

3D Parallel FEM (II)

Fortran

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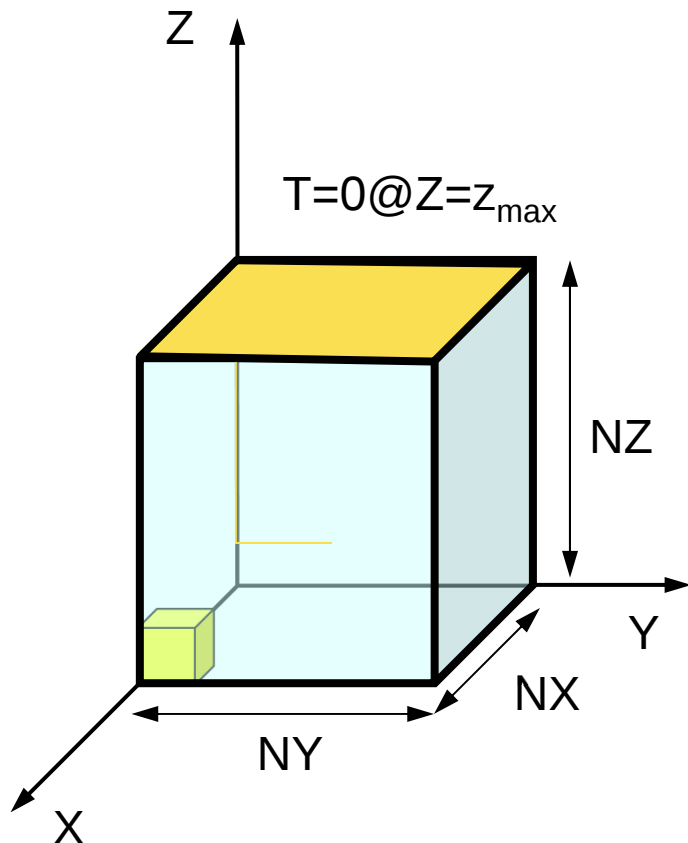
Technical & Scientific Computing II (4820-1028)

Seminar on Computer Science II (4810-1205)

Hybrid Distributed Parallel Computing (3747-111)

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)
 - $\dot{Q}(x, y, z) = QVOL|x_c + y_c|$

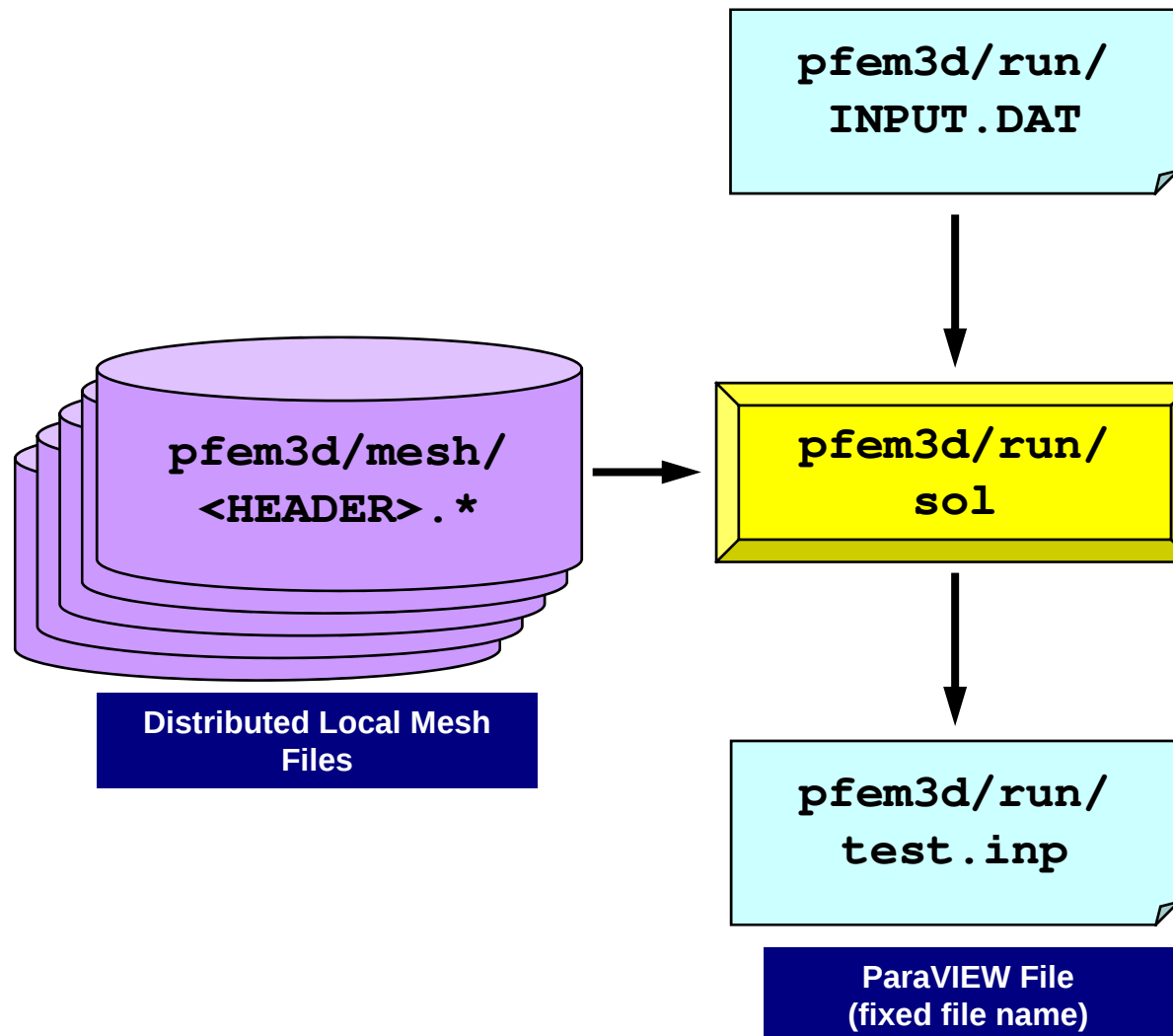
Finite-Element Procedures

- 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

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

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

<\$O-TOP>/pfem3d/run/go.sh

more stable with “export I_MPI_PERHOST=32”

```
#!/bin/sh
```

```
#PBS -q u-lecture
```

```
#PBS -N flat
```

```
#PBS -l select=4:mpiprocs=32
```

```
#PBS -Wgroup_list=gt26
```

```
#PBS -l walltime=00:05:00
```

```
#PBS -e err
```

```
#PBS -o test.lst
```

```
cd $PBS_O_WORKDIR
```

```
. /etc/profile.d/modules.sh
```

```
export I_MPI_PIN_DOMAIN=socket
```

```
export I_MPI_PERHOST=32
```

```
mpirun ./impimap.sh ./sol
```

Name of “QUEUE”

Job Name

node#, proc#/node

Group Name (Wallet)

Computation Time

Standard Error

Standard Outpt

go to current dir
(ESSENTIAL)

Execution on each socket

MPI proc#/node (=mpiprocs)

Exec's

```
#PBS -l select=1:mpiprocs=4
```

```
#PBS -l select=1:mpiprocs=16
```

```
#PBS -l select=1:mpiprocs=36
```

```
#PBS -l select=2:mpiprocs=32
```

```
#PBS -l select=4:mpiprocs=32
```

```
#PBS -l select=8:mpiprocs=36
```

1-node, 4-core's

1-node, 16-core's

1-node, 36-core's

2-nodes, 32x2=64-core's

4-nodes, 32x4=128-core's

8-nodes, 36x8=288-core's

<\$O-TOP>/pfem3d/run/go.sh

more stable with “export I_MPI_PERHOST=32”

```
#!/bin/sh
#PBS -q u-lecture
#PBS -N flat
#PBS -l select=4:mpiprocs=32
#PBS -Wgroup_list=gt26
#PBS -l walltime=00:05:00
#PBS -e err
#PBS -o test.lst
```

Name of “QUEUE”
Job Name
node#, proc#/node
Group Name (Wallet)
Computation Time
Standard Error
Standard Outpt

```
cd $PBS_O_WORKDIR
. /etc/profile.d/modules.sh
```

go to current dir
(ESSENTIAL)

