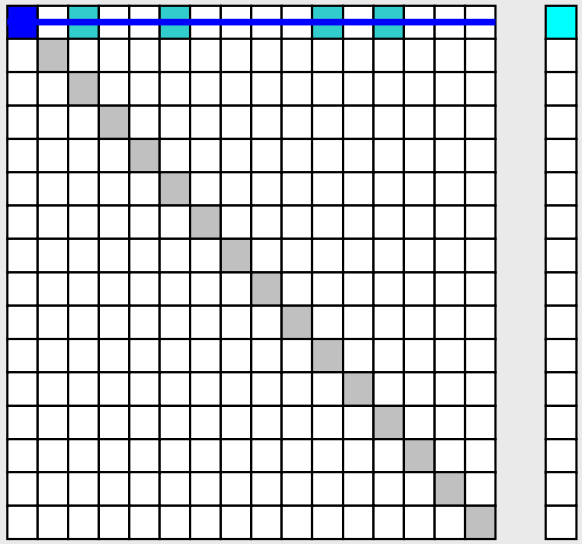
Dirichlet B.C. @ X=0

```
/*
// +--------------------+
// | BOUNDARY conditions |
// +--------------------+
*/

/* X=Xmin */
        i=0;
        jS= Index[i];
        AMat[jS]= 0.0;
        Diag[i ]= 1.0;
        Rhs [i ]= 0.0;

        for(k=0;k<NPLU;k++){
          if(Item[k]==0){AMat[k]=0.0;
          }}
```

$T_1=0$

Diagonal Component=1
RHS=0
Off-Diagonal Components= 0.

Erase !



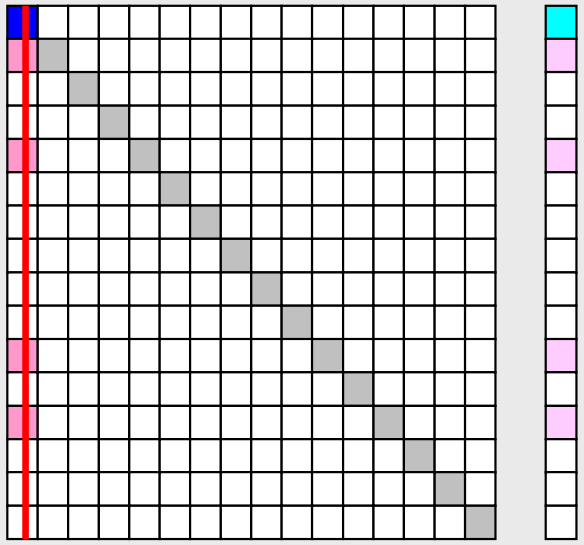
Program: 1d.c (6/6)
Dirichlet B.C. @ X=0

```
/*
// +--------------------+
// | BOUNDARY conditions |
// +--------------------+
*/

/* X=Xmin */
        i=0;
        jS= Index[i];
        AMat[jS]= 0.0;
        Diag[i ]= 1.0;
        Rhs [i ]= 0.0;

        for(k=0;k<NPLU;k++){
          if(Item[k]==0){AMat[k]=0.0;
          }}
```

$T_1=0$

Diagonal Component=1
RHS=0
Off-Diagonal Components= 0.

Elimination and Erase



Column components of boundary nodes (Dirichlet B.C.) are moved to RHS and eliminated for keeping symmetrical feature of the matrix (in this case just erase off-diagonal components)

if $T_1 \neq 0$

```
/*
// +--------------------+
// | BOUNDARY conditions |
// +--------------------+
*/
```

Column components of boundary nodes (Dirichlet B.C.) are moved to RHS and eliminated for keeping symmetrical feature of the matrix.

