3D Parallel FEM (II)
Fortran

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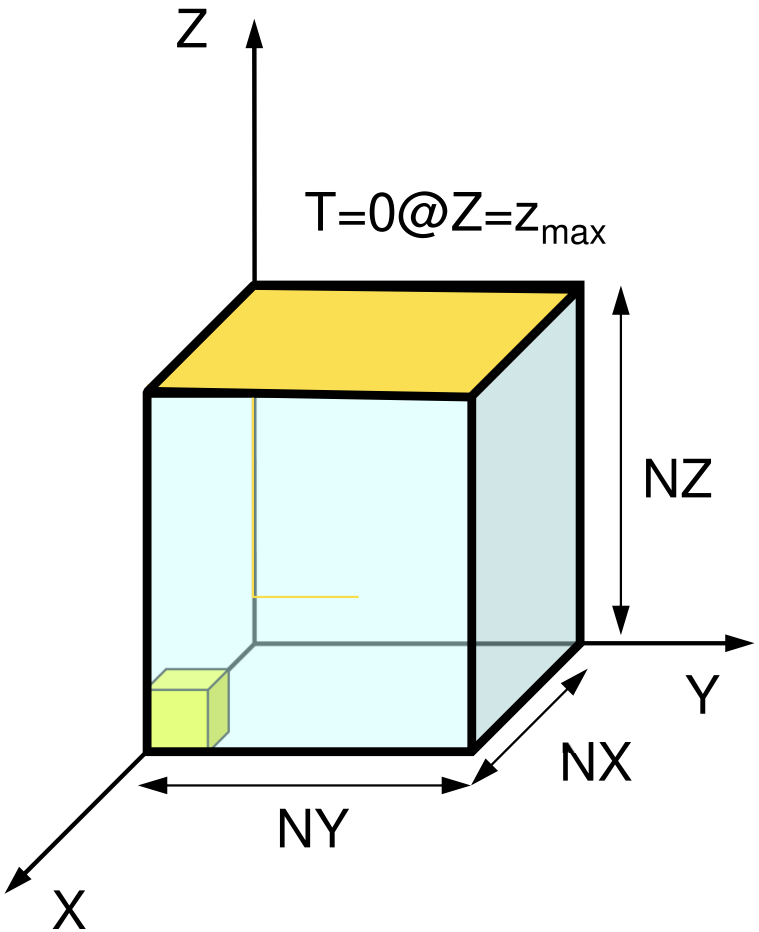
3D Steady-State Heat Conduction

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



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

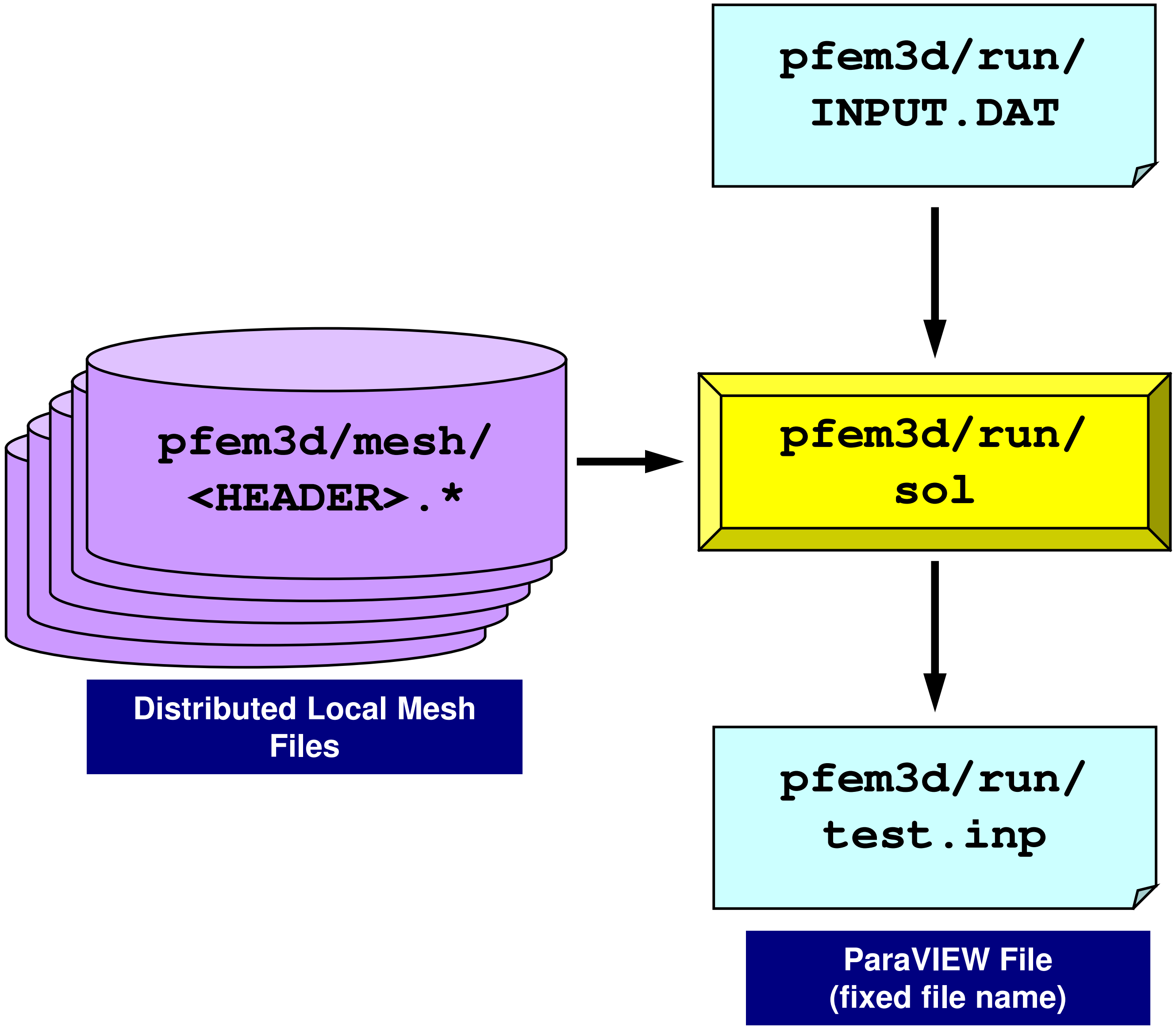
Finite-Element Procedures

- 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

Procedures for Parallel FEM



Control File: INPUT.DAT

```
INPUT.DAT

../mesh/aaa  HEADER
2000         ITER
1.0 1.0      COND, QVOL
1.0e-08      RESID
```

- HEADER : HEADER of distributed mesh files “HEADER”.my_rank
- ITER : Max. Iterations for CG
- COND : Thermal Conductivity
- QVOL : Heat Generation Rate
- RESID : Criteria for Convergence of CG

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

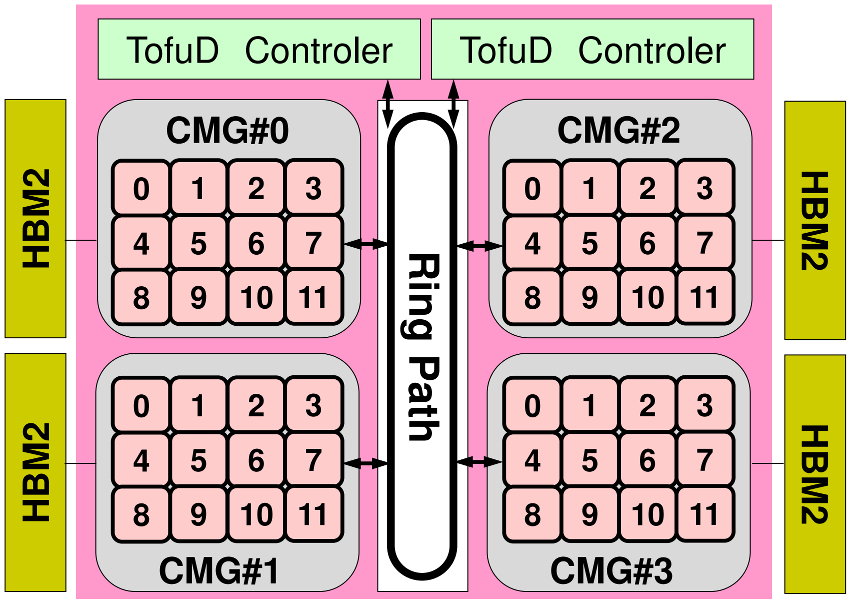
$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

pFEM/pfem3d/run/a08.sh

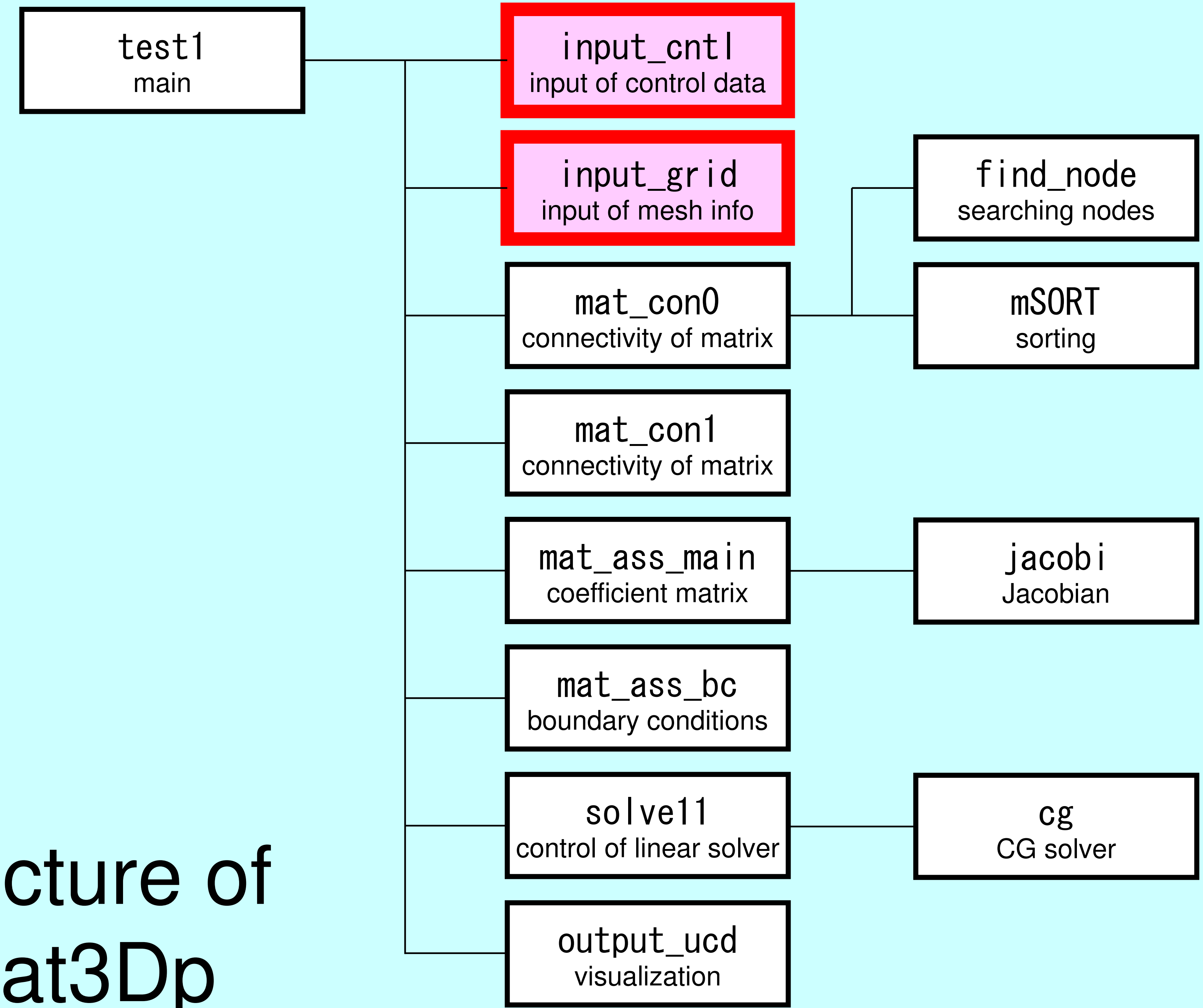
```
#!/bin/sh
#PJM -N "flat-08"                      Job Name
#PJM -L rscgrp=lecture8-o              Name of "Queue/Resource Group"
#PJM -L node=8                         Node #
#PJM -mpi proc=384                     Total MPI # (384/8= 48 per node)
#PJM -L elapse=00:15:00                Computation Time
#PJM -g gt18                           Group Name (Wallet)
#PJM -j
#PJM -e err                            Standard Error
#PJM -o a08.lst              Standard Output

module load fj
module load fjmpi

mpiexec ./sol
mpiexec numactl -l ./sol
```

Number of Processes

```
#PJM -L node=1;#PJM --mpi proc= 1    1-node, 1-proc, 1-proc/n
#PJM -L node=1;#PJM --mpi proc= 4    1-node, 4-proc, 4-proc/n
#PJM -L node=1;#PJM --mpi proc=12    1-node,12-proc,12-proc/n
#PJM -L node=1;#PJM --mpi proc=24    1-node,24-proc,24-proc/n
#PJM -L node=1;#PJM --mpi proc=48    1-node,48-proc,48-proc/n

#PJM -L node= 4;#PJM --mpi proc=192   4-node,192-proc,48-proc/n
#PJM -L node= 8;#PJM --mpi proc=384   8-node,384-proc,48-proc/n
#PJM -L node=12;#PJM --mpi proc=576  12-node,576-proc,48-proc/n
```



Structure of heat3Dp



Main Part

```
program heat3Dp

use solver11
use pfem_util

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

call PFEM_INIT

call INPUT_CNTL
call INPUT_GRID

call MAT_CON0
call MAT_CON1

call MAT_ASS_MAIN
call MAT_ASS_BC

call SOLVE11

call OUTPUT_UCD

call PFEM_FINALIZE

end program heat3Dp
```

Global Variables: pfem_util.f (1/4)

Name	Type	Size	I/O	Definition
fname	C	(80)	I	Name of mesh file
N,NP	I		I	# Node (N: Internal, NP: Internal + External)
ICELTOT	I		I	# Element
NODGRPtot	I		I	# Node Group
XYZ	R	(NP,3)	I	Node Coordinates
ICELNOD	I	(ICELTOT,8)	I	Element Connectivity
NODGRP_INDEX	I	(0:NODGRPtot)	I	# Node in each Node Group
NODGRP_ITEM	I	(NODGRP_INDEX(NODGRPTOT))	I	Node ID in each Node Group
NODGRP_NAME	C80	(NODGRP_INDEX(NODGRPTOT))	I	Name of NodeGroup
NLU	I		O	# Non-Zero Off-Diagonals at each node
NPLU	I		O	# Non-Zero Off-Diagonals
D	R	(NP)	O	Diagonal Block of Global Matrix
B,X	R	(NP)	O	RHS, Unknown Vector

Global Variables: pfem_util.f (2/4)

Name	Type	Size	I/O	Definition
AMAT	R	(NPLU)	O	Non-Zero Off-Diagonal Components of Global Matrix
index	I	(0:NP)	O	# Non-Zero Off-Diagonal Components
item	I	(NPLU)	O	Column ID of Non-Zero Off-Diagonal Components
INLU	I	(NP)	O	Number of Non-Zero Off-Diagonal Components at Each Node
IALU	I	(NP,NLU)	O	Column ID of Non-Zero Off-Diagonal Components at Each Node
IWKX	I	(NP,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.f (3/4)

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

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

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

Global Variables: pfem_util.f (4/4)

Name	Type	Size	I/O	Definition
PETOT	I		O	Number of PE's
my_rank	I		O	Process ID of MPI
errno	I		O	Error Flag
NEIBPETOT	I		I	Number of Neighbors
NEIBPE	I	(NEIBPETOT)	I	ID of Neighbor
IMPORT_INDEX **EXPORT_INEDX**	I	(0:NEIBPETOT)	I	Size of Import/Export Arrays for Communication Table
IMPORT_ITEM	I	(Npimport)	I	Receiving Table (External Points) NPimport=IMPORT_INDEX(NEIBPETOT))
EXPORT_ITEM	I	(Npexport)	I	Sending Table (Boundary Points) NPexport=EXPORT_INDEX(NEIBPETOT))
ICELTOT_INT	**I**		**I**	**Number of Local Elements**
intELEM_list	**I**	**(ICELTOT_INT)**	**I**	**List of Local Elements**

Start/End: MPI_Init/Finalize

```
subroutine PFEM_INIT
use pfem_util
implicit REAL*8 (A-H,O-Z)

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

pfemRarray= 0.d0
pfemIarray= 0

return
end
```

```
subroutine PFEM_FINALIZE
use pfem_util
implicit REAL*8 (A-H,O-Z)

call MPI_FINALIZE (errno)
if (my_rank.eq.0) stop ' * normal termination'

return
end
```