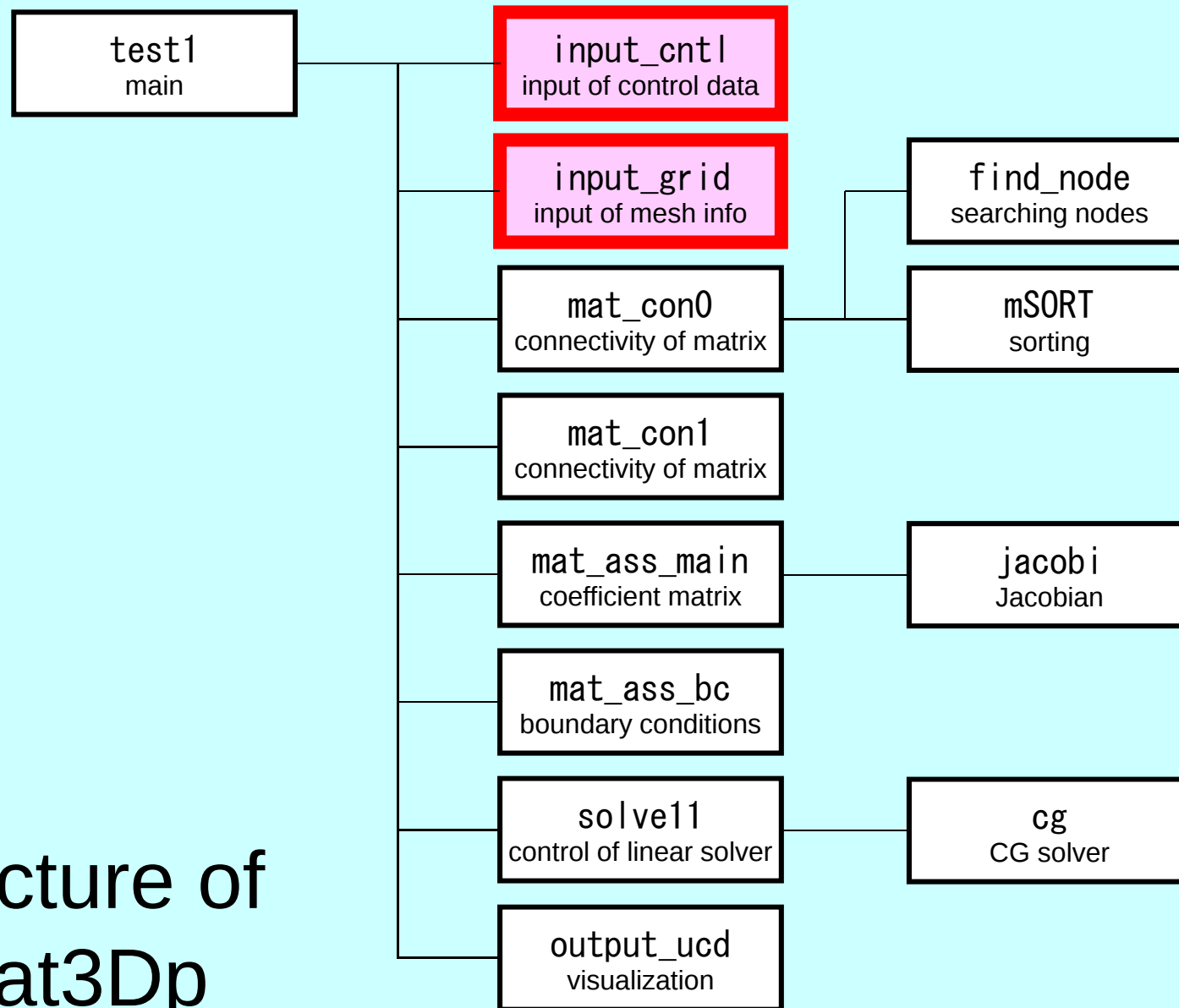
```
export I_MPI_PIN_DOMAIN=socket
export I_MPI_PERHOST=32
mpirun ./impimap.sh ./sol
```

Execution on each socket
MPI proc#/node (=mpiprocs)
Exec's

```
#PBS -l select=1:mpiprocs=4
#PBS -l select=1:mpiprocs=16
#PBS -l select=1:mpiprocs=36
#PBS -l select=2:mpiprocs=32
#PBS -l select=4:mpiprocs=32
#PBS -l select=8:mpiprocs=36
```

1-node, 4-core's
1-node, 16-core's
1-node, 36-core's
2-nodes, 32x2=64-core's
4-nodes, 32x4=128-core's
8-nodes, 36x8=288-core's

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_CONO
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)	○	Non-Zero Off-Diagonal Components of Global Matrix
index	I	(0:NP)	○	# Non-Zero Off-Diagonal Components
item	I	(NPLU)	○	Column ID of Non-Zero Off-Diagonal Components
INLU	I	(NP)	○	Number of Non-Zero Off-Diagonal Components at Each Node
IALU	I	(NP, NLU)	○	Column ID of Non-Zero Off-Diagonal Components at Each Node
IWKX	I	(NP, 2)	○	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)	○	Integer Parameter Array
pfemRarray	R	(100)	○	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	$N_i (i=1 \sim 8)$ 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

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

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

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

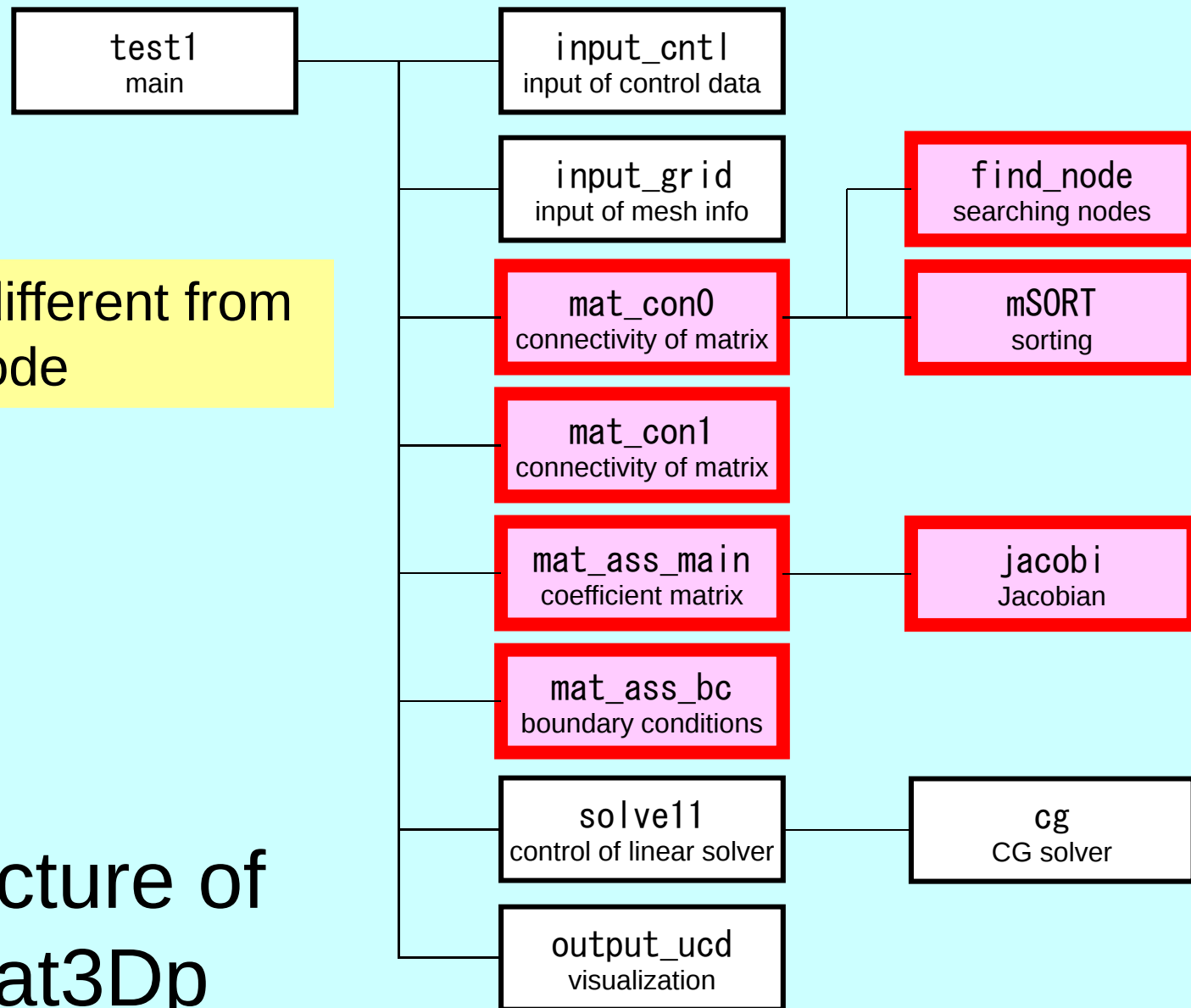
```

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

NOT so different from
1-CPU code

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
```

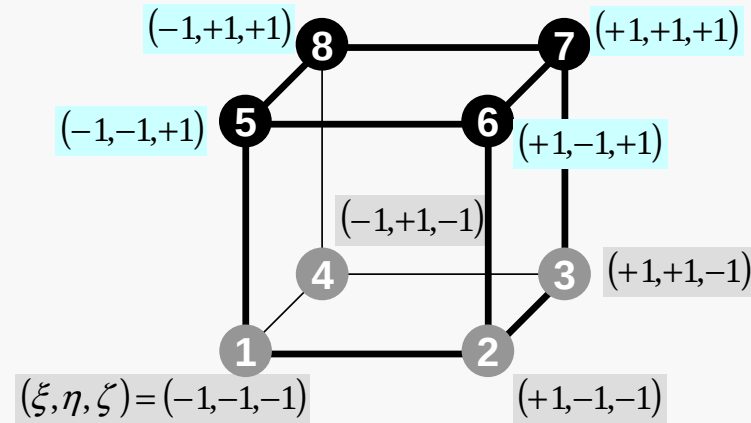
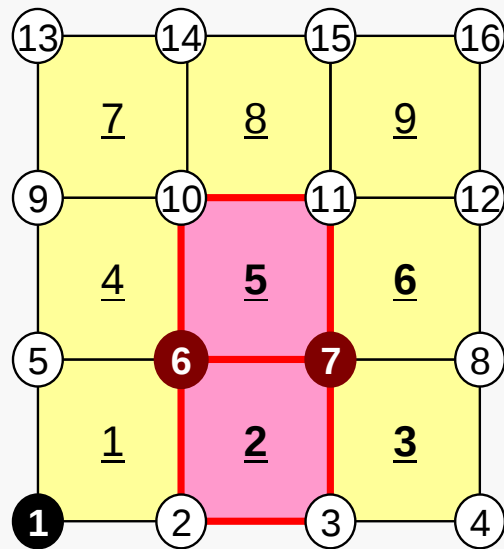
MAT_CON0: generates INU, IALU
MAT_CON1: generates index, item