$$Diag_j \phi_j + \sum_{k=Index[j]}^{Index[j+1]-1} Amat_k \ \phi_{Item[k]} = Rhs_j$$

```
/* X=Xmin */
        i=0;
        jS= Index[i];
        AMat[jS]= 0.0;
        Diag[i ]= 1.0;
        Rhs [i ]= PHImin;

          for(j=1;i<N;i++){
            for (k=Index[j];k<Index[j+1];k++){
              if(Item[k]==0){
                 Rhs [j]= Rhs[j] - Amat[k]*PHImin;
                 AMat[k]= 0.0;
            }}
```

if $T_1 \neq 0$

```
/*
// +--------------------+
// | BOUNDARY conditions |
// +--------------------+
*/



/* X=Xmin */
        i=0;
        jS= Index[i];
        AMat[jS]= 0.0;
        Diag[i ]= 1.0;
        Rhs [i ]= PHImin;

          for(j=1;i<N;i++){
            for (k=Index[j];k<Index[j+1];k++){
              if(Item[k]==0){
                 Rhs [j]= Rhs[j] - Amat[k]*PHImin;
                 AMat[k]= 0.0;
            }}
```

$$Diag_j \phi_j + \sum_{k=Index[j],k\neq k_s}^{Index[j+1]-1} Amat_k \ \phi_{Item[k]}$$

$$= Rhs_j - Amat_{k_s} \phi_{Item[k_s]}$$

$$= Rhs_j - Amat_{k_s} \phi_{\min} \quad where\ Item[k_s] = 0$$

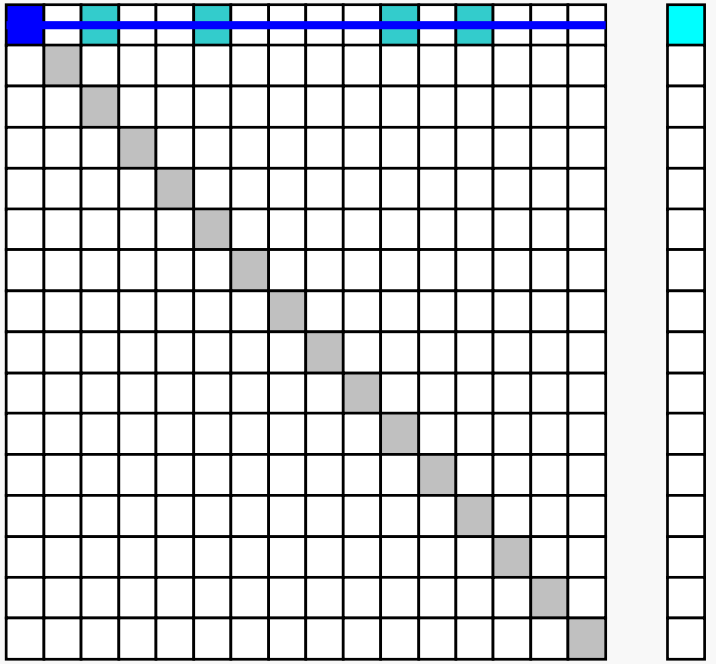
Column components of boundary nodes (Dirichlet B.C.) are moved to RHS and eliminated for keeping symmetrical feature of the matrix.

MAT_ASS_BC (2/2)

```
for(in=0;in<N;in++){
   if( IWKX[in][0] == 1 ){
     B[in]= 0.e0;
     D[in]= 1.e0;
     for(k=indexLU[in];k<indexLU[in+1];k++){
       AMAT[k]= 0.e0;
     }
   }
 }

 for(in=0;in<N;in++){
   for(k=indexLU[in];k<indexLU[in+1];k++){
     if (IWKX[itemLU[k]][0] == 1 ) {
       AMAT[k]= 0.e0;
     }
   }
 }
}
```

Boundary Nodes: IWKX[in-1][0]=1

Erase !!