Reading Control File: INPUT_CNTL

```
      subroutine INPUT_CNTL
      use pfem_util

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

      if (my_rank.eq.0) then
        open (11,file= 'INPUT.DAT', status='unknown')
        read (11,'(a80)') HEADER
        read (11,*) ITER
        read (11,*) COND, QVOL
        read (11,*) RESID
        close (11)
      endif

      call MPI_BCAST (HEADER, 80, MPI_CHARACTER, 0, MPI_COMM_WORLD,ierr)
      call MPI_BCAST (ITER   , 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr)
      call MPI_BCAST (COND   , 1, MPI_DOUBLE_PRECISION, 0,
     &                                  MPI_COMM_WORLD, ierr)
      call MPI_BCAST (QVOL   , 1, MPI_DOUBLE_PRECISION, 0,
     &                                  MPI_COMM_WORLD, ierr)
      call MPI_BCAST (RESID  , 1, MPI_DOUBLE_PRECISION, 0,
     &                                  MPI_COMM_WORLD, ierr)

      pfemRarray(1)= RESID
      pfemIarray(1)= ITER

      return
      end
```

Reading Meshes: INPUT_GRID (1/3)

```
      subroutine INPUT_GRID
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      call define_file_name (HEADER, fname, my_rank)
      open (11, file= fname, status= 'unknown', form= 'formatted')

!C
!C-- NEIB-PE
      read (11,'(10i10)') kkk
      read (11,'(10i10)') NEIBPETOT
      allocate (NEIBPE(NEIBPETOT))

      read (11,'(10i10)') (NEIBPE(i), i= 1, NEIBPETOT)

      do i= 1, NEIBPETOT
        if (NEIBPE(i).gt.PETOT-1) then
          call ERROR_EXIT (202, my_rank)
        endif
      enddo
```

Name of Distributed Local Mesh File: DEFINE_FILE_NAME HEADER + Rank ID

```
subroutine DEFINE_FILE_NAME (HEADERo, filename, my_rank)

character (len=80) ::  HEADERo, filename
character (len=80) ::  HEADER
character (len= 1) ::  SUBindex1
character (len= 2) ::  SUBindex2
character (len= 3) ::  SUBindex3
integer:: LENGTH, ID

HEADER= adjustL (HEADERo)
LENGTH= len_trim(HEADER)

if (my_rank.le.9) then
  ID= 1
  write(SUBindex1 ,'(i1.1)') my_rank
 else if (my_rank.le.99) then
  ID= 2
  write(SUBindex2 ,'(i2.2)') my_rank
 else if (my_rank.le.999) then
  ID= 3
  write(SUBindex3 ,'(i3.3)') my_rank
endif

if (ID.eq.1) filename= HEADER(1:LENGTH)//'.'//SUBindex1
if (ID.eq.2) filename= HEADER(1:LENGTH)//'.'//SUBindex2
if (ID.eq.3) filename= HEADER(1:LENGTH)//'.'//SUBindex3

end subroutine define_file_name
```

allocate, deallocate for C

```
#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 );
}

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 );
}
```

Same interface with FORTRAN

Reading Meshes: INPUT_GRID (2/3)

```
!C
!C-- NODE
      read (11,'(10i10)')  NP, N
      allocate (XYZ(NP,3), NODE_ID(NP,2))
      XYZ= 0.d0
        do i= 1, NP
          read (11,*) NODE_ID(i,1), NODE_ID(i,2), (XYZ(i,kk),kk=1,3)
        enddo

!C
!C-- ELEMENT
      read (11,*)  ICELTOT, ICELTOT_INT

      allocate (ICELNOD(ICELTOT,8), intELEM_list(ICELTOT))
      allocate (ELEM_ID(ICELTOT,2))
      read (11,'(10i10)') (NTYPE, i= 1, ICELTOT)
      do icel= 1, ICELTOT
        read (11,'(i10,2i5,8i10)') (ELEM_ID(icel,jj),jj=1,2),           &
     &                       IMAT, (ICELNOD(icel,k), k= 1, 8)
      enddo

      read (11,'(10i10)') (intELEM_list(ic0), ic0= 1, ICELTOT_INT)
```

Reading Meshes: INPUT_GRID (3/3)

```
!C-- COMMUNICATION table
      allocate (IMPORT_INDEX(0:NEIBPETOT))
      allocate (EXPORT_INDEX(0:NEIBPETOT))

      IMPORT_INDEX= 0
      EXPORT_INDEX= 0

      if (PETOT.ne.1) then
      read (11,'(10i10)') (IMPORT_INDEX(i), i= 1, NEIBPETOT)
      nn= IMPORT_INDEX(NEIBPETOT)
      allocate (IMPORT_ITEM(nn))
      do i= 1, nn
        read (11,*) IMPORT_ITEM(i)
      enddo

      read (11,'(10i10)') (EXPORT_INDEX(i), i= 1, NEIBPETOT)
      nn= EXPORT_INDEX(NEIBPETOT)
      allocate (EXPORT_ITEM(nn))
      do i= 1, nn
        read (11,*) EXPORT_ITEM(i)
      enddo
      endif
!C-- NODE grp. info.
      read (11,'(10i10)') NODGRPtot
      allocate (NODGRP_INDEX(0:NODGRPtot),NODGRP_NAME(NODGRPtot))
      NODGRP_INDEX= 0

      read (11,'(10i10)') (NODGRP_INDEX(i), i= 1, NODGRPtot)
      nn= NODGRP_INDEX(NODGRPtot)
      allocate (NODGRP_ITEM(nn))

      do k= 1, NODGRPtot
        iS= NODGRP_INDEX(k-1) + 1
        iE= NODGRP_INDEX(k  )
        read (11,'(a80)') NODGRP_NAME(k)
        nn= iE - iS + 1
        if (nn.ne.0) then
          read (11,'(10i10)') (NODGRP_ITEM(kk),kk=iS, iE)
        endif
      enddo
```

Parallel 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 heat3Dp

NOT so different from 1-CPU code

- test1 — main
  - input_cntl — input of control data
  - input_grid — input of mesh info
  - mat_con0 — connectivity of matrix
    - find_node — searching nodes
    - mSORT — sorting
  - mat_con1 — connectivity of matrix
  - mat_ass_main — coefficient matrix
    - jacobi — Jacobian
  - mat_ass_bc — boundary conditions
  - solve11 — control of linear solver
    - cg — CG solver
  - output_ucd — visualization

Main Part

```
program heat3Dp

use solver11
use pfem_util

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

call PFEM_INIT
call INPUT_CNTL
call INPUT_GRID

call MAT_CON0
call MAT_CON1

call MAT_ASS_MAIN
call MAT_ASS_BC

call SOLVE11

call OUTPUT_UCD

call PFEM_FINALIZE

end program heat3Dp
```

MAT_CON0: generates INU, IALU

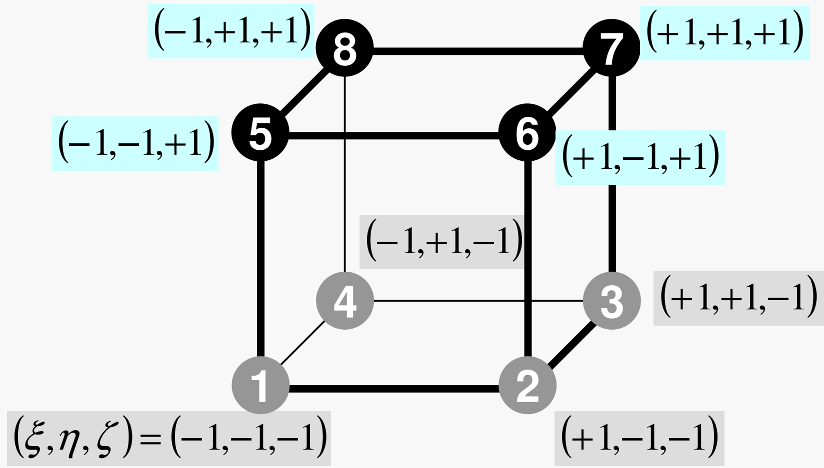
MAT_CON1: generates index, item

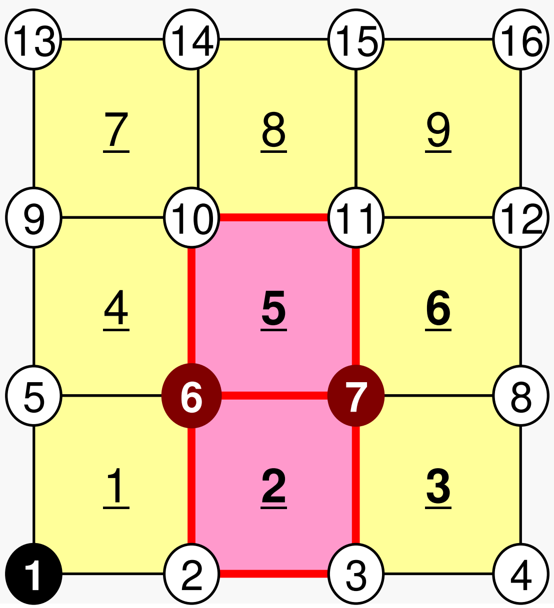
Please compare parallel/serial codes

```
$ cd /work/t87XYZ/pFEM/pfem3d/src

$ diff mat_con1.f ../../fem3d/src/mat_con0.f
$ diff mat_con0.f ../../fem3d/src/mat_con1.f
$ diff mat_ass_main.f ../../fem3d/src/mat_ass_main.f
$ diff mat_ass_bc.f ../../fem3d/src/mat_ass_bc.f
```

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)

```
!C
!C***
!C*** MAT_CON0
!C***
!C
      subroutine MAT_CON0
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      NLU= 26

      allocate (INLU(NP), IALU(NP,NLU))

      INLU= 0
      IALU= 0
```

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

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

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

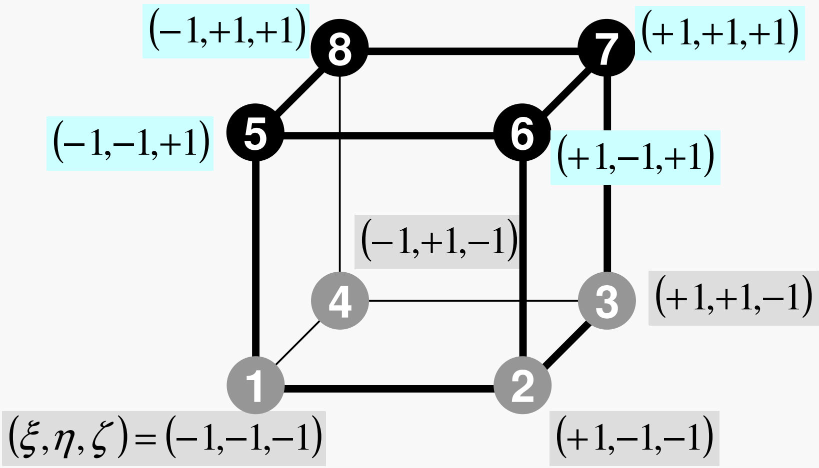
Generating Connectivity of Matrix MAT_CON0 (1/4)

```
!C
!C***
!C*** MAT_CON0
!C***
!C
      subroutine MAT_CON0
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      NLU= 26

      allocate (INLU(NP), IALU(NP,NLU))

      INLU= 0
      IALU= 0
```

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

Generating Connectivity of Matrix MAT_CON0 (2/4)

```
do icel= 1, ICELTOT
  in1= ICELNOD(icel,1)
  in2= ICELNOD(icel,2)
  in3= ICELNOD(icel,3)
  in4= ICELNOD(icel,4)
  in5= ICELNOD(icel,5)
  in6= ICELNOD(icel,6)
  in7= ICELNOD(icel,7)
  in8= ICELNOD(icel,8)

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

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

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



FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search

```
!C
!C***
!C*** FIND_TS_NODE
!C***
!C
      subroutine FIND_TS_NODE (ip1,ip2)

        do kk= 1, INLU(ip1)
          if (ip2.eq.IALU(ip1,kk)) return
        enddo

        icou= INLU(ip1) + 1
        IALU(ip1,icou)= ip2
        INLU(ip1     )= icou

        return

      end subroutine FIND_TS_NODE
```

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

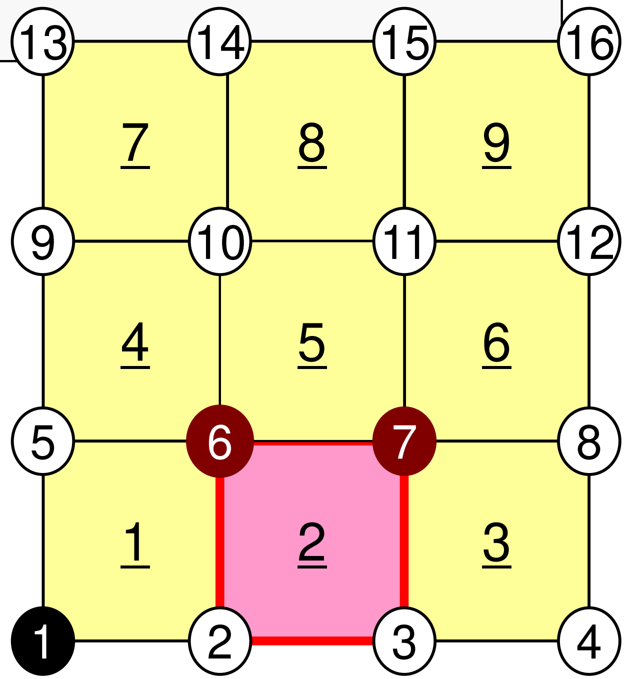
FIND_TS_NODE: Search Connectivity

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

```
!C
!C***
!C*** FIND_TS_NODE
!C***
!C
      subroutine FIND_TS_NODE (ip1,ip2)

        do kk= 1, INLU(ip1)
          if (ip2.eq.IALU(ip1,kk)) return
        enddo

        icou= INLU(ip1) + 1
        IALU(ip1,icou)= ip2
        INLU(ip1     )= icou

        return

      end subroutine FIND_TS_NODE
```

Checking whether ip2 is included in IALU(ip1,kk), or not

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

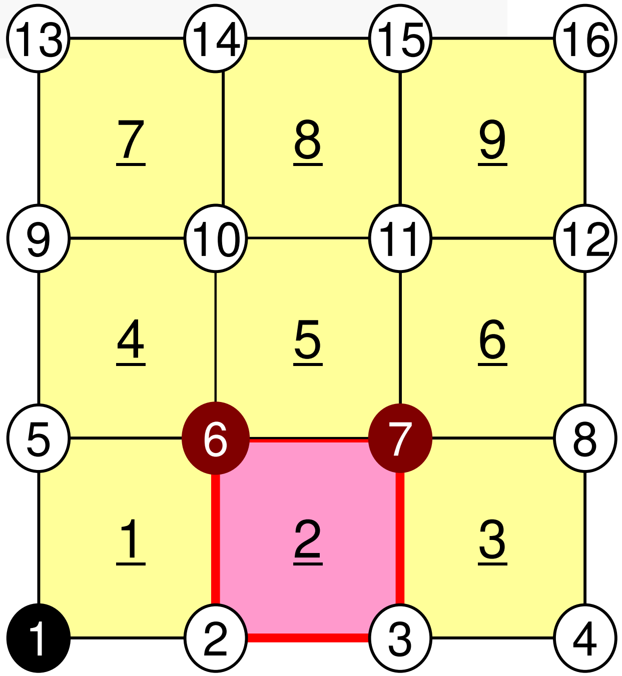


FIND_TS_NODE: Search Connectivity

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

```
!C
!C***
!C*** FIND_TS_NODE
!C***
!C
      subroutine FIND_TS_NODE (ip1,ip2)

        do kk= 1, INLU(ip1)
          if (ip2.eq.IALU(ip1,kk)) return
        enddo

        icou= INLU(ip1) + 1
        IALU(ip1,icou)= ip2
        INLU(ip1     )= icou

        return

      end subroutine FIND_TS_NODE
```

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



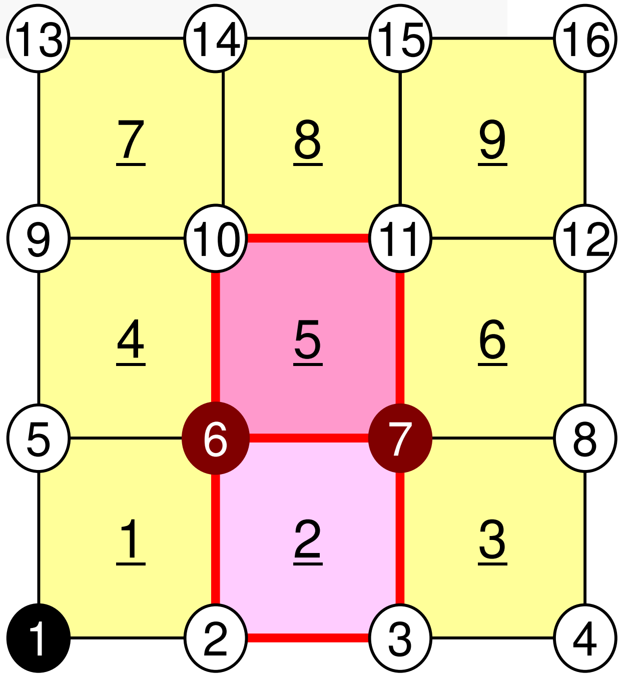
ip1: No.6 node
ip2: No.7 node

FIND_TS_NODE: Search Connectivity

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