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)

```

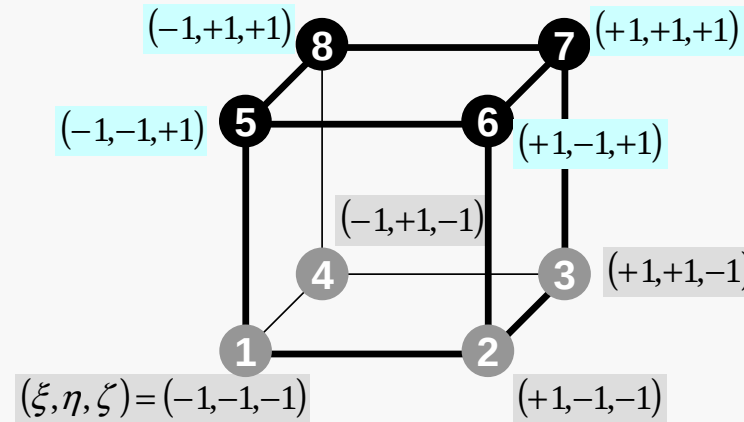
do icel= 1, ICELTOT
  in1= ICELNOD(icel, 1)
  in2= ICELNOD(icel, 2)
  in3= ICELNOD(icel, 3)
  in4= ICELNOD(icel, 4)
  in5= ICELNOD(icel, 5)
  in6= ICELNOD(icel, 6)
  in7= ICELNOD(icel, 7)
  in8= ICELNOD(icel, 8)

  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

```

!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

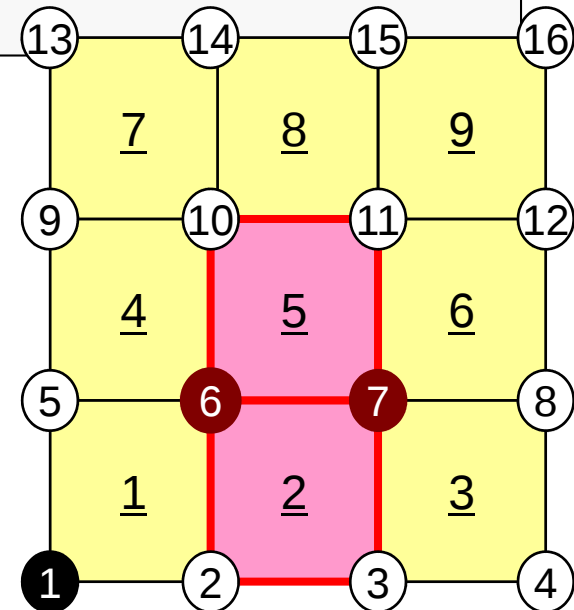
        icou= INLU(ip1) + 1
        IALU(ip1, icou)= ip2
        INLU(ip1      )= icou

        return

      end subroutine FIND_TS_NODE

```

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



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

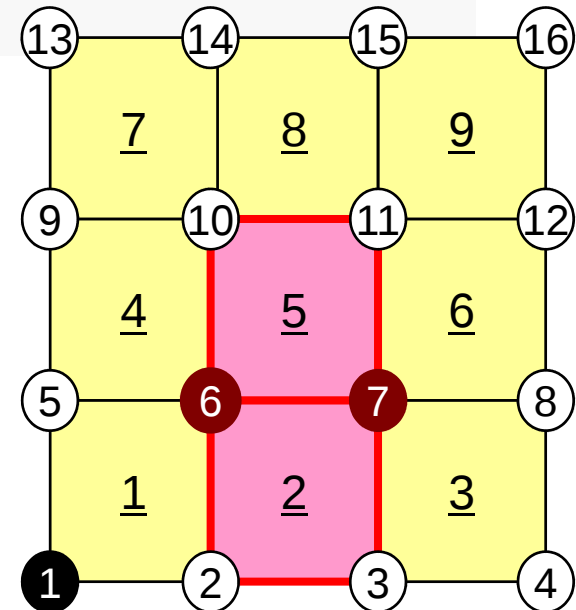
        icou= INLU(ip1) + 1
        IALU(ip1, icou)= ip2
        INLU(ip1) = icou

        return

      end subroutine FIND_TS_NODE

```

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



Generating Connectivity of Matrix MAT_CON0 (3/4)

```

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

```

```

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

```

```

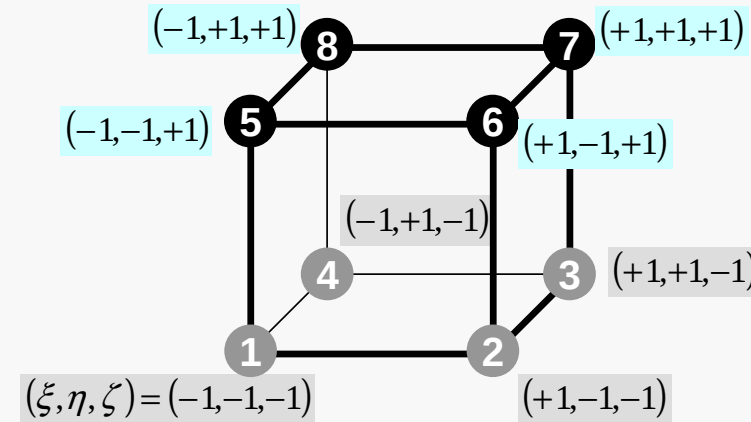
ca || FIND_TS_NODE (in6, in1)
ca || FIND_TS_NODE (in6, in2)
ca || FIND_TS_NODE (in6, in3)
ca || FIND_TS_NODE (in6, in4)
ca || FIND_TS_NODE (in6, in5)
ca || FIND_TS_NODE (in6, in7)
ca || FIND_TS_NODE (in6, in8)

```

```

ca || FIND_TS_NODE (in7, in1)
ca || FIND_TS_NODE (in7, in2)
ca || FIND_TS_NODE (in7, in3)
ca || FIND_TS_NODE (in7, in4)
ca || FIND_TS_NODE (in7, in5)
ca || FIND_TS_NODE (in7, in6)
ca || 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

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

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

FORTRAN

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

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

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  $\zeta$ -direction
  do jpn= 1, 2    Gaussian Quad. points in  $\eta$ -direction
    do ipn= 1, 2  Gaussian Quad. Points in  $\xi$ -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)

```

```

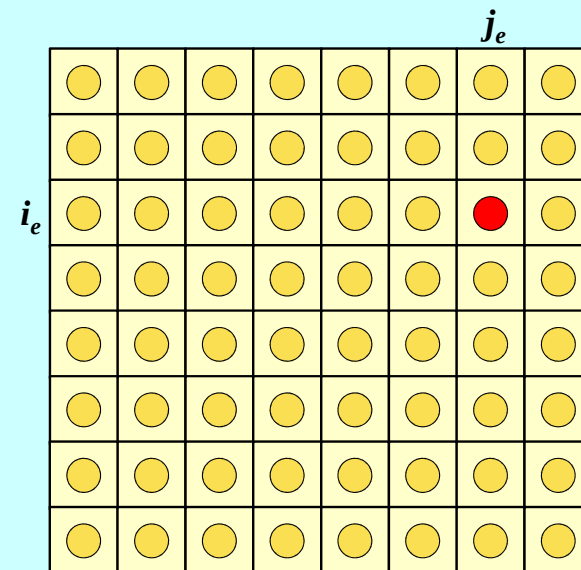
do ie= 1, 8          Local Node ID
  do je= 1, 8         Local Node ID
    Global Node ID: ip, jp
    Address of  $A_{ip, jp}$  in "item" : kk

```

```

    do kpn= 1, 2      Gaussian Quad. points in  $\zeta$ -direction
      do jpn= 1, 2    Gaussian Quad. points in  $\eta$ -direction
        do ipn= 1, 2  Gaussian Quad. points in  $\xi$ -direction
          integration on each element
          coefficients of element matrices
          accumulation to global matrix
        enddo
      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
      B= 0.d0
      X= 0.d0
      D= 0.d0

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

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

```

Non-Zero Off-Diagonal components (coef. matrix)
 RHS vector
 Unknowns
 Diagonal components (coef. matrix)

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))

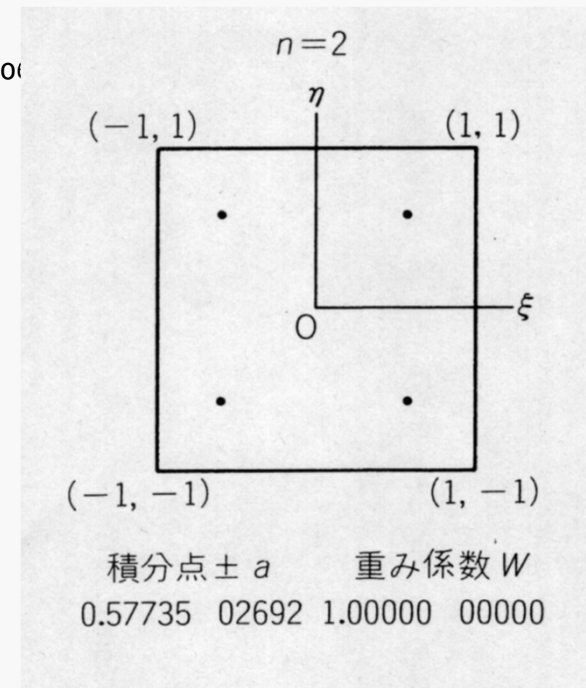
AMAT= 0. d0
B= 0. d0
X= 0. d0
D= 0. d0
```

Non-Zero Off-Diagonal components (coef. matrix)
 RHS vector
 Unknowns
 Diagonal components (coef. matrix)

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)= 08th * QM1 * EM1 * TM1
  SHAPE(ip, jp, kp, 2)= 08th * QP1 * EM1 * TM1
  SHAPE(ip, jp, kp, 3)= 08th * QP1 * EP1 * TM1
  SHAPE(ip, jp, kp, 4)= 08th * QM1 * EP1 * TM1
  SHAPE(ip, jp, kp, 5)= 08th * QM1 * EM1 * TP1
  SHAPE(ip, jp, kp, 6)= 08th * QP1 * EM1 * TP1
  SHAPE(ip, jp, kp, 7)= 08th * QP1 * EP1 * TP1
  SHAPE(ip, jp, kp, 8)= 08th * 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)= 08th * QM1 * EM1 * TM1
SHAPE(ip, jp, kp, 2)= 08th * QP1 * EM1 * TM1
SHAPE(ip, jp, kp, 3)= 08th * QP1 * EP1 * TM1
SHAPE(ip, jp, kp, 4)= 08th * QM1 * EP1 * TM1
SHAPE(ip, jp, kp, 5)= 08th * QM1 * EM1 * TP1
SHAPE(ip, jp, kp, 6)= 08th * QP1 * EM1 * TP1
SHAPE(ip, jp, kp, 7)= 08th * QP1 * EP1 * TP1
SHAPE(ip, jp, kp, 8)= 08th * QP1 * EP1 * TP1
```