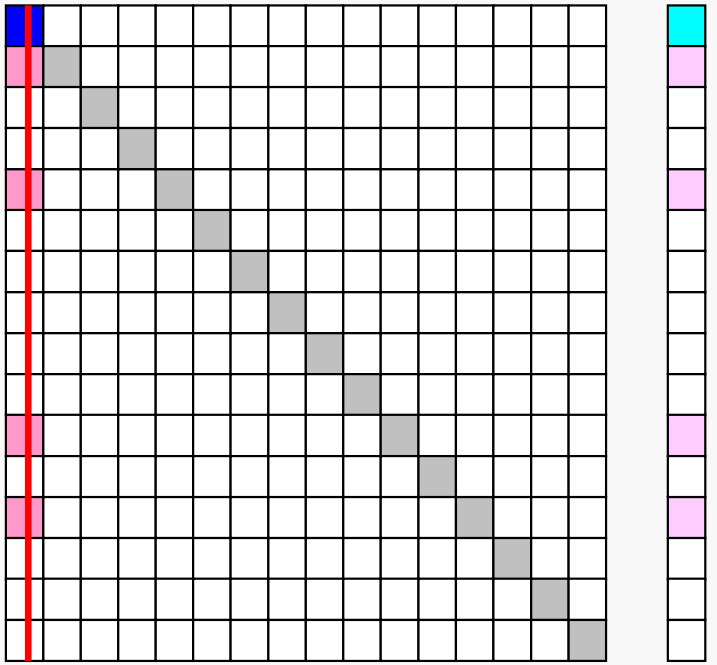


Same as 1D case

MAT_ASS_BC (2/2)

```
for(in=0;in<N;in++){
   if( IWKX[in][0] == 1 ){
     B[in]= 0.e0;
     D[in]= 1.e0;
     for(k=indexLU[in];k<indexLU[in+1];k++){
       AMAT[k]= 0.e0;
     }
   }
 }

 for(in=0;in<N;in++){
   for(k=indexLU[in];k<indexLU[in+1];k++){
     if (IWKX[itemLU[k]][0] == 1 ) {
       AMAT[k]= 0.e0;
     }
   }
 }
}
```