```
!C
!C***
!C*** FIND_TS_NODE
!C***
!C
      subroutine FIND_TS_NODE (ip1, ip2)

        do kk= 1, INLU(ip1)
          if (ip2.eq. IALU(ip1,kk)) return
        enddo

        icou= INLU(ip1) + 1
        IALU(ip1,icou)= ip2
        INLU(ip1    )= icou

        return

      end subroutine FIND_TS_NODE
```

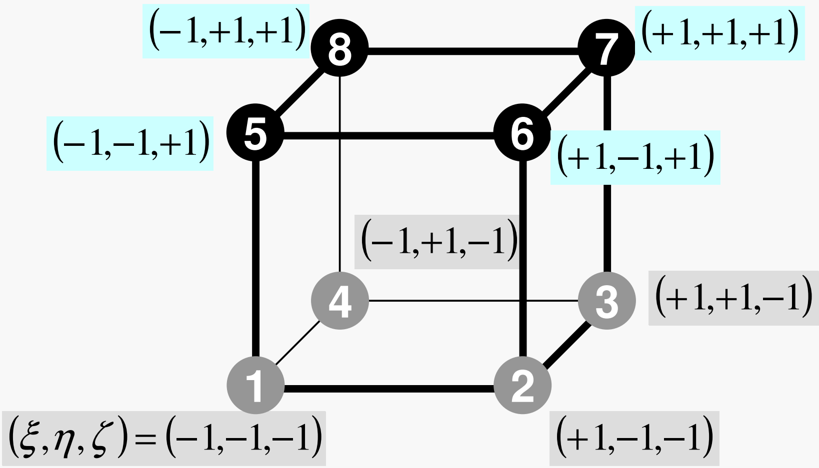
If the target node is already included in IALU, proceed to next pair of nodes



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

Generating Connectivity of Matrix MAT_CON0 (3/4)

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

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

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

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



Generating Connectivity of Matrix MAT_CON0 (4/4)

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

  do in= 1, N
    NN= INLU(in)
    do k= 1, NN
      NCOL1(k)= IALU(in,k)
    enddo
    call mSORT (NCOL1, NCOL2, NN)
    do k= NN, 1, -1
      IALU(in,NN-k+1)= NCOL1(NCOL2(k))
    enddo
  enddo
```

Sort IALU(i,k) in ascending order by “bubble” sorting for less than 100 components.

MAT_CON1: CRS format

```
!C
!C***
!C*** MAT_CON1
!C***
!C
      subroutine MAT_CON1
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      allocate (index(0:NP))
      index= 0

      do i= 1, NP
        index(i)= index(i-1) + INLU(i)
      enddo

      NPLU= index(NP)

      allocate (item(NPLU))

      do i= 1, NP
        do k= 1, INLU(i)
               kk = k + index(i-1)
          item(kk)=      IALU(i,k)
        enddo
      enddo

      deallocate (INLU, IALU)

      end subroutine MAT_CON1
```

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

```
!C
!C***
!C*** MAT_CON1
!C***
!C
      subroutine MAT_CON1
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      allocate (index(0:NP))
      index= 0

      do i= 1, NP
        index(i)= index(i-1) + INLU(i)
      enddo

      NPLU= index(NP)

      allocate (item(NPLU))

      do i= 1, NP
        do k= 1, INLU(i)
                kk = k + index(i-1)
          item(kk)=       IALU(i,k)
        enddo
      enddo

      deallocate (INLU, IALU)

      end subroutine MAT_CON1
```

NPLU=indexLU(NP)
Size of array: itemLU
Total number of non-zero off-diagonal blocks

MAT_CON1: CRS format

```
!C
!C***
!C*** MAT_CON1
!C***
!C
      subroutine MAT_CON1
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      allocate (index(0:NP))
      index= 0

      do i= 1, NP
        index(i)= index(i-1) + INLU(i)
      enddo

      NPLU= index(NP)

      allocate (item(NPLU))

      do i= 1, NP
        do k= 1, INLU(i)
                kk = k + index(i-1)
          item(kk)=      IALU(i,k)
        enddo
      enddo

      deallocate (INLU, IALU)

      end subroutine MAT_CON1
```

itemLU
store node ID starting from 1

MAT_CON1: CRS format

```
!C
!C***
!C*** MAT_CON1
!C***
!C
      subroutine MAT_CON1
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      allocate (index(0:NP))
      index= 0

      do i= 1, NP
        index(i)= index(i-1) + INLU(i)
      enddo

      NPLU= index(NP)

      allocate (item(NPLU))

      do i= 1, NP
        do k= 1, INLU(i)
                kk = k + index(i-1)
          item(kk)=      IALU(i,k)
        enddo
      enddo

      deallocate (INLU, IALU)

      end subroutine MAT_CON1
```

Not required any more

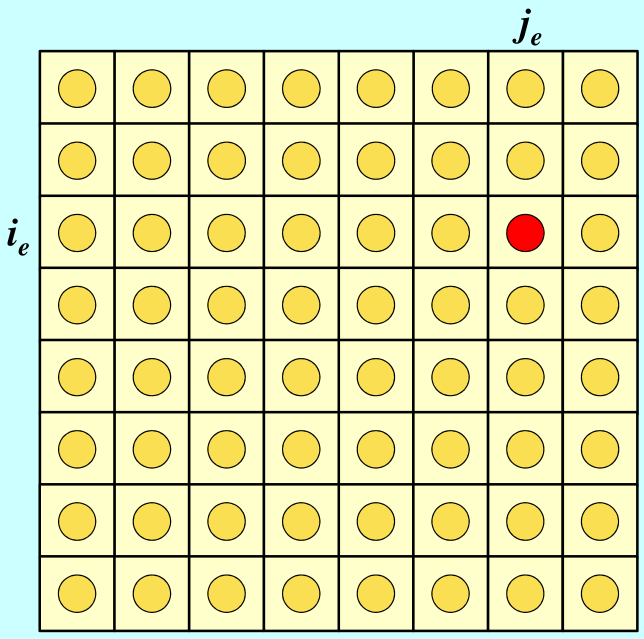
Main Part

```
program heat3Dp

use solver11
use pfem_util

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

call PFEM_INIT
call INPUT_CNTL
call INPUT_GRID

call MAT_CON0
call MAT_CON1

call MAT_ASS_MAIN
call MAT_ASS_BC

call SOLVE11

call OUTPUT_UCD

call PFEM_FINALIZE

end program heat3Dp
```

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 "item" : 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)

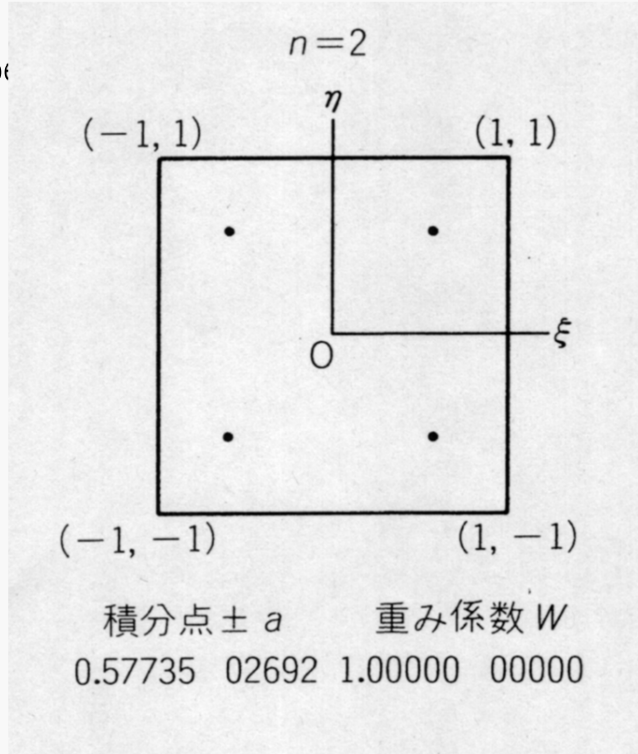
```
!C
!C***
!C*** MAT_ASS_MAIN
!C***
!C
      subroutine MAT_ASS_MAIN
      use pfem_util
      implicit REAL*8 (A-H,O-Z)
      integer(kind=kint), dimension(  8) :: nodLOCAL

      allocate (AMAT(NPLU))
      allocate (B(NP), D(NP), X(NP))

      AMAT= 0.d0                         Non-Zero Off-Diagonal components (coef. matrix)
         B= 0.d0                         RHS vector
         X= 0.d0                         Unknowns
         D= 0.d0                         Diagonal components (coef. matrix)

      WEI(1)= +1.0000000000D+00
      WEI(2)= +1.0000000000D+00

      POS(1)= -0.5773502692D+00
      POS(2)= +0.5773502692D+00
```

MAT_ASS_MAIN (1/6)

```
!C
!C***
!C*** MAT_ASS_MAIN
!C***
!C
      subroutine MAT_ASS_MAIN
      use pfem_util
      implicit REAL*8 (A-H,O-Z)
      integer(kind=kint), dimension(  8) :: nodLOCAL

      allocate (AMAT(NPLU))
      allocate (B(NP), D(NP), X(NP))

      AMAT= 0.d0                    Non-Zero Off-Diagonal components (coef. matrix)
         B= 0.d0                    RHS vector
         X= 0.d0                    Unknowns
         D= 0.d0                    Diagonal components (coe

      WEI(1)= +1.0000000000D+00
      WEI(2)= +1.0000000000D+00

      POS(1)= -0.5773502692D+00
      POS(2)= +0.5773502692D+00
```

POS : Quad. Point

WEI : Weighting Factor



MAT_ASS_MAIN (2/6)

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

      do kp= 1, 2
      do jp= 1, 2
      do ip= 1, 2

        QP1= 1.d0 + POS(ip)
        QM1= 1.d0 - POS(ip)
        EP1= 1.d0 + POS(jp)
        EM1= 1.d0 - POS(jp)
        TP1= 1.d0 + POS(kp)
        TM1= 1.d0 - POS(kp)

        SHAPE(ip,jp,kp,1)= O8th * QM1 * EM1 * TM1
        SHAPE(ip,jp,kp,2)= O8th * QP1 * EM1 * TM1
        SHAPE(ip,jp,kp,3)= O8th * QP1 * EP1 * TM1
        SHAPE(ip,jp,kp,4)= O8th * QM1 * EP1 * TM1
        SHAPE(ip,jp,kp,5)= O8th * QM1 * EM1 * TP1
        SHAPE(ip,jp,kp,6)= O8th * QP1 * EM1 * TP1
        SHAPE(ip,jp,kp,7)= O8th * QP1 * EP1 * TP1
        SHAPE(ip,jp,kp,8)= O8th * QP1 * EP1 * TP1
```

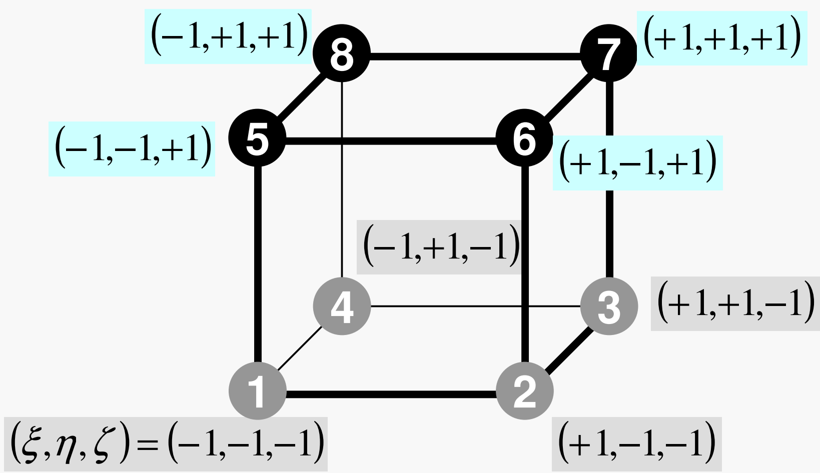
MAT_ASS_MAIN (2/6)

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

      do kp= 1, 2
      do jp= 1, 2
      do ip= 1, 2

        QP1= 1.d0 + POS(ip)
        QM1= 1.d0 - POS(ip)
        EP1= 1.d0 + POS(jp)
        EM1= 1.d0 - POS(jp)
        TP1= 1.d0 + POS(kp)
        TM1= 1.d0 - POS(kp)

        SHAPE(ip,jp,kp,1)= O8th * QM1 * EM1 * TM1
        SHAPE(ip,jp,kp,2)= O8th * QP1 * EM1 * TM1
        SHAPE(ip,jp,kp,3)= O8th * QP1 * EP1 * TM1
        SHAPE(ip,jp,kp,4)= O8th * QM1 * EP1 * TM1
        SHAPE(ip,jp,kp,5)= O8th * QM1 * EM1 * TP1
        SHAPE(ip,jp,kp,6)= O8th * QP1 * EM1 * TP1
        SHAPE(ip,jp,kp,7)= O8th * QP1 * EP1 * TP1
        SHAPE(ip,jp,kp,8)= O8th * QM1 * EP1 * TP1
```

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

MAT_ASS_MAIN (2/6)

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

      do kp= 1, 2
      do jp= 1, 2
      do ip= 1, 2

        QP1= 1.d0 + POS(ip)
        QM1= 1.d0 - POS(ip)
        EP1= 1.d0 + POS(jp)
        EM1= 1.d0 - POS(jp)
        TP1= 1.d0 + POS(kp)
        TM1= 1.d0 - POS(kp)

        SHAPE(ip,jp,kp,1)= O8th * QM1 * EM1 * TM1
        SHAPE(ip,jp,kp,2)= O8th * QP1 * EM1 * TM1
        SHAPE(ip,jp,kp,3)= O8th * QP1 * EP1 * TM1
        SHAPE(ip,jp,kp,4)= O8th * QM1 * EP1 * TM1
        SHAPE(ip,jp,kp,5)= O8th * QM1 * EM1 * TP1
        SHAPE(ip,jp,kp,6)= O8th * QP1 * EM1 * TP1
        SHAPE(ip,jp,kp,7)= O8th * QP1 * EP1 * TP1
        SHAPE(ip,jp,kp,8)= O8th * QP1 * EP1 * TP1
```



MAT_ASS_MAIN (2/6)

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

      do kp= 1, 2
      do jp= 1, 2
      do ip= 1, 2

        QP1= 1.d0 + POS(ip)
        QM1= 1.d0 - POS(ip)
        EP1= 1.d0 + POS(jp)
        EM1= 1.d0 - POS(jp)
        TP1= 1.d0 + POS(kp)
        TM1= 1.d0 - POS(kp)

        SHAPE(ip,jp,kp,1)= O8th * QM1 * EM1 * TM1
        SHAPE(ip,jp,kp,2)= O8th * QP1 * EM1 * TM1
        SHAPE(ip,jp,kp,3)= O8th * QP1 * EP1 * TM1
        SHAPE(ip,jp,kp,4)= O8th * QM1 * EP1 * TM1
        SHAPE(ip,jp,kp,5)= O8th * QM1 * EM1 * TP1
        SHAPE(ip,jp,kp,6)= O8th * QP1 * EM1 * TP1
        SHAPE(ip,jp,kp,7)= O8th * QP1 * EP1 * TP1
        SHAPE(ip,jp,kp,8)= O8th * QP1 * 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,1)= - O8th * EM1 * TM1
    PNQ(jp,kp,2)= + O8th * EM1 * TM1
    PNQ(jp,kp,3)= + O8th * EP1 * TM1
    PNQ(jp,kp,4)= - O8th * EP1 * TM1
    PNQ(jp,kp,5)= - O8th * EM1 * TP1
    PNQ(jp,kp,6)= + O8th * EM1 * TP1
    PNQ(jp,kp,7)= + O8th * EP1 * TP1
    PNQ(jp,kp,8)= - O8th * EP1 * TP1
    PNE(ip,kp,1)= - O8th * QM1 * TM1
    PNE(ip,kp,2)= - O8th * QP1 * TM1
    PNE(ip,kp,3)= + O8th * QP1 * TM1
    PNE(ip,kp,4)= + O8th * QM1 * TM1
    PNE(ip,kp,5)= - O8th * QM1 * TP1
    PNE(ip,kp,6)= - O8th * QP1 * TP1
    PNE(ip,kp,7)= + O8th * QP1 * TP1
    PNE(ip,kp,8)= + O8th * QM1 * TP1
    PNT(ip,jp,1)= - O8th * QM1 * EM1
    PNT(ip,jp,2)= - O8th * QP1 * EM1
    PNT(ip,jp,3)= - O8th * QP1 * EP1
    PNT(ip,jp,4)= - O8th * QM1 * EP1
    PNT(ip,jp,5)= + O8th * QM1 * EM1
    PNT(ip,jp,6)= + O8th * QP1 * EM1
    PNT(ip,jp,7)= + O8th * QP1 * EP1
    PNT(ip,jp,8)= + O8th * QM1 * EP1
  enddo
  enddo
  enddo

  do icel= 1, ICELTOT
    COND0= COND

    in1= ICELNOD(icel,1)
    in2= ICELNOD(icel,2)
    in3= ICELNOD(icel,3)
    in4= ICELNOD(icel,4)
    in5= ICELNOD(icel,5)
    in6= ICELNOD(icel,6)
    in7= ICELNOD(icel,7)
    in8= ICELNOD(icel,8)
```