$$\begin{aligned} QP1(i) &= (1 + \xi_i), & QM1(i) &= (1 - \xi_i) \\ EP1(j) &= (1 + \eta_j), & EM1(j) &= (1 - \eta_j) \\ TP1(k) &= (1 + \zeta_k), & TM1(k) &= (1 - \zeta_k) \end{aligned}$$

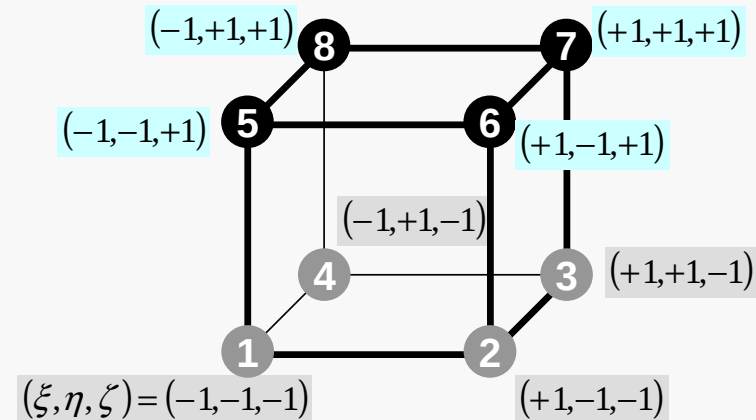
MAT_ASS_MAIN (2/6)

```
!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)= 08th * QM1 * EM1 * TM1
  SHAPE (ip, jp, kp, 2)= 08th * QP1 * EM1 * TM1
  SHAPE (ip, jp, kp, 3)= 08th * QP1 * EP1 * TM1
  SHAPE (ip, jp, kp, 4)= 08th * QM1 * EP1 * TM1
  SHAPE (ip, jp, kp, 5)= 08th * QM1 * EM1 * TP1
  SHAPE (ip, jp, kp, 6)= 08th * QP1 * EM1 * TP1
  SHAPE (ip, jp, kp, 7)= 08th * QP1 * EP1 * TP1
  SHAPE (ip, jp, kp, 8)= 08th * 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)= 08th * QM1 * EM1 * TM1
  SHAPE(ip, jp, kp, 2)= 08th * QP1 * EM1 * TM1
  SHAPE(ip, jp, kp, 3)= 08th * QP1 * EP1 * TM1
  SHAPE(ip, jp, kp, 4)= 08th * QM1 * EP1 * TM1
  SHAPE(ip, jp, kp, 5)= 08th * QM1 * EM1 * TP1
  SHAPE(ip, jp, kp, 6)= 08th * QP1 * EM1 * TP1
  SHAPE(ip, jp, kp, 7)= 08th * QP1 * EP1 * TP1
  SHAPE(ip, jp, kp, 8)= 08th * 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) = - 08th * EM1 * TM1
PNQ (jp, kp, 2) = + 08th * EM1 * TM1
PNQ (jp, kp, 3) = + 08th * EP1 * TM1
PNQ (jp, kp, 4) = - 08th * EP1 * TM1
PNQ (jp, kp, 5) = - 08th * EM1 * TP1
PNQ (jp, kp, 6) = + 08th * EM1 * TP1
PNQ (jp, kp, 7) = + 08th * EP1 * TP1
PNQ (jp, kp, 8) = - 08th * EP1 * TP1
PNE (ip, kp, 1) = - 08th * QM1 * TM1
PNE (ip, kp, 2) = - 08th * QP1 * TM1
PNE (ip, kp, 3) = + 08th * QP1 * TM1
PNE (ip, kp, 4) = + 08th * QM1 * TM1
PNE (ip, kp, 5) = - 08th * QM1 * TP1
PNE (ip, kp, 6) = - 08th * QP1 * TP1
PNE (ip, kp, 7) = + 08th * QP1 * TP1
PNE (ip, kp, 8) = + 08th * QM1 * TP1
PNT (ip, jp, 1) = - 08th * QM1 * EM1
PNT (ip, jp, 2) = - 08th * QP1 * EM1
PNT (ip, jp, 3) = - 08th * QP1 * EP1
PNT (ip, jp, 4) = - 08th * QM1 * EP1
PNT (ip, jp, 5) = + 08th * QM1 * EM1
PNT (ip, jp, 6) = + 08th * QP1 * EM1
PNT (ip, jp, 7) = + 08th * QP1 * EP1
PNT (ip, jp, 8) = + 08th * 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)

```

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

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

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

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

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

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

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

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

MAT_ASS_MAIN (3/6)

```

PNQ (jp, kp, 1) = - 08th * EM1 * TM1
PNQ (jp, kp, 2) = + 08th * EM1 * TM1
PNQ (jp, kp, 3) = + 08th * EP1 * TM1
PNQ (jp, kp, 4) = - 08th * EP1 * TM1
PNQ (jp, kp, 5) = - 08th * EM1 * TP1
PNQ (jp, kp, 6) = + 08th * EM1 * TP1
PNQ (jp, kp, 7) = + 08th * EP1 * TP1
PNQ (jp, kp, 8) = - 08th * EP1 * TP1
PNE (ip, kp, 1) = - 08th * QM1 * TM1
PNE (ip, kp, 2) = - 08th * QP1 * TM1
PNE (ip, kp, 3) = + 08th * QP1 * TM1
PNE (ip, kp, 4) = + 08th * QM1 * TM1
PNE (ip, kp, 5) = - 08th * QM1 * TP1
PNE (ip, kp, 6) = - 08th * QP1 * TP1
PNE (ip, kp, 7) = + 08th * QP1 * TP1
PNE (ip, kp, 8) = + 08th * QM1 * TP1
PNT (ip, jp, 1) = - 08th * QM1 * EM1
PNT (ip, jp, 2) = - 08th * QP1 * EM1
PNT (ip, jp, 3) = - 08th * QP1 * EP1
PNT (ip, jp, 4) = - 08th * QM1 * EP1
PNT (ip, jp, 5) = + 08th * QM1 * EM1
PNT (ip, jp, 6) = + 08th * QP1 * EM1
PNT (ip, jp, 7) = + 08th * QP1 * EP1
PNT (ip, jp, 8) = + 08th * QM1 * EP1

```

enddo
 enddo
 enddo

```

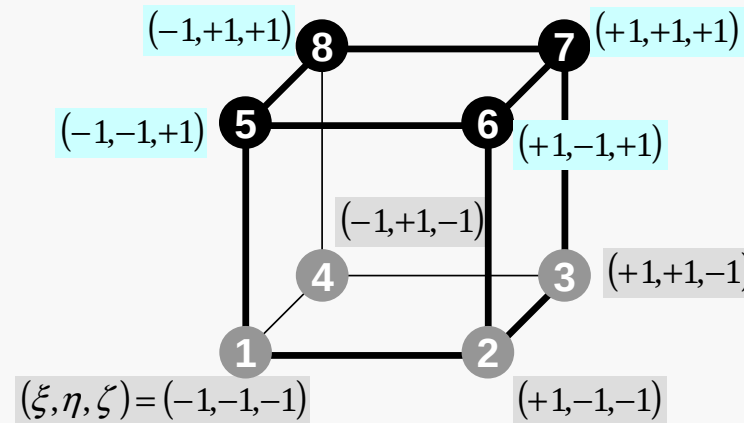
do icel= 1, ICELTOT
  CONDO= COND

```

```

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)

```



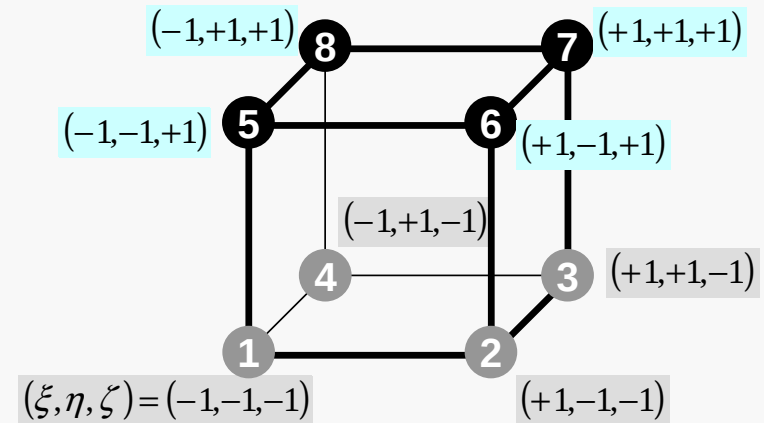
MAT_ASS_MAIN (4/6))

```

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