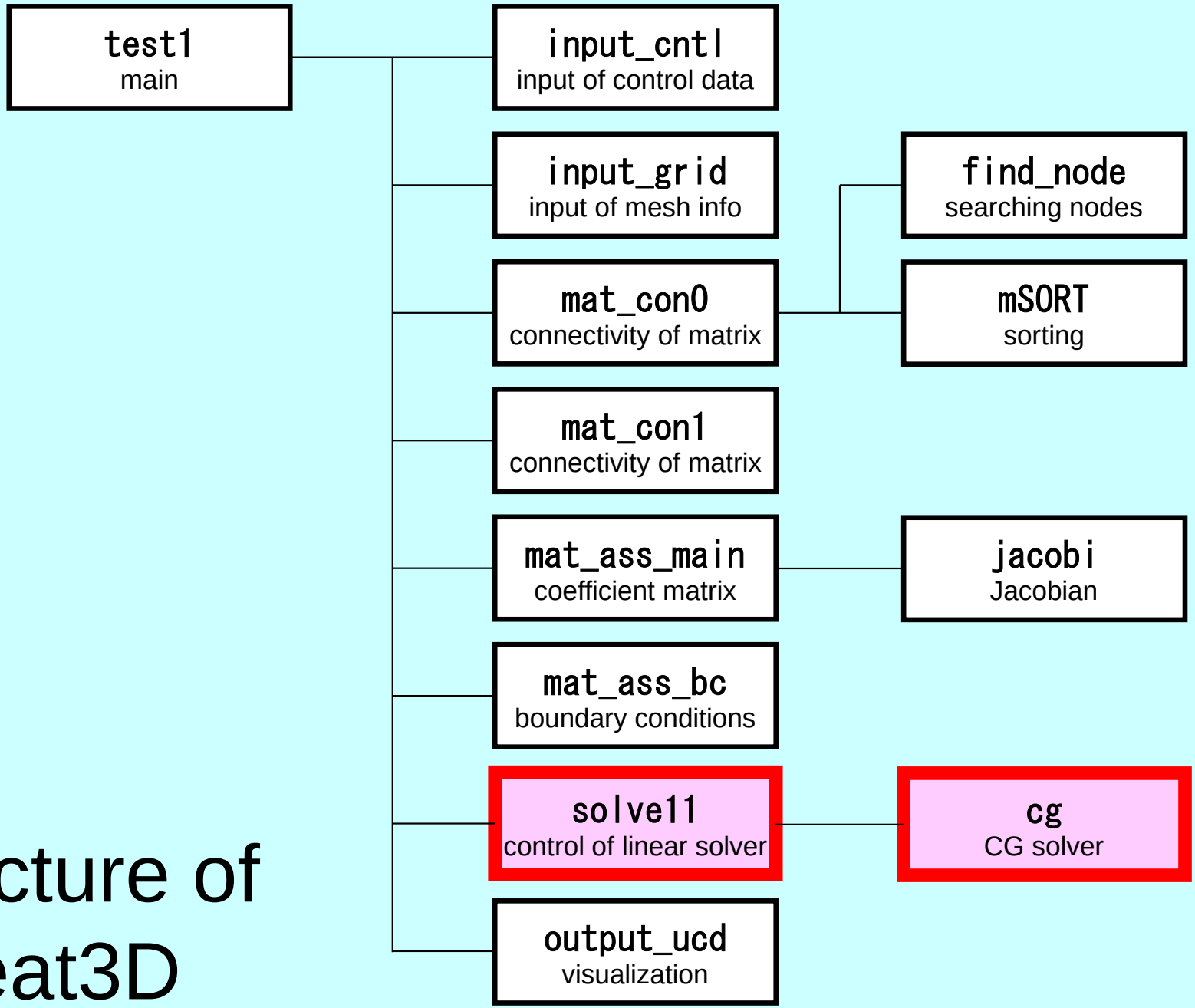
Boundary Nodes: IWKX[in-1][0]=1



Elimination and Erase

Same as 1D case

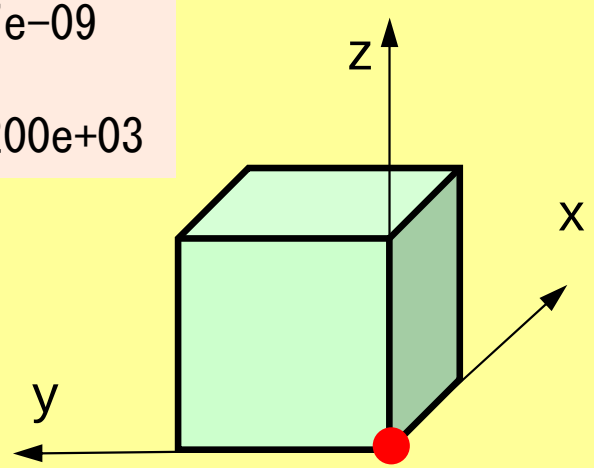
Structure of heat3D



Main Part

```
int main()
{
  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()  ;

  SOLVE11();

  OUTPUT_UCD()     ;
  for(i=0;i<N;i++){
    if (XYZ[i][0]==0.e0) {
    if (XYZ[i][1]==0.e0) {
    if (XYZ[i][2]==0.e0) {
      printf("%8d%16.6e¥n¥n¥n", i+1, X[i]);}
    }}}
}
```

```
1  4.025833e+00
2  3.628020e+00
3  3.319234e+00
4  3.073771e+00
(…)
55  9.238550e-07
56  3.876258e-07
57  1.854812e-07
58  1.062119e-07
59  3.541404e-08
60  1.284087e-08
61  6.073277e-09

1     3.391200e+03
```



SOLVE11

```
#include <stdio.h>
#include <string.h>
#include <math.h>
#include "pfem_util.h"
#include "allocate.h"
extern FILE *fp_log;
extern void CG();
void SOLVE11()
{
  int i,j,k,ii,L;

  int  ERROR, ICFLAG=0;
  CHAR_LENGTH BUF;

/**
   +------------+
   | PARAMETERs |
   +------------+
**/
  ITER      = pfemIarray[0];        Number of Iterations for CG
  RESID     = pfemRarray[0];        Convergence Criteria for CG

/**
   +------------------+
   | ITERATIVE solver |
   +------------------+
**/
  CG (N,NPLU, D, AMAT, indexLU, itemLU, B, X, RESID, ITER, &ERROR);
  ITERactual= ITER;
}
```

Preconditioned CG Solver

Diagonal Scaling/Point Jacobi Preconditioning

```
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
```