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

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

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

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

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

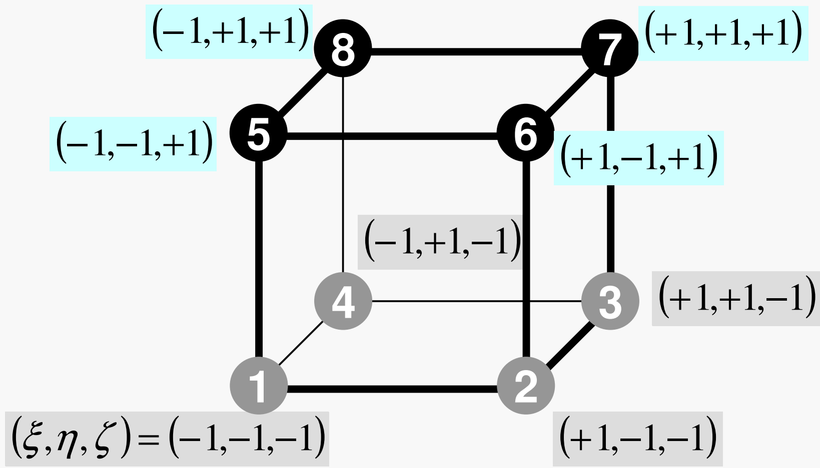
$$\frac{\partial N_3}{\partial \xi}(\xi_i,\eta_j,\zeta_k)=+\frac{1}{8}(1+\eta_j)(1-\zeta_k)$$

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

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

MAT_ASS_MAIN (3/6)

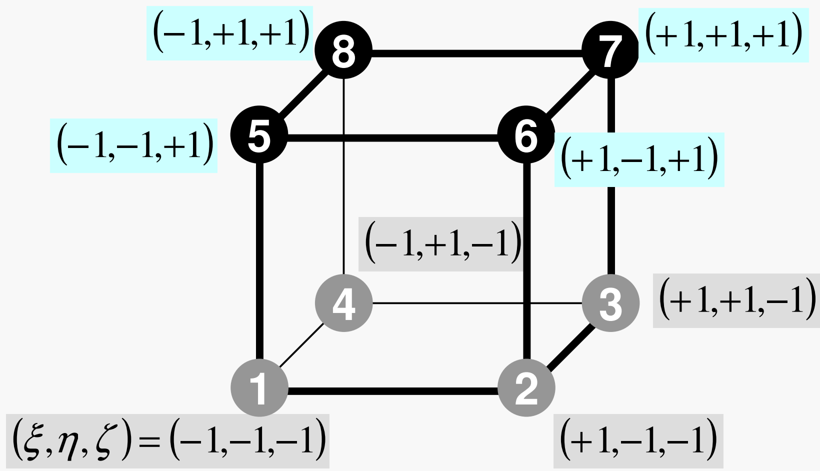
```
    PNQ(jp,kp,1)= - O8th * EM1 * TM1
    PNQ(jp,kp,2)= + O8th * EM1 * TM1
    PNQ(jp,kp,3)= + O8th * EP1 * TM1
    PNQ(jp,kp,4)= - O8th * EP1 * TM1
    PNQ(jp,kp,5)= - O8th * EM1 * TP1
    PNQ(jp,kp,6)= + O8th * EM1 * TP1
    PNQ(jp,kp,7)= + O8th * EP1 * TP1
    PNQ(jp,kp,8)= - O8th * EP1 * TP1
    PNE(ip,kp,1)= - O8th * QM1 * TM1
    PNE(ip,kp,2)= - O8th * QP1 * TM1
    PNE(ip,kp,3)= + O8th * QP1 * TM1
    PNE(ip,kp,4)= + O8th * QM1 * TM1
    PNE(ip,kp,5)= - O8th * QM1 * TP1
    PNE(ip,kp,6)= - O8th * QP1 * TP1
    PNE(ip,kp,7)= + O8th * QP1 * TP1
    PNE(ip,kp,8)= + O8th * QM1 * TP1
    PNT(ip,jp,1)= - O8th * QM1 * EM1
    PNT(ip,jp,2)= - O8th * QP1 * EM1
    PNT(ip,jp,3)= - O8th * QP1 * EP1
    PNT(ip,jp,4)= - O8th * QM1 * EP1
    PNT(ip,jp,5)= + O8th * QM1 * EM1
    PNT(ip,jp,6)= + O8th * QP1 * EM1
    PNT(ip,jp,7)= + O8th * QP1 * EP1
    PNT(ip,jp,8)= + O8th * QM1 * EP1
  enddo
  enddo
  enddo

  do icel= 1, ICELTOT
    CONDO= COND

    in1= ICELNOD(icel,1)
    in2= ICELNOD(icel,2)
    in3= ICELNOD(icel,3)
    in4= ICELNOD(icel,4)
    in5= ICELNOD(icel,5)
    in6= ICELNOD(icel,6)
    in7= ICELNOD(icel,7)
    in8= ICELNOD(icel,8)
```



MAT_ASS_MAIN (4/6))

```
      nodLOCAL(1)= in1
      nodLOCAL(2)= in2
      nodLOCAL(3)= in3
      nodLOCAL(4)= in4
      nodLOCAL(5)= in5
      nodLOCAL(6)= in6
      nodLOCAL(7)= in7
      nodLOCAL(8)= in8

      X1= XYZ(in1,1)
      X2= XYZ(in2,1)
      X3= XYZ(in3,1)
      X4= XYZ(in4,1)
      X5= XYZ(in5,1)
      X6= XYZ(in6,1)
      X7= XYZ(in7,1)
      X8= XYZ(in8,1)
      Y1= XYZ(in1,2)
      Y2= XYZ(in2,2)
      Y3= XYZ(in3,2)
      Y4= XYZ(in4,2)
      Y5= XYZ(in5,2)
      Y6= XYZ(in6,2)
      Y7= XYZ(in7,2)
      Y8= XYZ(in8,2)
      QVC= O8th * (X1+X2+X3+X4+X5+X6+X7+X8+
   &                Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)
      Z1= XYZ(in1,3)
      Z2= XYZ(in2,3)
      Z3= XYZ(in3,3)
      Z4= XYZ(in4,3)
      Z5= XYZ(in5,3)
      Z6= XYZ(in6,3)
      Z7= XYZ(in7,3)
      Z8= XYZ(in8,3)

      call 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)



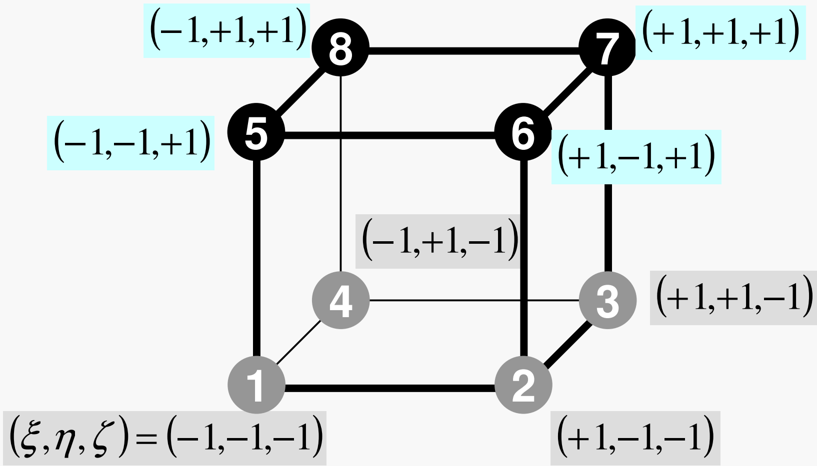
MAT_ASS_MAIN (4/6)

```
      nodLOCAL(1)= in1
      nodLOCAL(2)= in2
      nodLOCAL(3)= in3
      nodLOCAL(4)= in4
      nodLOCAL(5)= in5
      nodLOCAL(6)= in6
      nodLOCAL(7)= in7
      nodLOCAL(8)= in8

      X1= XYZ(in1,1)
      X2= XYZ(in2,1)
      X3= XYZ(in3,1)
      X4= XYZ(in4,1)
      X5= XYZ(in5,1)
      X6= XYZ(in6,1)
      X7= XYZ(in7,1)
      X8= XYZ(in8,1)
      Y1= XYZ(in1,2)
      Y2= XYZ(in2,2)
      Y3= XYZ(in3,2)
      Y4= XYZ(in4,2)
      Y5= XYZ(in5,2)
      Y6= XYZ(in6,2)
      Y7= XYZ(in7,2)
      Y8= XYZ(in8,2)
      QVC= O8th * (X1+X2+X3+X4+X5+X6+X7+X8+
     &              Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)
      Z1= XYZ(in1,3)
      Z2= XYZ(in2,3)
      Z3= XYZ(in3,3)
      Z4= XYZ(in4,3)
      Z5= XYZ(in5,3)
      Z6= XYZ(in6,3)
      Z7= XYZ(in7,3)
      Z8= XYZ(in8,3)

      call 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 )
```

X-Coordinates of 8 nodes

Y-Coordinates of 8 nodes

Z-Coordinates of 8 nodes

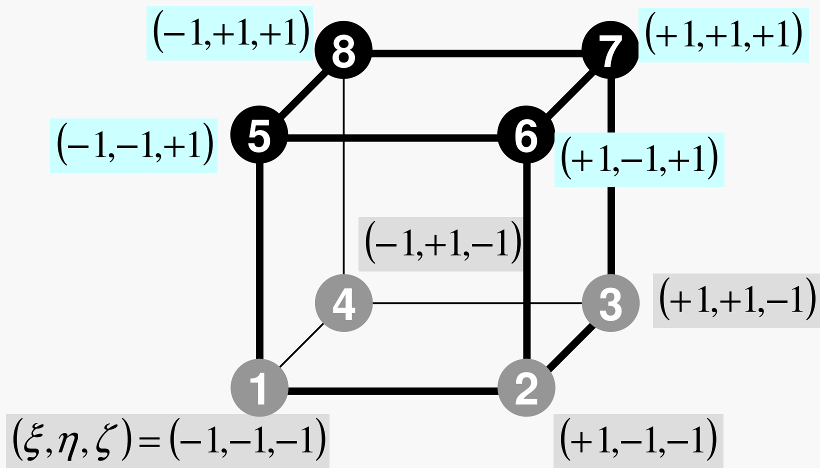


MAT_ASS_MAIN (4/6)

```
        nodLOCAL(1)= in1
        nodLOCAL(2)= in2
        nodLOCAL(3)= in3
        nodLOCAL(4)= in4
        nodLOCAL(5)= in5
        nodLOCAL(6)= in6
        nodLOCAL(7)= in7
        nodLOCAL(8)= in8

        X1= XYZ(in1,1)
        X2= XYZ(in2,1)
        X3= XYZ(in3,1)
        X4= XYZ(in4,1)
        X5= XYZ(in5,1)
        X6= XYZ(in6,1)
        X7= XYZ(in7,1)
        X8= XYZ(in8,1)
        Y1= XYZ(in1,2)
        Y2= XYZ(in2,2)
        Y3= XYZ(in3,2)
        Y4= XYZ(in4,2)
        Y5= XYZ(in5,2)
        Y6= XYZ(in6,2)
        Y7= XYZ(in7,2)
        Y8= XYZ(in8,2)
        QVC= O8th * (X1+X2+X3+X4+X5+X6+X7+X8+
     &               Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)
        Z1= XYZ(in1,3)
        Z2= XYZ(in2,3)
        Z3= XYZ(in3,3)
        Z4= XYZ(in4,3)
        Z5= XYZ(in5,3)
        Z6= XYZ(in6,3)
        Z7= XYZ(in7,3)
        Z8= XYZ(in8,3)

        call 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 )
```

X-Coordinates of 8 nodes

Y-Coordinates of 8 nodes



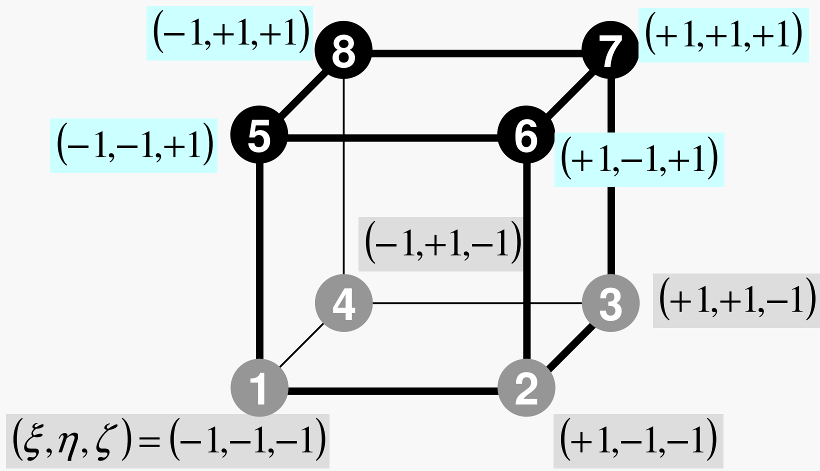
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\dot{Q}(x,y,z)=0$$

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

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

MAT_ASS_MAIN (4/6)

```
      nodLOCAL(1)= in1
      nodLOCAL(2)= in2
      nodLOCAL(3)= in3
      nodLOCAL(4)= in4
      nodLOCAL(5)= in5
      nodLOCAL(6)= in6
      nodLOCAL(7)= in7
      nodLOCAL(8)= in8

      X1= XYZ(in1,1)
      X2= XYZ(in2,1)
      X3= XYZ(in3,1)
      X4= XYZ(in4,1)
      X5= XYZ(in5,1)
      X6= XYZ(in6,1)
      X7= XYZ(in7,1)
      X8= XYZ(in8,1)
      Y1= XYZ(in1,2)
      Y2= XYZ(in2,2)
      Y3= XYZ(in3,2)
      Y4= XYZ(in4,2)
      Y5= XYZ(in5,2)
      Y6= XYZ(in6,2)
      Y7= XYZ(in7,2)
      Y8= XYZ(in8,2)
      QVC= O8th * (X1+X2+X3+X4+X5+X6+X7+X8+
    &              Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)
      Z1= XYZ(in1,3)
      Z2= XYZ(in2,3)
      Z3= XYZ(in3,3)
      Z4= XYZ(in4,3)
      Z5= XYZ(in5,3)
      Z6= XYZ(in6,3)
      Z7= XYZ(in7,3)
      Z8= XYZ(in8,3)

      call 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 )
```



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

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

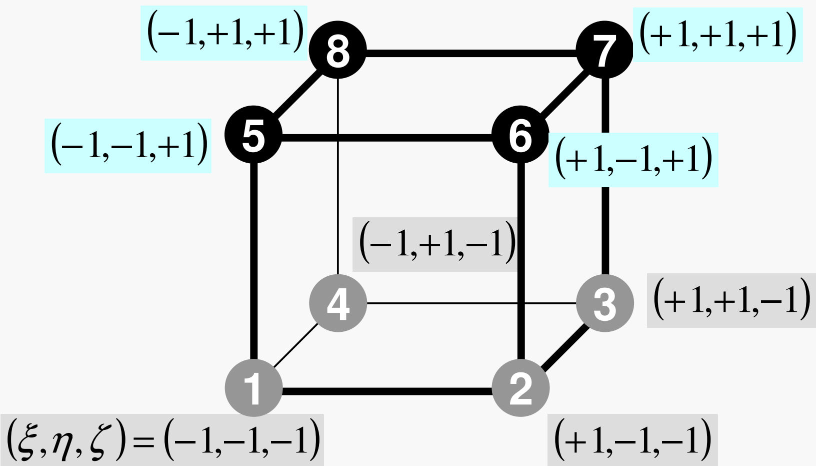
$$QVC=\left|x_C+y_C\right|$$

MAT_ASS_MAIN (4/6)

```
        nodLOCAL(1)= in1
        nodLOCAL(2)= in2
        nodLOCAL(3)= in3
        nodLOCAL(4)= in4
        nodLOCAL(5)= in5
        nodLOCAL(6)= in6
        nodLOCAL(7)= in7
        nodLOCAL(8)= in8