```

Node ID (Global)



```

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= 08th * (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 (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)

```

X-Coordinates
of 8 nodes

```

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)

```

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, 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)

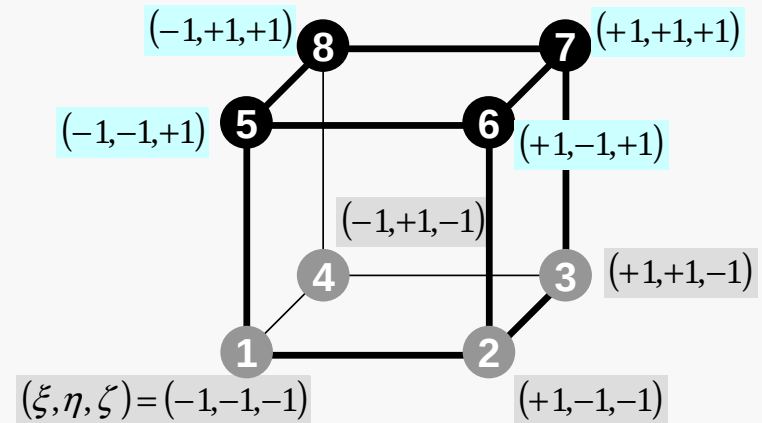
```

Z-Coordinates
of 8 nodes

```

&
&
&
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 (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)

```

X-Coordinates
of 8 nodes

```

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)

```

Y-Coordinates
of 8 nodes

```

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

```

```

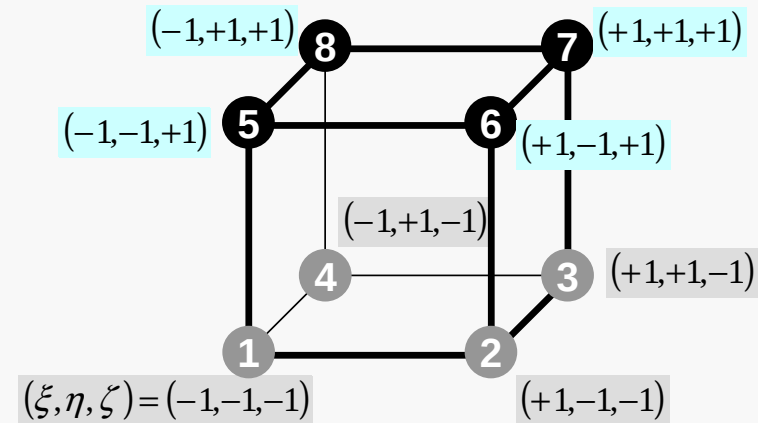
Z1= XYZ (in1, 3)
Z2= XYZ (in2, 3)
Z3= XYZ (in3, 3)
Z4= XYZ (in4, 3)
Z5= XYZ (in5, 3)
Z6= XYZ (in6, 3)
Z7= XYZ (in7, 3)
Z8= XYZ (in8, 3)

```

```

& call JACOBI (DETJ, PNQ, PNE, PNT, PNQ, 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 )

```



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

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

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

```

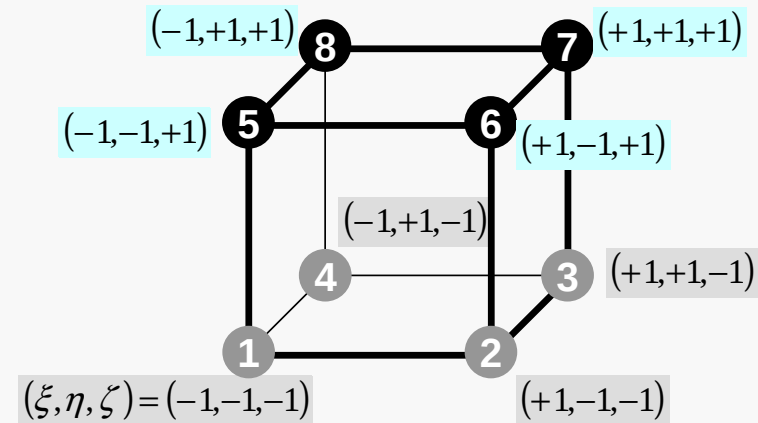
Z1= XYZ (in1, 3)
Z2= XYZ (in2, 3)
Z3= XYZ (in3, 3)
Z4= XYZ (in4, 3)
Z5= XYZ (in5, 3)
Z6= XYZ (in6, 3)
Z7= XYZ (in7, 3)
Z8= XYZ (in8, 3)

```

```

& 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 )

```



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

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

$$QVC = |x_c + y_c|$$

&
&
&

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= 08th * (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, PNQ, 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
endif
```

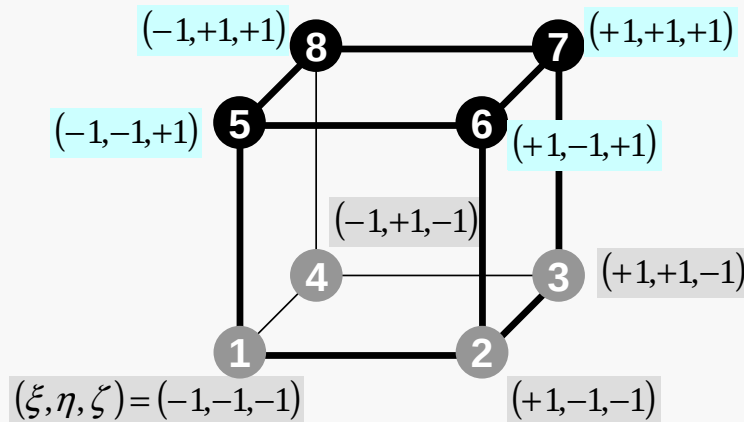
Non-Zero Off-Diagonal Block
in Global Matrix

$$A_{ip,jp}$$

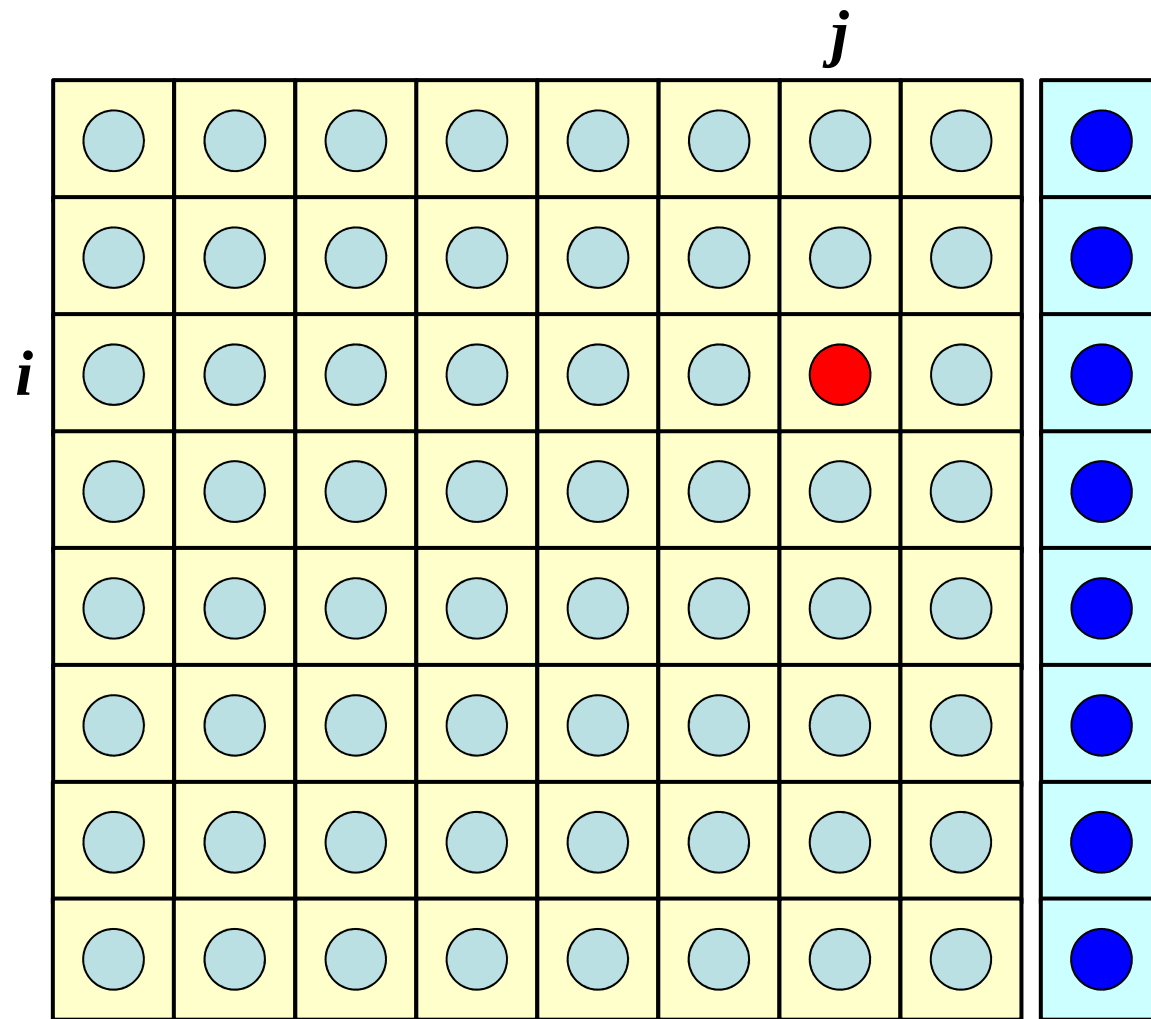
kk: address in “item”