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

Diagonal Scaling, Point-Jacobi

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

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

CG Solver (1/6)

```
#include <stdio.h>
#include <math.h>
#include "precision.h"
#include "allocate.h"
extern FILE *fp_log;

void  CG  (
           KINT N,KINT NPLU,KREAL D[],
           KREAL AMAT[],KINT indexLU[], KINT itemLU[],
           KREAL B[],KREAL X[],KREAL RESID,KINT ITER, KINT *ERROR)
{
  int i,j,k;
  int ieL,isL,ieU,isU;
  double WVAL;
  double BNRM20,BNRM2,DNRM20,DNRM2;
  double S1_TIME,E1_TIME;
  double ALPHA,BETA;
  double C1,C10,RH0,RH00,RH01;
  int    iterPRE;

  KREAL **WW;

  KINT R=0,Z=1,Q=1,P=2,DD=3;
  KINT MAXIT;
  KREAL TOL;
```

Variables/Arrays in CG Solver

Name	Type	Size	I/O	Definition
N,NP	I		I	# Node
NPLU	I		O	# Non-Zero Off-Diagonals
D	R	[N]	O	Diagonal Block of Global Matrix
B,X	R	[N]	O	RHS, Unknown Vector
AMAT	R	[NPLU]	O	Non-Zero Off-Diagonal Components of Global Matrix
indexLU	I	[N+1]	O	# Non-Zero Off-Diagonal Components
itemLU	I	[NPLU]	O	Column ID of Non-Zero Off-Diagonal Components
ITER	I		I/O	Number of CG Iterations (MAX: In, Actual: Out)
RESID	R		I/O	Convergence Criteria (In), Final Residual Norm (Out)
MAXIT	I		-	Maximum Number of CG Iterations
TOL	R		-	Convergence Criteria
WW	R	[4][N]	-	Work Arrays
P,Q,R,Z,DD	I		-	Vector ID for **WW** (1-4)

CG Solver (1/6)

```
#include <stdio.h>
#
#
e
v
                                                    U[]
                                                    ER,
{
  int i,j,k;
  int ieL,isL,ieU,isU;
  double WVAL;
  double BNRM20,BNRM2,DNRM20,DNRM2;
  double S1_TIME,E1_TIME;
  double ALPHA,BETA;
  double C1,C10,RHO,RHO0,RHO1;
  int    iterPRE;

  KREAL **WW;

  KINT R=0,Z=1,Q=1,P=2,DD=3;
  KINT MAXIT;
  KREAL TOL;
```

WW[0][i]= WW[R][i] ⇒ {r}
WW[1][i]= WW[Z][i] ⇒ {z}
WW[1][i]= WW[Q][i] ⇒ {q}
WW[2][i]= WW[P][i] ⇒ {p}
WW[3][i]= WW[DD][i] ⇒ 1/{D}

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

CG Solver (1/6)

```
  WW=(KREAL**) allocate_matrix(sizeof(KREAL),4,N);

  MAXIT  = ITER;
  TOL    = RESID;

  for(i=0;i<N;i++){
    X[i]=0.0;
  }
  for(i=0;i<N;i++) for(j=0;j<4;j++) WW[j][i]=0.0;
/**
   +---------------------+
   | {r0}= {b} - [A]{xini} |
   +---------------------+
**/
  for(j=0;j<N;j++){
    WW[DD][j]= 1.0/D[j];
    WVAL= B[j] - D[j]*X[j];

    for( k=indexLU[j];k<indexLU[j+1];k++){
      i= itemLU[k];
      WVAL+=  -AMAT[k]*X[i];
    }
    WW[R][j]= WVAL;
  }
```

```
WW[0][i]= WW[R][i] ⇒ {r}
WW[1][i]= WW[Z][i] ⇒ {z}
WW[1][i]= WW[Q][i] ⇒ {q}
WW[2][i]= WW[P][i] ⇒ {p}
WW[3][i]= WW[DD][i]⇒ 1/{D}
```

Reciprocal numbers（逆数）of diagonal components are stored in `WW[DD][i]`.
Computational cost for division is usually expensive.