        X1= XYZ(in1,1)
        X2= XYZ(in2,1)
        X3= XYZ(in3,1)
        X4= XYZ(in4,1)
        X5= XYZ(in5,1)
        X6= XYZ(in6,1)
        X7= XYZ(in7,1)
        X8= XYZ(in8,1)
        Y1= XYZ(in1,2)
        Y2= XYZ(in2,2)
        Y3= XYZ(in3,2)
        Y4= XYZ(in4,2)
        Y5= XYZ(in5,2)
        Y6= XYZ(in6,2)
        Y7= XYZ(in7,2)
        Y8= XYZ(in8,2)
        QVC= O8th * (X1+X2+X3+X4+X5+X6+X7+X8+
     &               Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)
        Z1= XYZ(in1,3)
        Z2= XYZ(in2,3)
        Z3= XYZ(in3,3)
        Z4= XYZ(in4,3)
        Z5= XYZ(in5,3)
        Z6= XYZ(in6,3)
        Z7= XYZ(in7,3)
        Z8= XYZ(in8,3)

        call 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 )
```

MAT_ASS_MAIN (5/6)

```
!C
!C== CONSTRUCT the GLOBAL MATRIX

        do ie= 1, 8
          ip = nodLOCAL(ie)
        do je= 1, 8
          jp = nodLOCAL(je)

          kk= 0
          if (jp.ne.ip) then
            iiS= index(ip-1) + 1
            iiE= index(ip  )
            do k= iiS, iiE
              if ( item(k).eq.jp ) then
                kk= k
                exit
              endif
            enddo
          endif
```



Non-Zero Off-Diagonal Block in Global Matrix

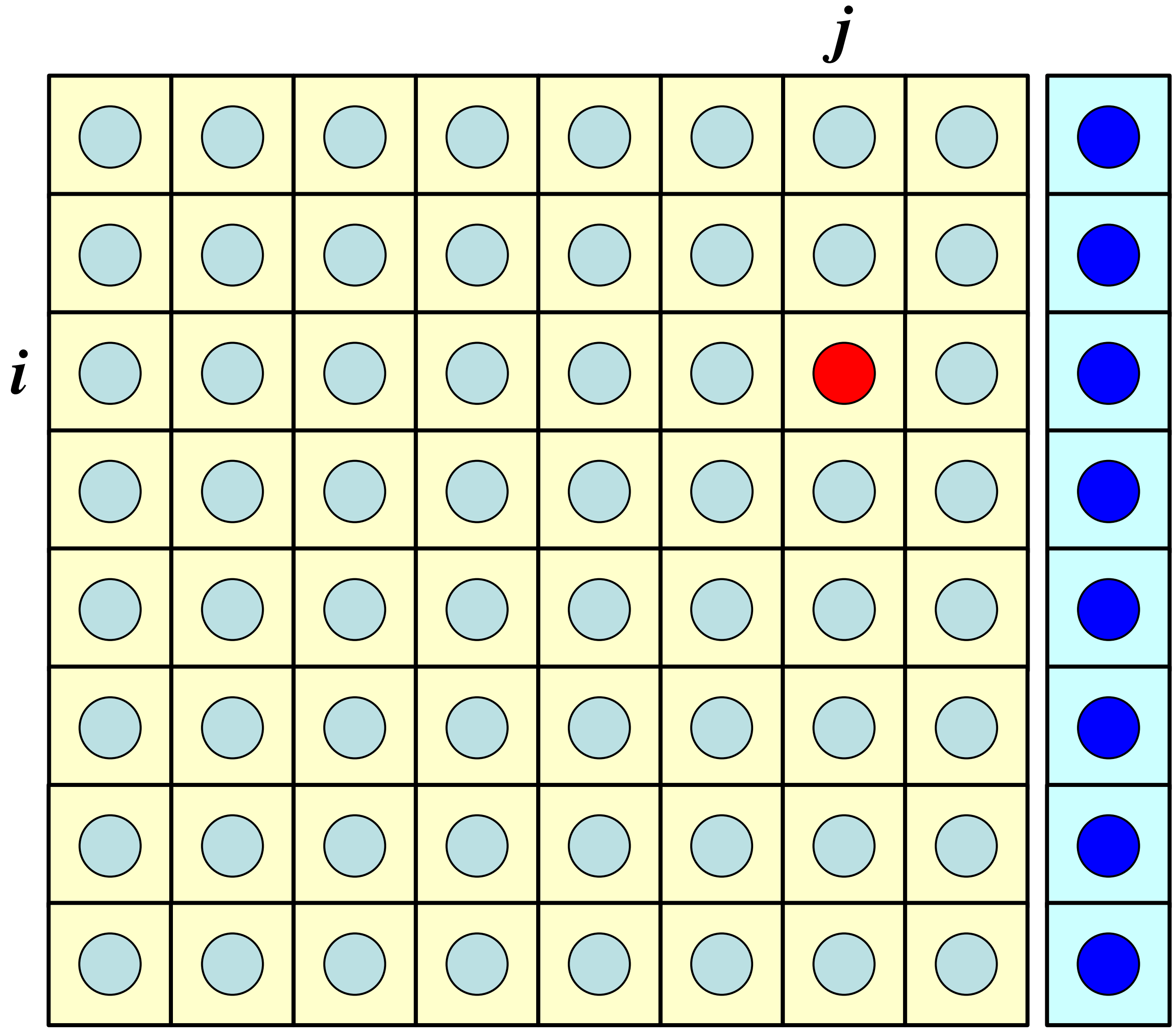
$$A_{ip,jp}$$

kk: address in "item"

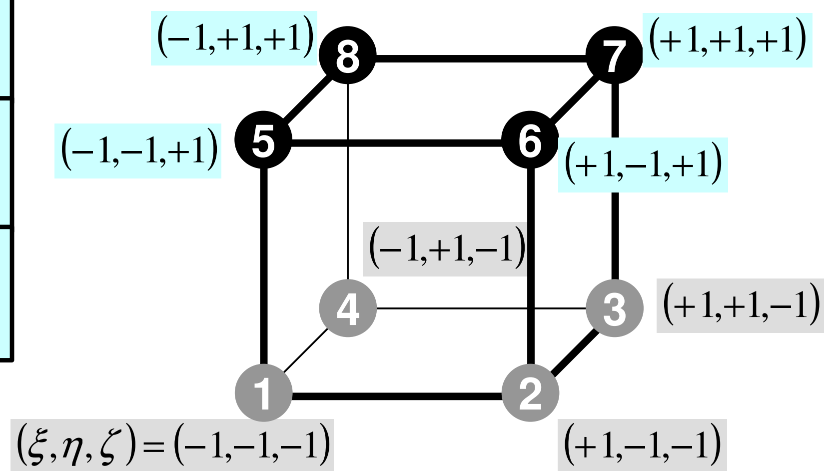
ip= nodLOCAL(ie)
jp= nodLOCAL(je)

Node ID (ip,jp) starting from 1

Element Matrix: 8x8



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



MAT_ASS_MAIN (5/6)

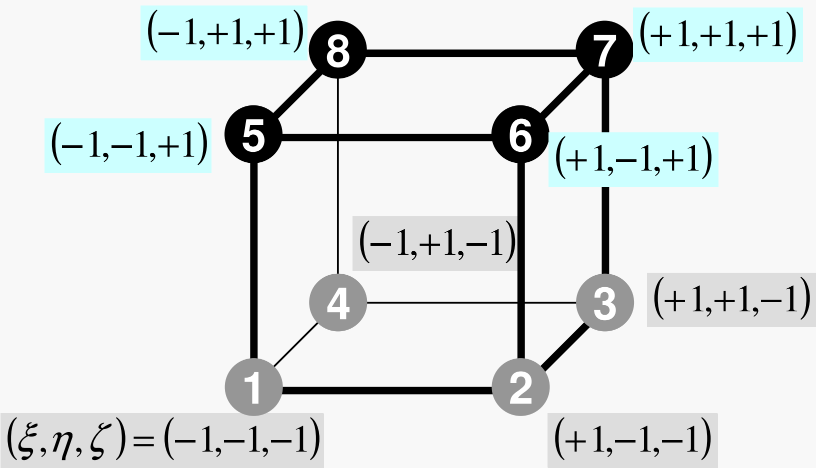
```
!C
!C== CONSTRUCT the GLOBAL MATRIX

        do ie= 1, 8
          ip = nodLOCAL(ie)
        do je= 1, 8
          jp = nodLOCAL(je)

          kk= 0
          if (jp.ne.ip) then
            iiS= index(ip-1) + 1
            iiE= index(ip  )
            do k= iiS, iiE
              if ( item(k).eq.jp ) then
                kk= k
                exit
              endif
            enddo
          endif
```

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

kk : address in "item" starting from "1"

k: starting from "1"

ip,jp: starting from "1"



MAT_ASS_MAIN (6/6)

```
      QVO   = 0.d0
      COEFij= 0.d0
      do kpn= 1, 2
      do jpn= 1, 2
      do ipn= 1, 2
        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= COEFij + coef * CONDO *
 &                      (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
 &                       DETJ(ipn,jpn,kpn)

        SHi= SHAPE(ipn,jpn,kpn,ie)
        QVO= QVO + SHi * QVOL * coef * DETJ(ipn,jpn,kpn)
      enddo
      enddo
      enddo

      if (jp.eq.ip) then
        D(ip)= D(ip) + COEFij
        B(ip)= B(ip) + QVO*QVC
       else
        AMAT(kk)= AMAT(kk) + COEFij
      endif
    enddo
    enddo
  enddo

  return
  end
```

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

MAT_ASS_MAIN (6/6)

```
        QVO   = 0.d0
        COEFij= 0.d0
        do kpn= 1, 2
        do jpn= 1, 2
        do ipn= 1, 2
          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= COEFij + coef * CONDO *
     &                     (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
     &                      DETJ(ipn,jpn,kpn)

          SHi= SHAPE(ipn,jpn,kpn,ie)
          QVO= QVO + SHi * QVOL * coef * DETJ(ipn,jpr
        enddo
        enddo
        enddo

        if (jp.eq.ip) then
          D(ip)= D(ip) + COEFij
          B(ip)= B(ip) + QVO*QVC
         else
          AMAT(kk)= AMAT(kk) + COEFij
        endif
      enddo
      enddo
    enddo

    return
    end
```

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

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

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

MAT_ASS_MAIN (6/6)

```
  do kpn= 1, 2
  do jpn= 1, 2
  do ipn= 1, 2
    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= COEFij + coef * CONDO * (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
 &                                   DETJ(ipn,jpn,kpn)

  enddo
  enddo
  enddo
```

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

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

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

MAT_ASS_MAIN (6/6)

```
    do kpn= 1, 2
    do jpn= 1, 2
    do ipn= 1, 2
      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= COEFij + coef * CONDO * (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
  &                           DETJ(ipn,jpn,kpn)

    enddo
    enddo
    enddo
```

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

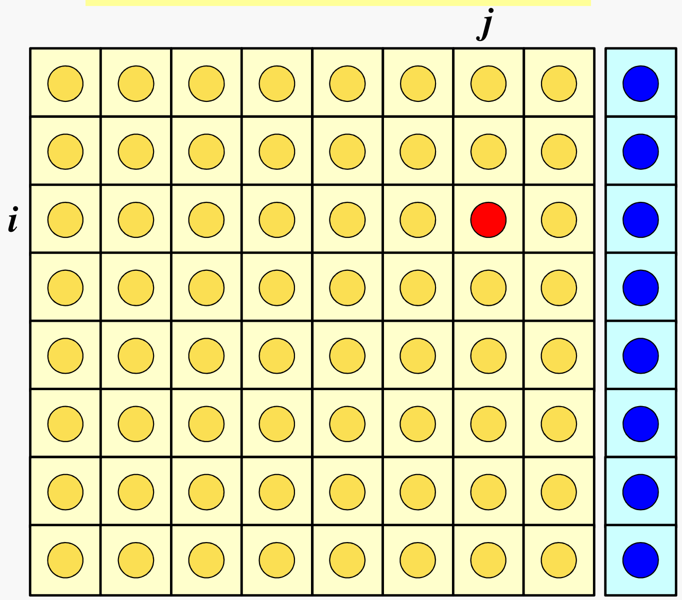
$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N}\left[W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k) \right]$$

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

MAT_ASS_MAIN (6/6)

```
      QVO    = 0.d0
      COEFij= 0.d0
      do kpn= 1, 2
      do jpn= 1, 2
      do ipn= 1, 2
        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= COEFij + coef * CONDO *
&                        (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
&                         DETJ(ipn,jpn,kpn)

        SHi= SHAPE(ipn,jpn,kpn,ie)
        QVO= QVO + SHi * QVOL * coef * DETJ(ipn,jpn,kpn)
      enddo
      enddo
      enddo

      if (jp.eq.ip) then
        D(ip)= D(ip) + COEFij
        B(ip)= B(ip) + QVO*QVC
       else
        AMAT(kk)= AMAT(kk) + COEFij
      endif
    enddo
    enddo
  enddo

  return
  end
```

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



MAT_ASS_MAIN（6/6）

```
      QVO    = 0.d0
      COEFij= 0.d0
      do kpn= 1, 2
      do jpn= 1, 2
      do ipn= 1, 2
        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= COEFij + coef * CONDO *
&                        (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
&                         DETJ(ipn,jpn,kpn)

        SHi= SHAPE(ipn,jpn,kpn,ie)
        QVO= QVO + SHi * QVOL * coef * DETJ(ipn,jpn,kpn)
      enddo
      enddo
      enddo

      if (jp.eq.ip) then
        D(ip)= D(ip) + COEFij
        B(ip)= B(ip) + QVO*QVC
       else
        AMAT(kk)= AMAT(kk) + COEFij
      endif
    enddo
    enddo
  enddo

  return
  end
```

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

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

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

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

MAT_ASS_MAIN (6/6)

```
do kpn= 1, 2
do jpn= 1, 2
do ipn= 1, 2
  coef= WEI(ipn)*WEI(jpn)*WEI(kpn)

  SHi= SHAPE(ipn,jpn,kpn,ie)
  QVO= QVO + SHi * QVOL * coef * DETJ(ipn,jpn,kpn)

enddo
enddo
enddo
```

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

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

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

MAT_ASS_MAIN (6/6)

```
    do kpn= 1, 2
    do jpn= 1, 2
    do ipn= 1, 2
      coef= WEI(ipn)*WEI(jpn)*WEI(kpn)

      SHi= SHAPE(ipn,jpn,kpn,ie)
      QV0= QV0 + SHi * QVOL * coef * DETJ(ipn,jpn,kpn)

    enddo
    enddo
    enddo
```

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

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

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

MAT_ASS_MAIN (6/6)

```
      QV0    = 0.d0
      COEFij= 0.d0
      do kpn= 1, 2
      do jpn= 1, 2
      do ipn= 1, 2
        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= COEFij + coef * CONDO *
&                        (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj) *
&                         DETJ(ipn,jpn,kpn)

        SHi= SHAPE(ipn,jpn,kpn,ie)
        QV0= QV0 + SHi * QVOL * coef * DETJ(ipn,jpn,kpn)
      enddo
      enddo
      enddo

      if (jp.eq.ip) then
        D(ip)= D(ip) + COEFij
        B(ip)= B(ip) + QV0*QVC
       else
        AMAT(kk)= AMAT(kk) + COEFij
      endif
    enddo
    enddo
  enddo

  return
  end
```

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

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

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

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

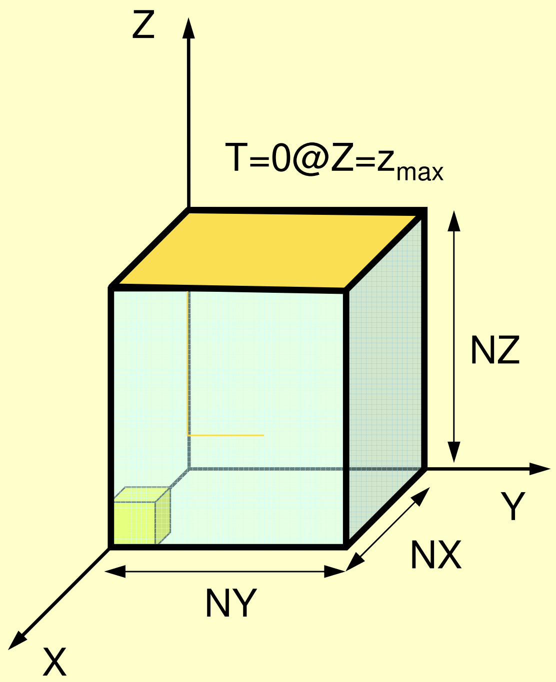
$$QVC = |x_C + y_C|$$

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

MAT_ASS_BC: Overview

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

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

do i= 1, NP Loop for Nodes
  do k= index(i-1)+1, index(i)       Non-Zero Off-Diagonal Nodes
    if (IWKX(item(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)