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

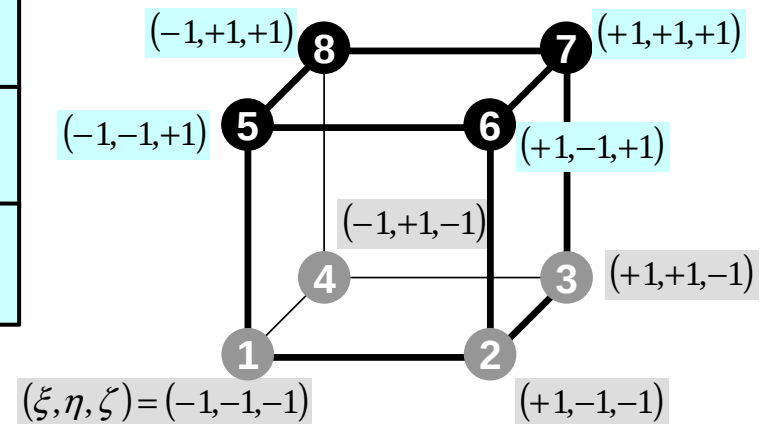
Node ID (ip,jp)
starting from 1



Element Matrix: 8x8



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



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)

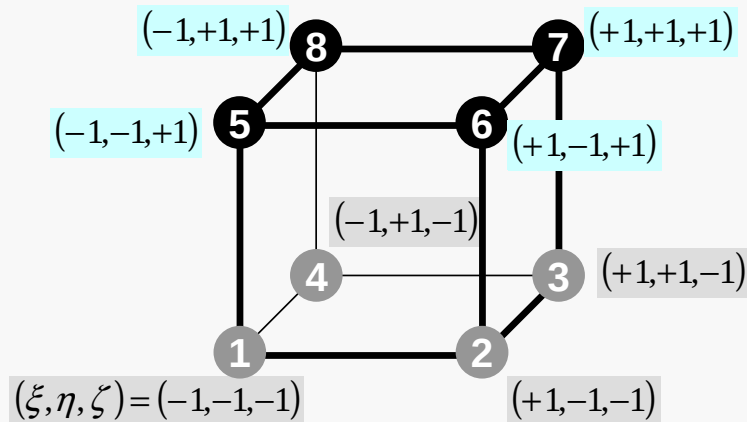
  kk= 0
  if (jp.ne.ip) then
    iiS= index(ip-1) + 1
    iiE= index(ip )
    do k= iiS, iiE
      if ( item(k).eq.jp ) then
        kk= k
        exit
      endif
    enddo
  endif
endif
```

Element Matrix ($i_e \sim j_e$): Local ID
Global Matrix ($i_p \sim j_p$): Global ID

kk: address in “item” starting from “1”

k: starting from “1”

ip,jp: starting from “1”



MAT_ASS_MAIN (6/6)

```

QV0 = 0. d0
COEFij= 0. d0
do kpn= 1, 2
do jpn= 1, 2
do ipn= 1, 2
  coef= dabs (DETJ (ipn, jpn, kpn)) *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)

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

```

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

MAT_ASS_MAIN (6/6)

```

QV0 = 0. d0
COEFij= 0. d0
do kpn= 1, 2
do jpn= 1, 2
do ipn= 1, 2
coef= dabs (DETJ (ipn, jpn, kpn)) *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)

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

```

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

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

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

MAT_ASS_MAIN (6/6)

```

QV0 = 0. d0
COEFij= 0. d0
do kpn= 1, 2
do jpn= 1, 2
do ipn= 1, 2
  coef= dabs(DETJ(ipn, jpn, kpn))*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)

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

```

$$\text{coef} = W_i \cdot W_j \cdot W_k \cdot \det|J(\xi_i, \eta_j, \zeta_k)|$$

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

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

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

MAT_ASS_MAIN (6/6)

```

QV0 = 0. d0
COEFij= 0. d0
do kpn= 1, 2
do jpn= 1, 2
do ipn= 1, 2
  coef= dabs (DETJ (ipn, jpn, kpn)) *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)

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

```

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

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

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

$$QVC = |x_C + y_C|$$

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

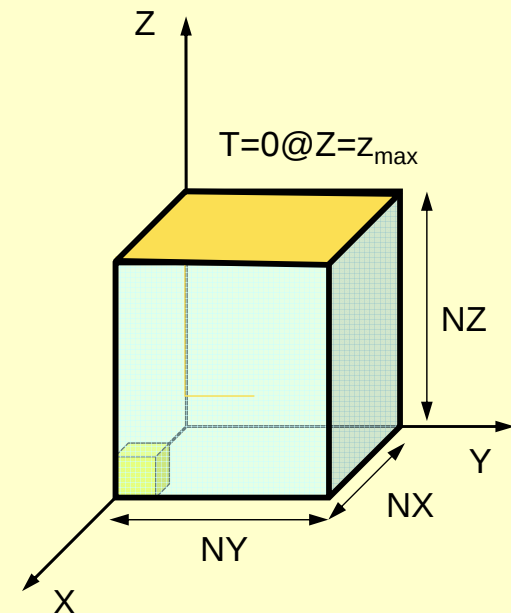
$$[f]^{(e)} = QV0 \cdot QVC$$

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 (IWXX(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 (IWXX(item(k),1).eq.1) then
      AMAT(k)= 0.d0
    endif
  enddo
enddo

!C==
return
end
```

MAT_ASS_BC (2/2)

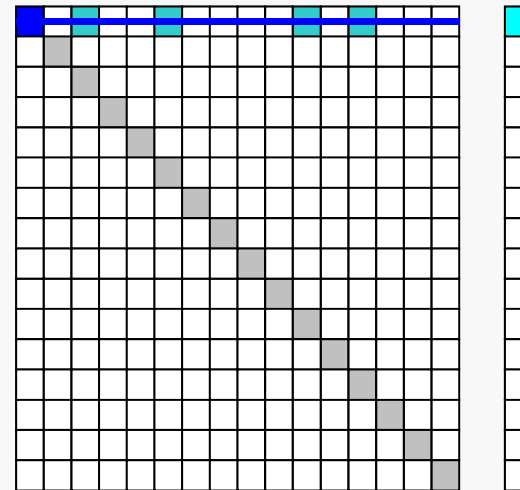
```
do in= 1, NP
  if (IWKX(in,1).eq.1) then
    B(in)= 0. d0
    D(in)= 1. d0
```

Boundary Nodes: IWKX(in,1)=1

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

Erase !!

```
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
```



Same as 1CPU case

境界条件 : MAT_ASS_BC (2/2)

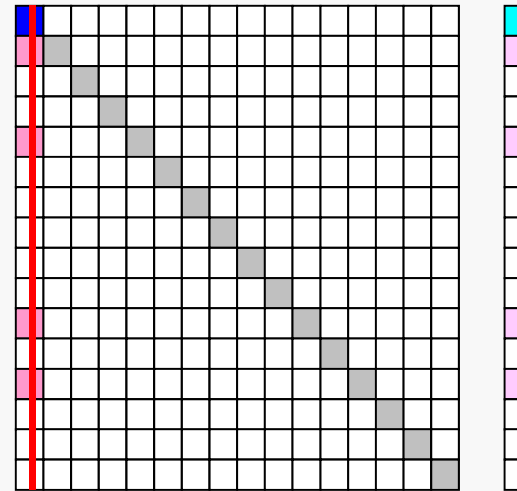
```
do in= 1, NP
  if (IWKX(in,1).eq.1) then
    B(in)= 0. d0
    D(in)= 1. d0
```

```
    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



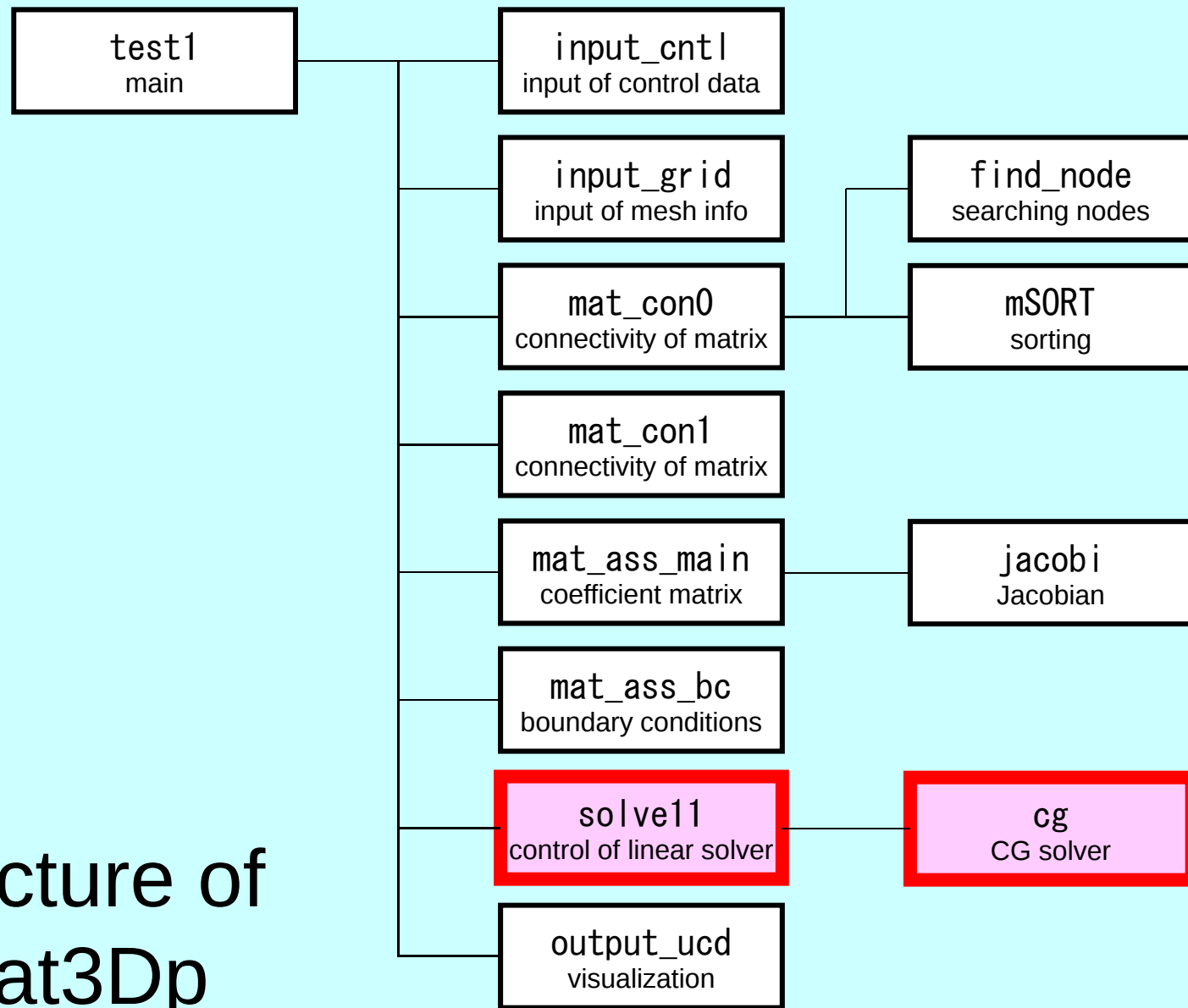
Elimination and Erase

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
```