CG Solver (2/6)

```
  WW=(KREAL**) allocate_matrix(sizeof(KREAL),4,N);

  MAXIT  = ITER;
  TOL    = RESID;

  for(i=0;i<N;i++){
    X[i]=0.0;
  }
  for(i=0;i<N;i++) for(j=0;j<4;j++) WW[j][i]=0
/**
   +---------------------+
   | {r0}= {b} - [A]{xini} |
   +---------------------+
**/
  for(j=0;j<N;j++){
    WW[DD][j]= 1.0/D[j];
    WVAL= B[j] - D[j]*X[j];

    for( k=indexLU[j];k<indexLU[j+1];k++){
      i= itemLU[k];
      WVAL+=  -AMAT[k]*X[i];
    }
    WW[R][j]= WVAL;
  }
```

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

CG Solver (3/6)

```
  BNRM2= 0.e0;
  for(i=0;i<N;i++){
    BNRM2+= B[i]*B[i];
  }
```

BNRM2=|b|²
for convergence criteria of CG solvers

```
  if (BNRM2 == 0.e0) BNRM2= 1.e0;

  ITER = 0;

  for( ITER=1;ITER<= MAXIT;ITER++){
/**
********************************************** Conjugate Gradient Iteration
**/

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

CG Solver (3/6)

```
  BNRM2= 0.e0;
  for(i=0;i<N;i++){
    BNRM2+= B[i]*B[i];
  }



  if (BNRM2 == 0.e0) BNRM2= 1.e0;

  ITER = 0;

  for( ITER=1;ITER<= MAXIT;ITER++){
/**
************************************************
**/

/**
   +---------------+
   | {z}= [Minv]{r} |
   +---------------+
**/
  for(i=0;i<N;i++){
    WW[Z][i]= WW[DD][i]*WW[R][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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  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

CG Solver (4/6)

```
/**
   +---------------+
   | {RHO}= {r}{z} |
   +---------------+
**/
  RHO= 0.e0;

  for(i=0;i<N;i++){
    RHO+= WW[R][i]*WW[Z][i];
  }

/**
   +-----------------------------+
   | {p} = {z} if      ITER=1    |
   | BETA= RHO / RHO1  otherwise |
   +-----------------------------+
**/
  if( ITER == 1 ){
    for(i=0;i<N;i++){
      WW[P][i]=WW[Z][i];
    }
  }else{
    BETA= RHO / RHO1;
    for(i=0;i<N;i++){
      WW[P][i]=WW[Z][i] + BETA*WW[P][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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  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

CG Solver (5/6)

```
/**
   +-------------+
   | {q}= [A]{p} |
   +-------------+
**/
  for( j=0;j<N;j++){
    WVAL= D[j] * WW[P][j];
    for(k=indexLU[j];k<indexLU[j+1];k++){
      i=itemLU[k];
      WVAL+= AMAT[k] * WW[P][i];
    }
    WW[Q][j]=WVAL;
  }

/**
   +---------------------+
   | ALPHA= RHO / {p}{q} |
   +---------------------+
**/
  C1= 0.e0;
  for(i=0;i<N;i++){
    C1+=WW[P][i]*WW[Q][i];
  }


  ALPHA= RHO / C1;
```

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

CG Solver (6/6)

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

  DNRM2= 0.e0;
  for(i=0;i<N;i++){
    DNRM2+=WW[R][i]*WW[R][i];
  }

  RESID= sqrt(DNRM2/BNRM2);

  if ( RESID <= TOL   ) break;
  if ( ITER  == MAXIT ) *ERROR= -300;

  RHO1 = RHO ;
}
```

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

CG Solver (6/6)

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

  DNRM2= 0.e0;
  for(i=0;i<N;i++){
    DNRM2+=WW[R][i]*WW[R][i];
  }

  RESID= sqrt(DNRM2/BNRM2);

  if ( RESID <= TOL   ) break;
  if ( ITER  == MAXIT ) *ERROR= -300;

  RHO1 = RHO ;
}
```

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

$$\mathrm{Resid} = \sqrt{\frac{\mathrm{DNorm2}}{\mathrm{BNorm2}}} = \frac{|r|}{|b|} = \frac{|b-Ax|}{|b|} \leq \mathrm{Tol}$$