```
      subroutine MAT_ASS_BC
      use pfem_util
      implicit REAL*8 (A-H,O-Z)

      allocate (IWKX(NP,2))
      IWKX= 0

!C
!C== Z=Zmax

      do in= 1, NP
        IWKX(in,1)= 0
      enddo

      ib0= -1
      do ib0= 1, NODGRPtot
        if (NODGRP_NAME(ib0).eq.'Zmax') exit
      enddo

      do ib= NODGRP_INDEX(ib0-1)+1, NODGRP_INDEX(ib0)
        in= NODGRP_ITEM(ib)
        IWKX(in,1)= 1
      enddo
```

If the node "in" is included in the node group "Zmax"

IWKX(in,1)= 1

MAT_ASS_BC (2/2)

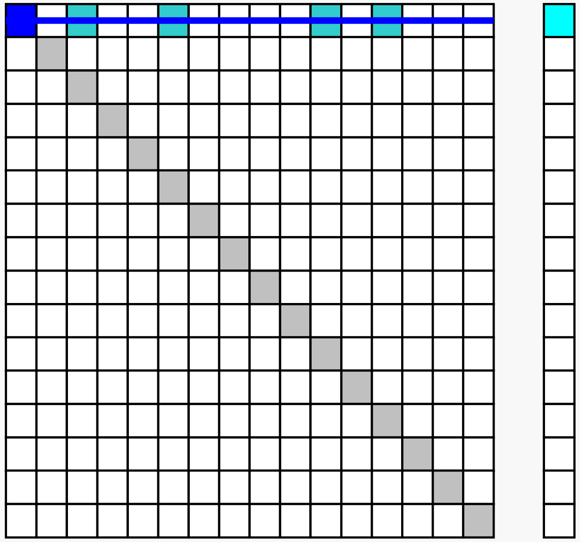
```
      do in= 1, NP
        if (IWKX(in,1).eq.1) then
          B(in)= 0.d0
          D(in)= 1.d0

          iS= index(in-1) + 1
          iE= index(in  )
          do k= iS, iE
            AMAT(k)= 0.d0
          enddo
        endif
      enddo

      do in= 1, NP
        iS= index(in-1) + 1
        iE= index(in  )
        do k= iS, iE
          if (IWKX(item(k),1).eq.1) then
            AMAT(k)= 0.d0
          endif
        enddo
      enddo
!C==
      return
      end
```

MAT_ASS_BC (2/2)

```
      do in= 1, NP
        if (IWKX(in,1).eq.1) then
          B(in)= 0.d0
          D(in)= 1.d0

          iS= index(in-1) + 1
          iE= index(in  )
          do k= iS, iE
            AMAT(k)= 0.d0
          enddo
        endif
      enddo

      do in= 1, NP
        iS= index(in-1) + 1
        iE= index(in  )
        do k= iS, iE
          if (IWKX(item(k),1).eq.1) then
            AMAT(k)= 0.d0
          endif
        enddo
      enddo
!C==
      return
      end
```

Boundary Nodes: IWKX(in,1)=1

Erase !!

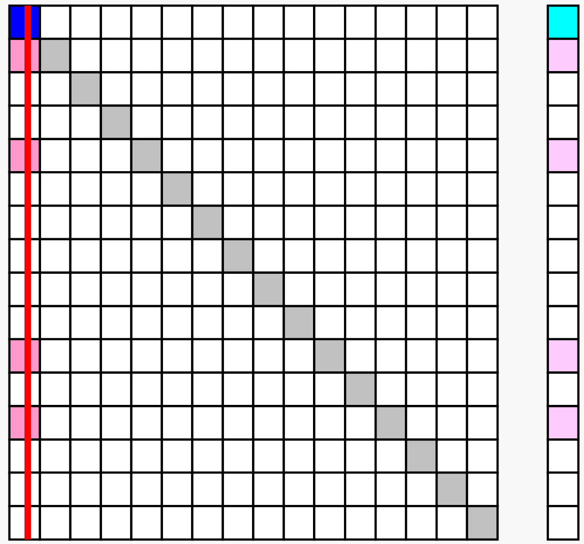


Same as 1CPU case

境界条件：MAT_ASS_BC（2/2）

```
      do in= 1, NP
        if (IWKX(in,1).eq.1) then
          B(in)= 0.d0
          D(in)= 1.d0

          iS= index(in-1) + 1
          iE= index(in  )
          do k= iS, iE
            AMAT(k)= 0.d0
          enddo
        endif
      enddo

      do in= 1, NP
        iS= index(in-1) + 1
        iE= index(in  )
        do k= iS, iE
          if (IWKX(item(k),1).eq.1) then
            AMAT(k)= 0.d0
          endif
        enddo
      enddo
!C==
      return
      end
```

Boundary Nodes: IWKX(in,1)=1



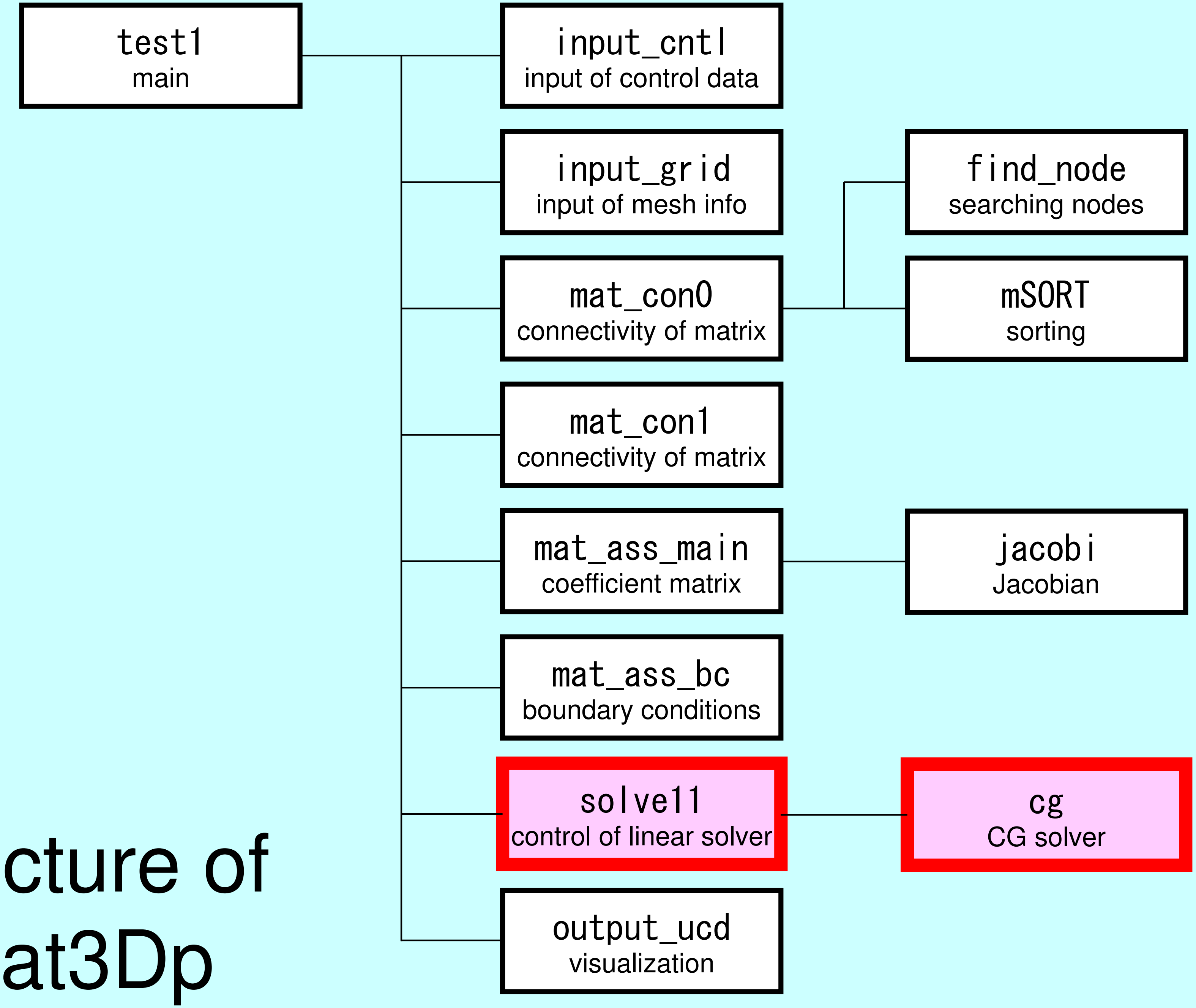
Elimination and Erase

Same as 1CPU case

Parallel 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 heat3Dp



Main Part

```
program heat3Dp

use solver11
use pfem_util

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

call PFEM_INIT
call INPUT_CNTL
call INPUT_GRID

call MAT_CON0
call MAT_CON1

call MAT_ASS_MAIN
call MAT_ASS_BC

call SOLVE11

call OUTPUT_UCD

call PFEM_FINALIZE

end program heat3Dp
```

SOLVE11

```
      module SOLVER11

       contains
         subroutine SOLVE11

         use pfem_util
         use solver_CG

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

         integer :: ERROR, ICFLAG
         character(len=char_length) :: BUF

         data ICFLAG/0/

!C
!C +------------+
!C | PARAMETERs |
!C +------------+
!C===
         ITER      = pfemIarray(1)               Max. Iterations for CG
         RESID     = pfemRarray(1)               Convergence Criteria for CG
!C===

!C
!C +------------------+
!C | ITERATIVE solver |
!C +------------------+
!C===
         call CG                                                     &
     &      ( N, NP, NPLU, D, AMAT, index, item, B, X,  RESID,       &
     &        ITER, ERROR, my_rank,                                  &
     &        NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,          &
     &                           EXPORT_INDEX, EXPORT_ITEM)
       ITERactual= ITER
!C===

       end subroutine SOLVE11
       end module SOLVER11
```

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)

```
      subroutine CG                                                    &
     &   (N, NP, NPLU, D, AMAT, index, item, B, X, RESID,              &
     &     ITER, ERROR, my_rank,                                       &
     &    NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,                &
     &                       EXPORT_INDEX, EXPORT_ITEM)

      use  solver_SR

      implicit REAL*8(A-H,O-Z)
      include  'precision.inc'
      include  'mpif.h'

      integer(kind=kint ), intent(in):: N, NP, NPLU, my_rank
      integer(kind=kint ), intent(in):: NEIBPETOT
      integer(kind=kint ), intent(inout):: ITER, ERROR
      real   (kind=kreal), intent(inout):: RESID

      real(kind=kreal), dimension(NP)   , intent(inout):: B, X, D
      real(kind=kreal), dimension(NPLU), intent(inout):: AMAT

      integer(kind=kint ), dimension(0:NP),intent(in) :: index
      integer(kind=kint ), dimension(NPLU),intent(in) :: item

      integer(kind=kint ), pointer :: NEIBPE(:)
      integer(kind=kint ), pointer :: IMPORT_INDEX(:), IMPORT_ITEM(:)
      integer(kind=kint ), pointer :: EXPORT_INDEX(:), EXPORT_ITEM(:)

      real(kind=kreal), dimension(:),    allocatable:: WS, WR          Sending/Receiving Buffer
      real(kind=kreal), dimension(:,:),  allocatable:: WW

      integer(kind=kint), parameter ::  R= 1
      integer(kind=kint), parameter ::  Z= 2
      integer(kind=kint), parameter ::  Q= 2
      integer(kind=kint), parameter ::  P= 3
      integer(kind=kint), parameter :: DD= 4

      integer(kind=kint ) :: MAXIT
      real   (kind=kreal) :: TOL, W, SS
```

Variables/Arrays in CG Solver (1/2)

Name	Type	Size	I/O	Definition
N,NP	I		I	# Node (Internal, Internal+External)
NPLU	I		O	# Non-Zero Off-Diagonals
D	R	(NP)	O	Diagonal Block of Global Matrix
B,X	R	(NP)	O	RHS, Unknown Vector
AMAT	R	(NPLU)	O	Non-Zero Off-Diagonal Components of Global Matrix
index	I	(0:NP)	O	# Non-Zero Off-Diagonal Components
item	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	(NP,4)	–	Work Arrays
P,Q,R,Z,DD	I		–	Vector ID for **WW** (1-4)

Variables/Arrays in CG Solver (2/2)

Name	Type	Size	I/O	Definition
PETOT	I		I	Number of PE's
my_rank	I		I	Process ID of MPI
NEIBPETOT	I		I	Number of Neighbors
NEIBPE	I	(NEIBPETOT)	I	ID of Neighbor
IMPORT_INDEX **EXPORT_INEDX**	I	(0:NEIBPETOT)	I	Size of Import/Export Arrays for Communication Table
IMPORT_ITEM	I	(NPimport)	I	Receiving Table (External Points) NPimport=IMPORT_INDEX(NEIBPETOT))
EXPORT_ITEM	I	(NPexport)	I	Sending Table (Boundary Points) NPexport=EXPORT_INDEX(NEIBPETOT))
WR, WS	R	(NP)		Receiving/Sending Buffer for Point-to-Point Communications

CG Solver (2/6)

```
 COMMtime= 0.d0
      COMPtime= 0.d0

      ERROR= 0

      allocate (WW(NP,4),WR(NP),WS(NP))

      MAXIT  = ITER
       TOL   = RESID

      X = 0.d0
      WS= 0.d0
      WR= 0.d0
!C
!C +----------------------+
!C | {r0}= {b} - [A]{xini} |
!C +----------------------+
!C===

      call SOLVER_SEND_RECV
     &   ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,
     &     EXPORT_INDEX, EXPORT_ITEM, WS, WR, X , my_rank)

      do j= 1, N
        WW(j,DD)= 1.d0/D(j)
        WVAL= B(j) - D(j)*X(j)
        do k= index(j-1)+1, index(j)
          i= item(k)
          WVAL= WVAL - AMAT(k)*X(i)
        enddo
        WW(j,R)= WVAL
      enddo

      BNRM20= 0.d0
      do i= 1, N
        BNRM20= BNRM20 + B(i)**2
      enddo
      call MPI_Allreduce (BNRM20, BNRM2, 1, MPI_DOUBLE_PRECISION,       &
     &                    MPI_SUM, MPI_COMM_WORLD, ierr)
```

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

SOLVER_SEND_RECV (1/2)

```
      subroutine  SOLVER_SEND_RECV                                   &
     &            ( N, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM, &
     &                                    EXPORT_INDEX, EXPORT_ITEM, &
     &              WS, WR, X, my_rank)

      implicit REAL*8 (A-H,O-Z)
      include  'mpif.h'
      include  'precision.inc'
      integer(kind=kint )                   , intent(in)   :: N
      integer(kind=kint )                   , intent(in)   :: NEIBPETOT
      integer(kind=kint ), pointer :: NEIBPE      (:)
      integer(kind=kint ), pointer :: IMPORT_INDEX(:)
      integer(kind=kint ), pointer :: IMPORT_ITEM  (:)
      integer(kind=kint ), pointer :: EXPORT_INDEX(:)
      integer(kind=kint ), pointer :: EXPORT_ITEM  (:)
      real   (kind=kreal), dimension(N), intent(inout):: WS
      real   (kind=kreal), dimension(N), intent(inout):: WR
      real   (kind=kreal), dimension(N), intent(inout):: X
      integer                          , intent(in)   :: my_rank
      integer(kind=kint ), dimension(:,:), save, allocatable :: sta1, sta2, req1, req2
      integer(kind=kint ), save :: NFLAG
      data NFLAG/0/

      if (NFLAG.eq.0) then
        allocate (sta1(MPI_STATUS_SIZE,NEIBPETOT), sta2(MPI_STATUS_SIZE,NEIBPETOT))
        allocate (req1(NEIBPETOT), req2(NEIBPETOT))
        NFLAG= 1
      endif

      do neib= 1, NEIBPETOT
        istart= EXPORT_INDEX(neib-1)
        inum  = EXPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
           ii   = EXPORT_ITEM(k)
           WS(k)= X(ii)
        enddo

        call MPI_Isend (WS(istart+1), inum, MPI_DOUBLE_PRECISION,     &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req1(neib),   &
     &                  ierr)
      enddo
```

SOLVER_SEND_RECV (2/2)

```
      do neib= 1, NEIBPETOT
        istart= IMPORT_INDEX(neib-1)
        inum  = IMPORT_INDEX(neib  ) - istart
        call MPI_Irecv (WR(istart+1), inum, MPI_DOUBLE_PRECISION,      &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req2(neib),    &
     &                  ierr)
      enddo

      call MPI_Waitall (NEIBPETOT, req2, sta2, ierr)

      do neib= 1, NEIBPETOT
        istart= IMPORT_INDEX(neib-1)
        inum  = IMPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
            ii = IMPORT_ITEM(k)
          X(ii)= WR(k)
        enddo
      enddo

      call MPI_Waitall (NEIBPETOT, req1, sta1, ierr)

      end subroutine solver_send_recv
      end module     solver_SR
```

CG Solver (3/6)

```
 do iter= 1, MAXIT

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

!C
!C +---------------+
!C | {RHO}= {r}{z} |
!C +---------------+
      RHO0= 0.d0

      do i= 1, N
        RHO0= RHO0 + WW(i,R)*WW(i,Z)
      enddo

      call MPI_Allreduce (RHO0, RHO, 1, MPI_DOUBLE_PRECISION,
     &                    MPI_SUM, MPI_COMM_WORLD, ierr)