Preconditioned CG Solver

Diagonal Scaling/Point Jacobi Preconditioning

```

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

```

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

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
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

```

Sending/Receiving Buffer

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 $i = 1, 2, \dots$

 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 +-----+
```

```
RH00= 0.d0
```

```
do i= 1, N
  RH00= RH00 + WW(i,R)*WW(i,Z)
enddo
```

```
call MPI_Allreduce (RH00, RHO, 1, MPI_DOUBLE_PRECISION,
& MPI_SUM, MPI_COMM_WORLD, ierr)
```

```
!C
!C +-----+
!C | {p} = {z} if      ITER=1
!C | BETA= RHO / RH01 otherwise
!C +-----+
```

```
if ( ITER.eq.1 ) then
```

```
do i= 1, N
  WW(i,P)= WW(i,Z)
enddo
```

```
else
```

```
BETA= RHO / RH01
```

```
do i= 1, N
  WW(i,P)= WW(i,Z) + BETA*WW(i,P)
enddo
```

```
endif
```

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

for $i = 1, 2, \dots$

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 +-----+
!C
!C call SOLVER_SEND_RECV
!C & ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,
!C & EXPORT_INDEX, EXPORT_ITEM, WS, WR, WW(1,P),
!C & my_rank)
!C
!C do j= 1, N
!C   WVAL= D(j)*WW(j,P)
!C   do k= index(j-1)+1, index(j)
!C     i= item(k)
!C     WVAL= WVAL + AMAT(k)*WW(i,P)
!C   enddo
!C   WW(j,Q)= WVAL
!C enddo
!C
!C +-----+
!C | ALPHA= RHO / {p} {q} |
!C +-----+
!C
!C C10= 0.d0
!C do i= 1, N
!C   C10= C10 + WW(i,P)*WW(i,Q)
!C enddo
!C call MPI_Allreduce (C10, C1, 1, MPI_DOUBLE_PRECISION,
!C & MPI_SUM, MPI_COMM_WORLD, ierr)
!C
!C ALPHA= RHO / C1

```

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

for $i = 1, 2, \dots$

 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)

```

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

      DNRM2= 0.d0
      do i= 1, N
        DNRM2= DNRM2 + WW(i, R)**2
      enddo
      call MPI_Allreduce (DNRM2, 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

!C==
      enddo

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 $i = 1, 2, \dots$

 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)

```

!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

      RH01 = 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)    &

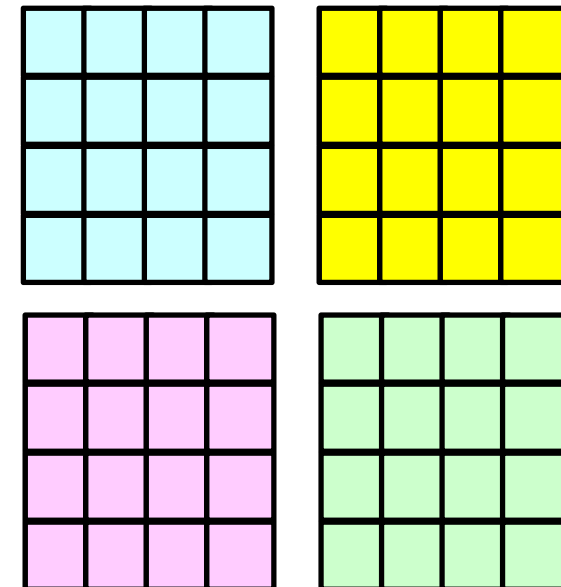
    deallocate (WW,WR,WS)

  end subroutine      CG
end module      solver_CG

```

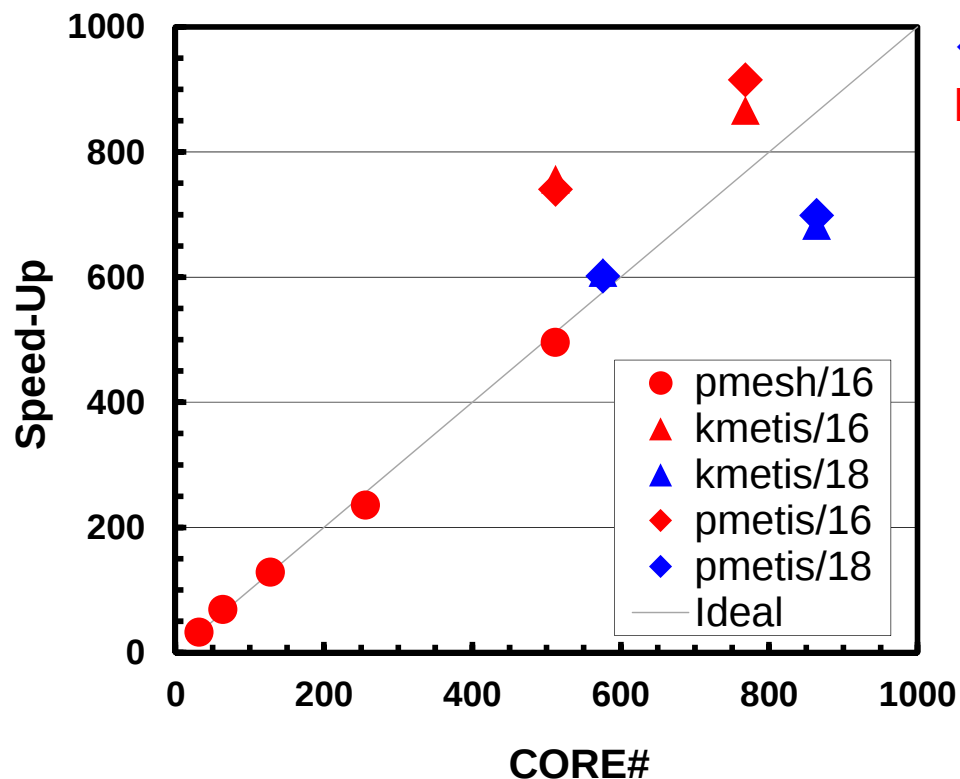
OUTPUT_UCD for Visualization

- 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



Example: Strong Scaling: Fortran

- $256 \times 128 \times 128$ nodes
 - 4,194,304 nodes, 4,112,895 elements
- 32~864 cores
- Linear Solver



- pmesh/16: pmesh 16 cores/socket
- ▲ kmetis/16: kmetis 16 cores/socket
- ▲ kmetis/18: kmetis 18 cores/socket
- ◆ pmetis/16: pmetis 16 cores/sockets
- ◆ pmetis/18: pmetis 18 cores/sockets

Performance of pmesh/16 w/32 cores= 32.0

```
256 128 128
  8  2  2
pcube
```

```
select=1:
mpiprocs=32
```