!C
!C +-----------------------------+
!C | {p} = {z} if      ITER=1    |
!C | BETA= RHO / RHO1  otherwise |
!C +-----------------------------+
      if ( ITER.eq.1 ) then
        do i= 1, N
          WW(i,P)= WW(i,Z)
        enddo
       else
         BETA= RHO / RHO1
         do i= 1, N
           WW(i,P)= WW(i,Z) + BETA*WW(i,P)
         enddo
      endif
```

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)

```
!C
!C +--------------+
!C | {q}= [A]{p}  |
!C +--------------+
      call SOLVER_SEND_RECV
     &   ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,
     &     EXPORT_INDEX, EXPORT_ITEM, WS, WR, WW(1,P),
     &     my_rank)

      do j= 1, N
        WVAL= D(j)*WW(j,P)
        do k= index(j-1)+1, index(j)
            i= item(k)
           WVAL= WVAL + AMAT(k)*WW(i,P)
        enddo
        WW(j,Q)= WVAL
      enddo

!C
!C +---------------------+
!C | ALPHA= RHO / {p}{q} |
!C +---------------------+
      C10= 0.d0
      do i= 1, N
        C10= C10 + WW(i,P)*WW(i,Q)
      enddo
      call MPI_Allreduce (C10, C1, 1, MPI_DOUBLE_PRECISION,
     &                    MPI_SUM, MPI_COMM_WORLD, ierr)

      ALPHA= RHO / C1
```

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

for $i= 1, 2, \ldots$

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

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

  if $i=1$

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

  else

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

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

  endif

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

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

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

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

  check convergence $|r|$

end

CG Solver (5/6)

```
!C
!C +----------------------+
!C | {x}= {x} + ALPHA*{p} |
!C | {r}= {r} - ALPHA*{q} |
!C +----------------------+
      do i= 1, N
         X(i)  = X (i)    + ALPHA * WW(i,P)
        WW(i,R)= WW(i,R) - ALPHA * WW(i,Q)
      enddo

      DNRM20= 0.d0
      do i= 1, N
        DNRM20= DNRM20 + WW(i,R)**2
      enddo
      call MPI_Allreduce (DNRM20, DNRM2, 1,
     &                    MPI_DOUBLE_PRECISION,
     &                    MPI_SUM, MPI_COMM_WORLD, ierr)

      RESID= dsqrt(DNRM2/BNRM2)
        if ( RESID.le.TOL   ) exit
        if ( ITER .eq.MAXIT ) ERROR= -300

        RHO1 = RHO

      enddo
!C===

   30 continue

      call SOLVER_SEND_RECV
     &   ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,
     &     EXPORT_INDEX, EXPORT_ITEM, WS, WR, X , my_rank)

      deallocate (WW,WR,WS)

      end subroutine        CG
      end module     solver_CG
```

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

for $i= 1, 2, \ldots$

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

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

  if $i=1$

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

   else

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

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

  endif

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

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

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

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

  check convergence |r|

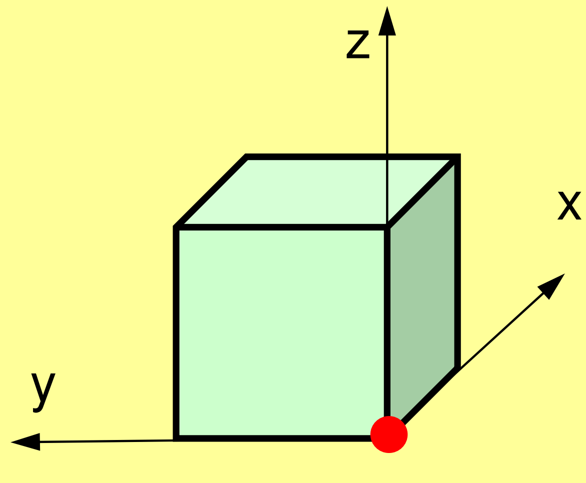
end

CG Solver (6/6)

```
!C
!C +-----------------------+
!C | {x}= {x} + ALPHA*{p} |
!C | {r}= {r} - ALPHA*{q} |
!C +-----------------------+
      do i= 1, N
          X(i)  = X (i)    + ALPHA * WW(i,P)
        WW(i,R)= WW(i,R) - ALPHA * WW(i,Q)
      enddo

      DNRM20= 0.d0
      do i= 1, N
        DNRM20= DNRM20 + WW(i,R)**2
      enddo
      call MPI_Allreduce (DNRM20, DNRM2, 1,
     &                     MPI_DOUBLE_PRECISION,
     &                     MPI_SUM, MPI_COMM_WORLD, ierr)

      RESID= dsqrt(DNRM2/BNRM2)
        if ( RESID.le.TOL   ) exit
        if ( ITER .eq.MAXIT ) ERROR= -300

        RHO1 = RHO

      enddo
!C===

   30 continue

      call SOLVER_SEND_RECV                                        & Updated temperature for external nodes

     &   ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,       &
     &     EXPORT_INDEX, EXPORT_ITEM, WS, WR, X , my_rank)

      deallocate (WW,WR,WS)

      end subroutine        CG
      end module     solver_CG
```

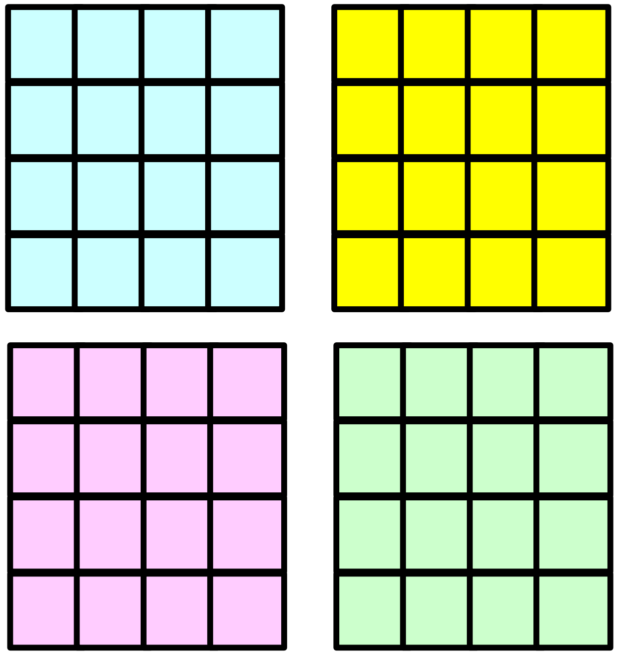
Final Output & Validation

```
   call SOLVE11
   call OUTPUT_UCD

   do i= 1, N
     if (XYZ(i,1).eq.0.d0.and.XYZ(i,2).eq.0.d0.
  &                           and.XYZ(i,3).eq.0.d0) then
       write (*,'(2i8,1pe16.6)') my_rank, i, X(i)
     endif
   enddo

   call PFEM_FINALIZE

   end program heat3Dp
```



OUTPUT_UCD for Visualization

- Gather information of elements in “intELEM_list” on each process
- Gather the following information to process #0 using MPI_Allgatherv
  - Nodes: Coordinates, Displacement
  - Element: Connectivity
- Some overlapping in part of node information
- Not good for large-scale problems
  - Entire model on a single process
  - parallel visualization



Time for Computation

```
!C
!C +-------------------+
!C | MATRIX assemble |
!C +-------------------+
!C===
      START_TIME= MPI_WTIME()

        call MAT_ASS_MAIN
        call MAT_ASS_BC

      END_TIME= MPI_WTIME()
      if (my_rank.eq.0) then
        write (*, '("*** matrix ass.   ", 1pe16.6, " sec.",/)')           &
     &          END_TIME-START_TIME
      endif
!C===

!C
!C +---------+
!C | SOLVER |
!C +---------+
!C===
      START_TIME= MPI_WTIME()
        call SOLVE11
      END_TIME= MPI_WTIME()

      if (my_rank.eq.0) then
        write (*, '("*** real  COMP.   ", 1pe16.6, " sec.",/)')           &
     &          END_TIME-START_TIME
      endif
!C===
```

Example

- (256x256x192) nodes = 12,582,912
- (255x255x191) elements = 12,419,775
- 8 nodes, 48-processes/node, 384-processes

k-MeTis (1/2): 48x8= 384 part's

```
>$ cd /work/gt18/t18XXX/pFEM/pfem3d/mesh

<modify inp_mg, mg.sh, inp_kmetis>
<modify part_kmetis.sh>

>$ pjsub mg.sh
>$ pjsub part_kmetis.sh
```

inp_mg

```
255 255 191
```

inp_kmetis

```
cube.0
2
384
aaa
```

255x255x191 elements
256x256x192 nodes
48x8= 384 partitions

k-MeTis (2/2): 48x8= 384 part's

```
>$ cd ../run
<modify INPUT.DAT, a08k.sh>

>$ pjsub a08k.sh
```

INPUT.DAT

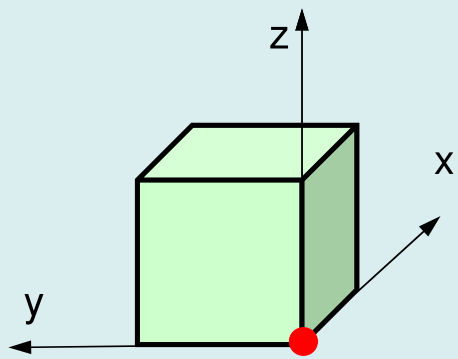
```
../mesh/aaa
2000
1.0 1.0
1.0e-08
```

a08k.sh

```
#!/bin/sh
#PJM -N "flat-08"
#PJM -L rscgrp=lecture8-o
#PJM -L node=8
#PJM --mpi proc=384
#PJM -L elapse=00:15:00
#PJM -g gt18
#PJM -j
#PJM -e err
#PJM -o a08k.lst

module load fj
module load fjmpi

mpiexec ./sol
mpiexec numactl -l ./sol
```

a08k.lst

```
*** matrix conn.      3.516576E-02 sec.
*** matrix ass.       4.487921E-02 sec.

    1     1.370663E+01
    2     1.356864E+01
    3     1.343335E+01
    4     1.330067E+01
    5     1.317050E+01
(…)
  668     1.366236E-08
  669     1.264988E-08
  670     1.162203E-08
  671     1.062147E-08
  672     9.649164E-09
*** real  COMP.       2.035819E+00 sec.

      265        1    3.526204E+06
 * normal termination
```



pmesh (1/2): 48x8= 384 part's

```
>$ cd /work/gt18/t18XXX/pFEM/pfem3d/pmesh

<modify mesh.inp, mg.sh>

>$ pjsub mg.sh
```

mesh.inp

```
256 256 192
  8   8   6
pcube
```

255x255x191 elements
256x256x192 nodes
48x8= 384 partitions

mg.sh

```
#!/bin/sh
#PJM -N "pmg"
#PJM -L rscgrp=lecture8-o
#PJM -L node=8
#PJM --mpi proc=384
#PJM -L elapse=00:10:00
#PJM -g gt18
#PJM -j
#PJM -e err
#PJM -o pmg.lst

module load fj
module load fjmpi

mpiexec ./pmesh
rm wk.*
```

pmesh (2/2): 48x8= 384 part's

```
>$ cd ../run
<modify INPUT.DAT, a08.sh>

>$ pjsub a08.sh
```

INPUT.DAT

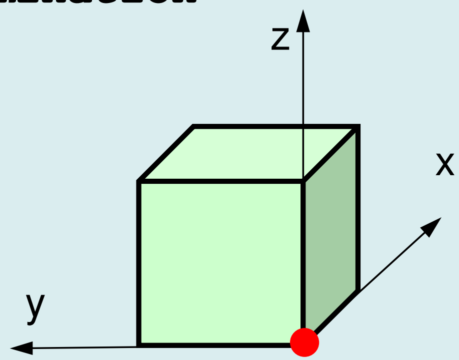
```
../pmesh/pcube
2000
1.0 1.0
1.0e-08
```

a08.sh

```
#!/bin/sh
#PJM -N "flat-08"
#PJM -L rscgrp=lecture8-o
#PJM -L node=8
#PJM --mpi proc=384
#PJM -L elapse=00:15:00
#PJM -g gt18
#PJM -j
#PJM -e err
#PJM -o a08.lst

module load fj
module load fjmpi

mpiexec ./sol
mpiexec numactl -l ./sol
```

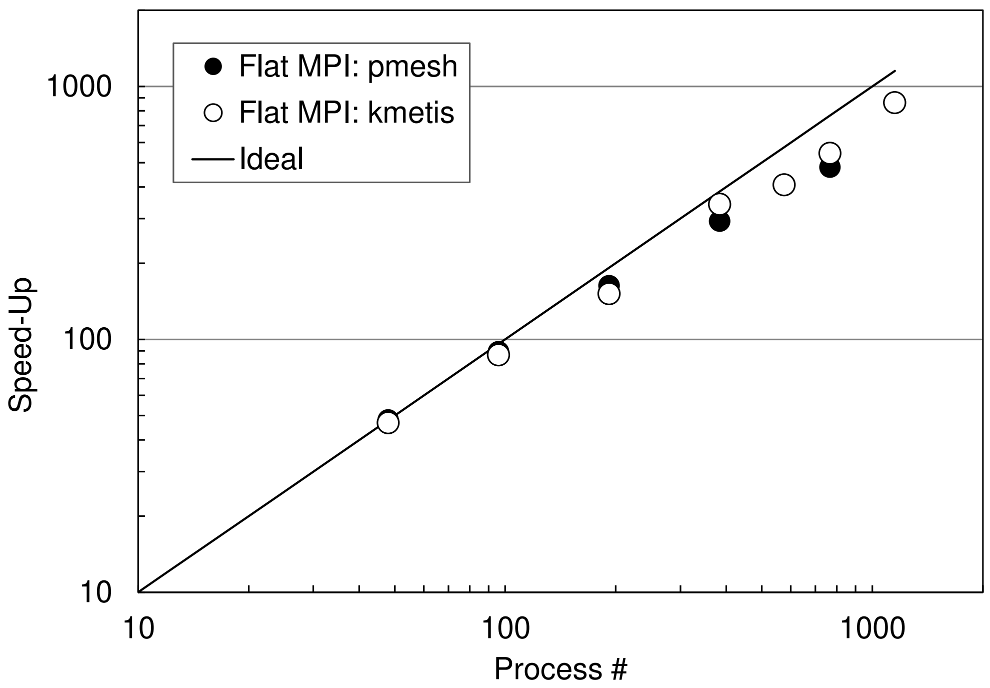
a08.lst

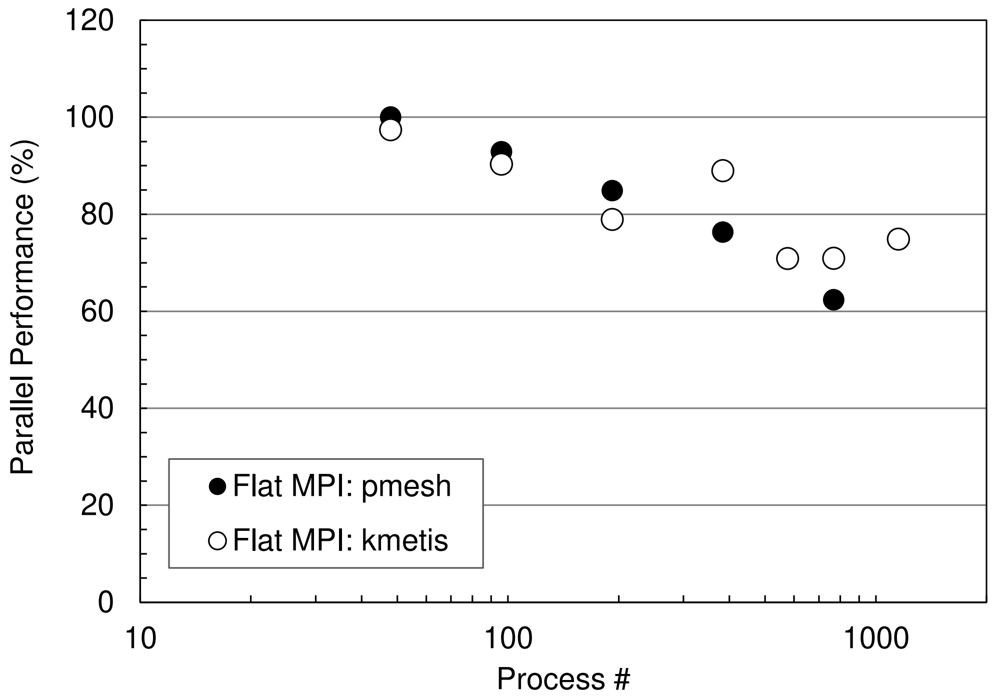
```
*** matrix conn.      3.516576E-02 sec.
*** matrix ass.       4.487921E-02 sec.

     1     1.370663E+01
     2     1.356864E+01
     3     1.343335E+01
     4     1.330067E+01
     5     1.317050E+01
(…)
   668     1.366236E-08
   669     1.264988E-08
   670     1.162203E-08
   671     1.062147E-08
   672     9.649164E-09
*** real  COMP.       2.058311E+00 sec.

       0       1      3.526204E+06
 * normal termination
```



Example: Strong Scaling: C

- 256×256×192 nodes, 12,582,912 DOF
- 48～1,152 cores (1~24 nodes), Flat MPI
- Linear Solver

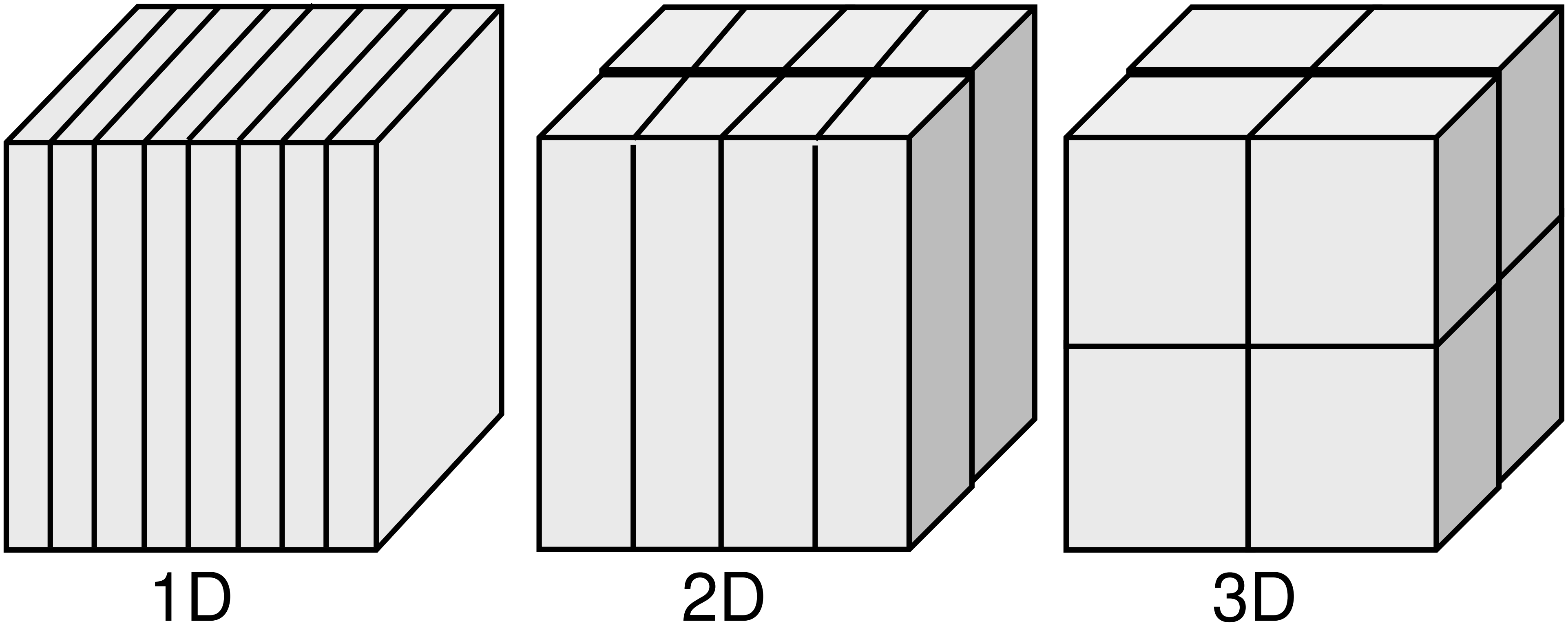




Exercise (1/2)

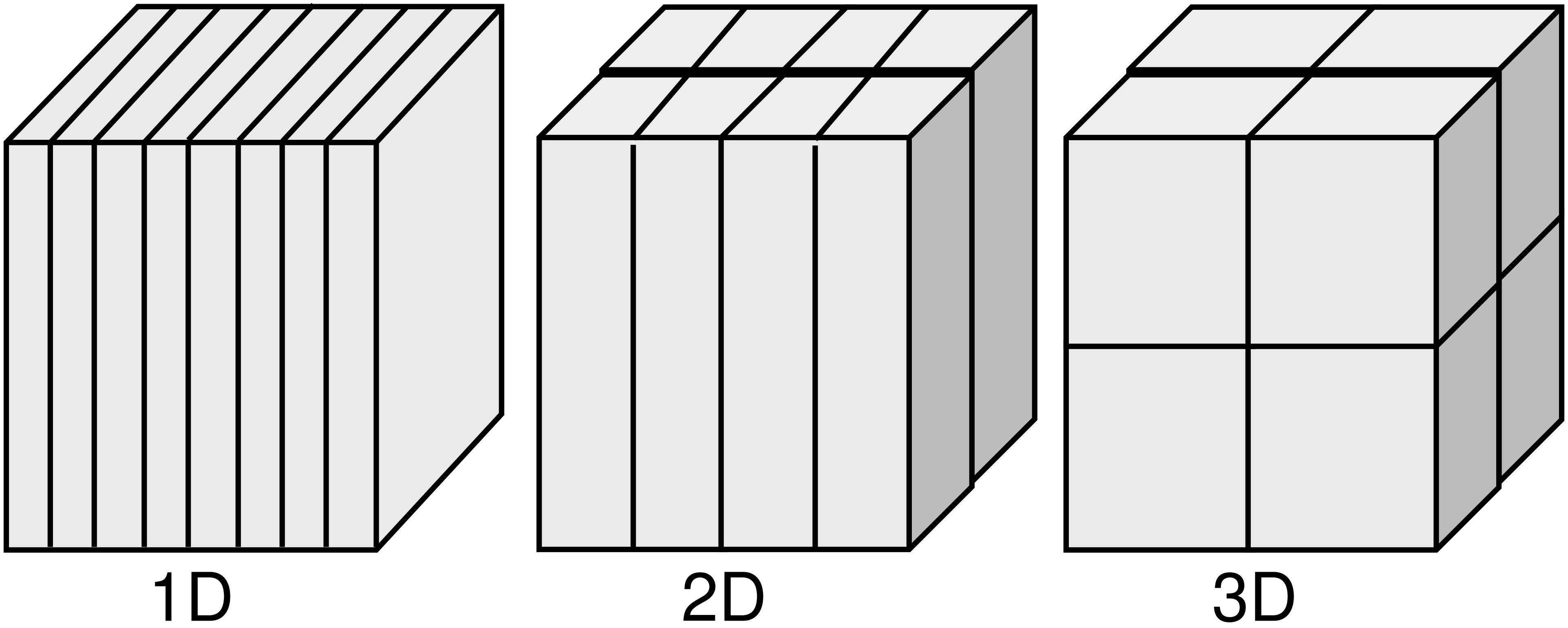
- Evaluation behavior and performance of “sol”
- Example
  - Strong Scaling
    - Fixed entire problem size
  - Weak Scaling
    - Fixed problem size/core, time for 1 iterations
  - Parameters
    - Problem size
    - Domain decomposition (1D-3D, kmetis, pmetis)
- “*.inp” may take long time.
  - delete “call OUTPUT_UCD”
  - src, part

1D-3D Decomposition



1D-3D Decomposition

Amount of comm.: each edge has 4N points, 8 domains



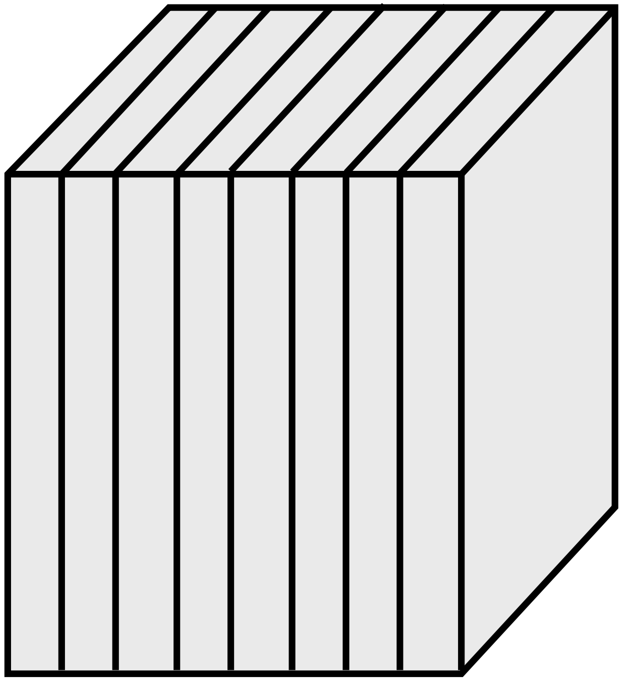
$16\ N^2 \times 7 = 112\ N^2$

$16\ N^2 \times 4 = 64\ N^2$

$16\ N^2 \times 3 = 48\ N^2$

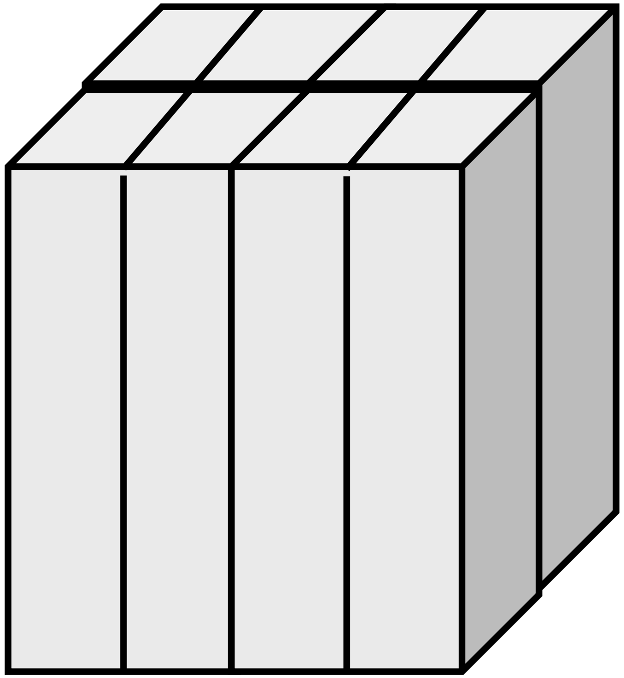
1D-3D Decomposition

mesh.inp



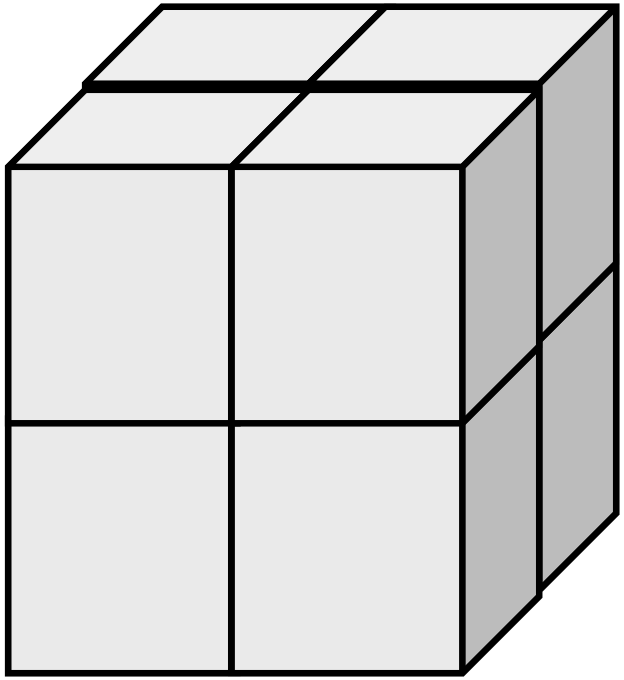
1D

```
 64  64  64
  8   1   1
pcube
```



2D

```
 64  64  64
  4   2   1
pcube
```



3D

```
 64  64  64
  2   2   2
pcube
```

Exercise (2/2)

- Improve PE-to-PE communication part (solver_SR)
  - Copying to receiving buffer, Combining MPI_Wait_all
- Actually, numbering of external nodes in each neighboring domain is continuous
- You can also apply this to 1D case

```
      do neib= 1, NEIBPETOT
        istart= IMPORT_INDEX(neib-1)
        inum  = IMPORT_INDEX(neib  ) - istart
        call MPI_Irecv (WR(istart+1), inum, MPI_DOUBLE_PRECISION,       &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req2(neib),    &
     &                  ierr)
      enddo

      call MPI_Waitall (NEIBPETOT, req2, sta2, ierr)

      do neib= 1, NEIBPETOT
        istart= IMPORT_INDEX(neib-1)
        inum  = IMPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
            ii = IMPORT_ITEM(k)
          X(ii)= WR(k)
        enddo
      enddo
```

SEND/RECV (Original)

```
!C
!C-- INIT.
      allocate (sta1(MPI_STATUS_SIZE,NEIBPETOT), sta2(MPI_STATUS_SIZE,NEIBPETOT))
      allocate (req1(NEIBPETOT), req2(NEIBPETOT))

!C
!C-- SEND
      do neib= 1, NEIBPETOT
        istart= EXPORT_INDEX(neib-1)
        inum  = EXPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
          WS(k)= X(EXPORT_ITEM(k))
        enddo
        call MPI_ISEND (WS(istart+1), inum, MPI_DOUBLE_PRECISION,          &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req1(neib), ierr)
      enddo

!C
!C-- RECEIVE
      do neib= 1, NEIBPETOT
        istart= IMPORT_INDEX(neib-1)
        inum  = IMPORT_INDEX(neib  ) - istart
        call MPI_IRECV (WR(istart+1), inum, MPI_DOUBLE_PRECISION,          &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req2(neib), ierr)
      enddo
      call MPI_WAITALL (NEIBPETOT, req2, sta2, ierr)

      do neib= 1, NEIBPETOT
        istart= IMPORT_INDEX(neib-1)
        inum  = IMPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
          X(IMPORT_ITEM(k))= WR(k)
        enddo
      enddo
      call MPI_WAITALL (NEIBPETOT, req1, sta1, ierr)
```

If numbering of external nodes is continuous in each neighboring process ...

	84	81	85	82	83	86	88	87	
96	57	58	59	60	61	62	63	64	73
95	49	50	51	52	53	54	55	56	74
94	41	42	43	44	45	46	47	48	80
93	33	34	35	36	37	38	39	40	79
92	25	26	27	28	29	30	31	32	78
91	17	18	19	20	21	22	23	24	77
90	9	10	11	12	13	14	15	16	76
89	1	2	3	4	5	6	7	8	75
	65	66	67	68	69	70	71	72	

SEND/RECV (NEW:1)

```
!C
!C-- INIT.
        allocate (sta1(MPI_STATUS_SIZE,2*NEIBPETOT))
        allocate (req1(2*NEIBPETOT))

!C
!C-- SEND
      do neib= 1, NEIBPETOT
        istart= EXPORT_INDEX(neib-1)
        inum  = EXPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
          WS(k)= X(EXPORT_ITEM(k))
        enddo
      enddo

      do neib= 1, NEIBPETOT
        istart= EXPORT_INDEX(neib-1)
        inum  = EXPORT_INDEX(neib  ) - istart
        call MPI_ISEND (WS(istart+1), inum, MPI_DOUBLE_PRECISION,          &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req1(neib), ierr)
      enddo

!C
!C-- RECEIVE
      do neib= 1, NEIBPETOT
        inum  = IMPORT_INDEX(neib) - STACK_IMPORT(neib-1)
        istart= IMPORT_ITEM(IMPORT_INDEX(neib-1)+1)

        call MPI_IRECV (X(istart), inum, MPI_DOUBLE_PRECISION,             &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req1(NEIBPETOT+neib), ierr)
      enddo

      call MPI_WAITALL (2*NEIBPETOT, req1, sta1, ierr)
```

SEND/RECV (NEW:2), N0: int. node

N0: Total Number of Internal Nodes

```
!C
!C-- INIT.
        allocate (sta1(MPI_STATUS_SIZE,2*NEIBPETOT))
        allocate (req1(2*NEIBPETOT))

!C
!C-- SEND
      do neib= 1, NEIBPETOT
        istart= EXPORT_INDEX(neib-1)
        inum  = EXPORT_INDEX(neib  ) - istart
        do k= istart+1, istart+inum
          WS(k)= X(EXPORT_ITEM(k))
        enddo
      enddo

      do neib= 1, NEIBPETOT
        istart= EXPORT_INDEX(neib-1)
        inum  = EXPORT_INDEX(neib  ) - istart
        call MPI_ISEND (WS(istart+1), inum, MPI_DOUBLE_PRECISION,                &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req1(neib), ierr)
      enddo

!C
!C-- RECEIVE
      do neib= 1, NEIBPETOT
        inum  = IMPORT_INDEX(neib) - IMPORT_INDEX(neib-1)
        istart= IMPORT_INDEX(neib-1) + N0 + 1

        call MPI_IRECV (X(istart), inum, MPI_DOUBLE_PRECISION,                   &
     &                  NEIBPE(neib), 0, MPI_COMM_WORLD, req1(NEIBPETOT+neib), ierr)
      enddo

      call MPI_WAITALL (2*NEIBPETOT, req1, sta1, ierr)
```