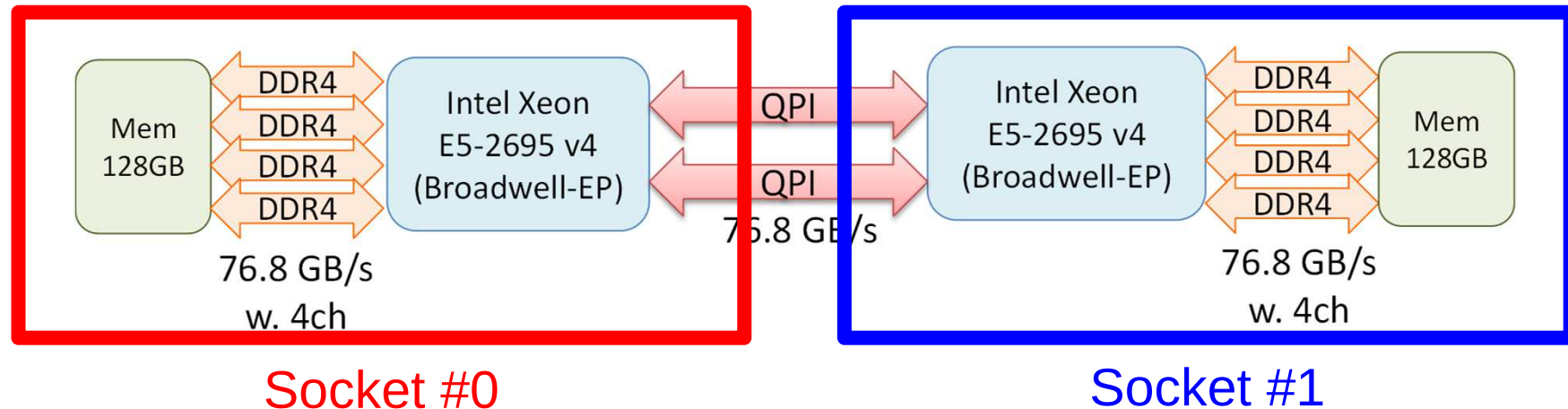
```
256 128 128
  8  4  2
pcube
```

```
select=2:
mpiprocs=32
```

```
256 128 128
 16  4  4
pcube
```

```
select=8:
mpiprocs=32
```

1 Node = 2 Sockets (CPU's)

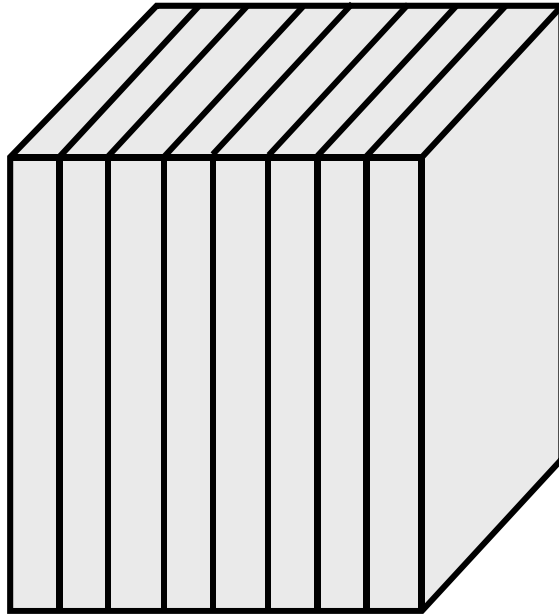


- Each Node of Reedbush-U
 - 2 Sockets (CPU's) of Intel Broadwell-EP
 - Each socket has 18 cores
- Each core of a socket can access to the memory on the other socket : NUMA (Non-Uniform Memory Access)
 - `I_MPI_PIN_DOMAIN=socket`, `impimap.sh`: local memory to be used

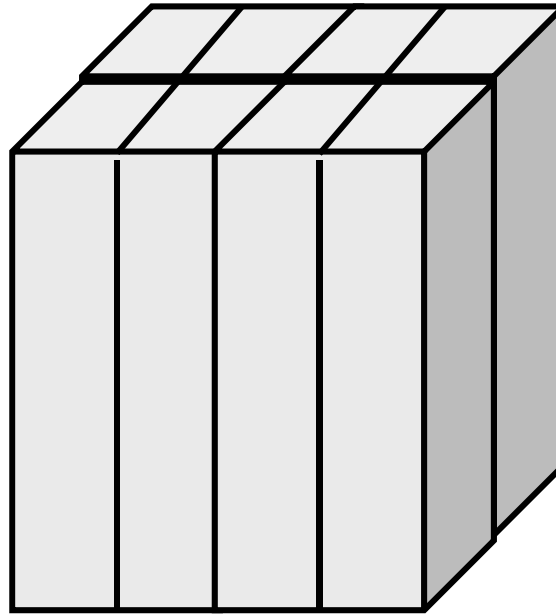
Exercise (1/2)

- 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

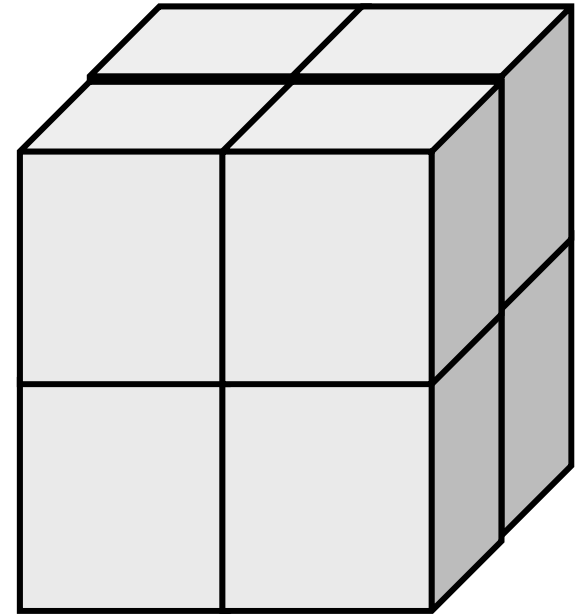
1D-3D Decomposition



1D



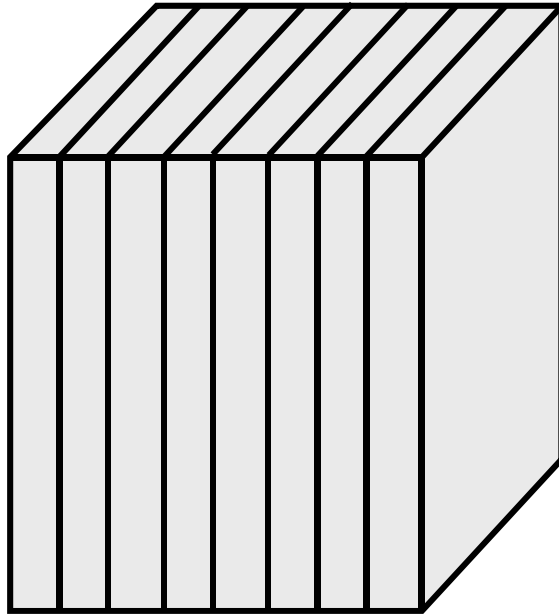
2D



3D

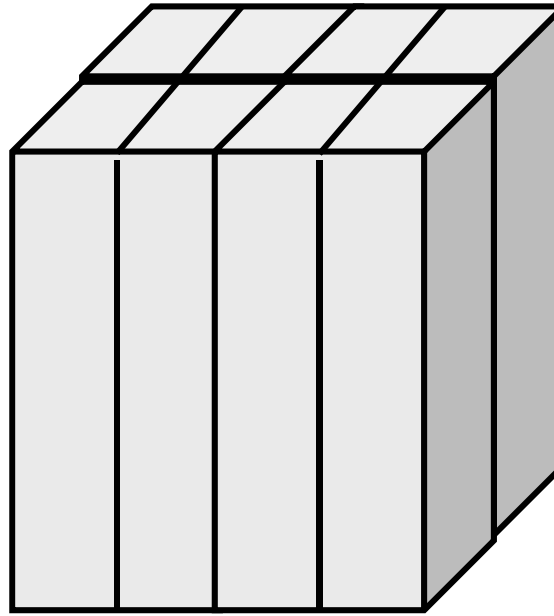
1D-3D Decomposition

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



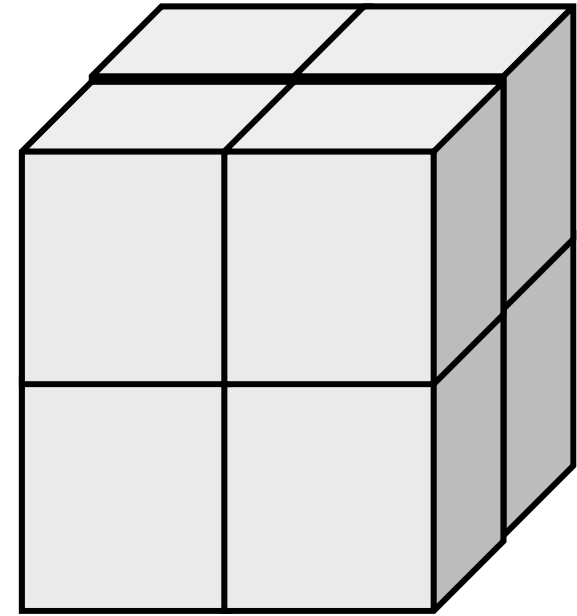
1D

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



2D

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

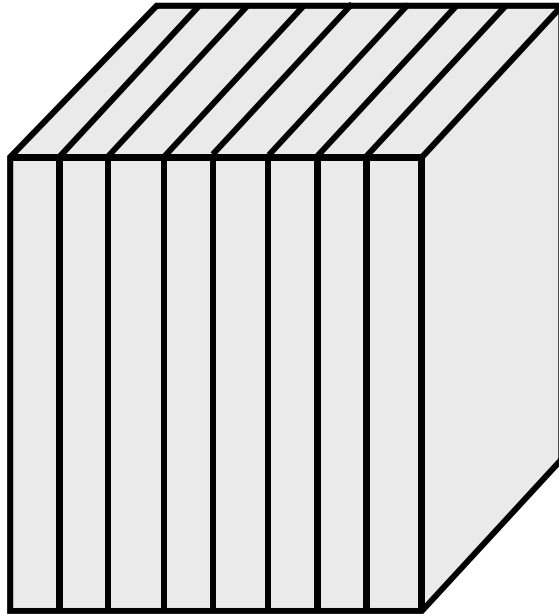


3D

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

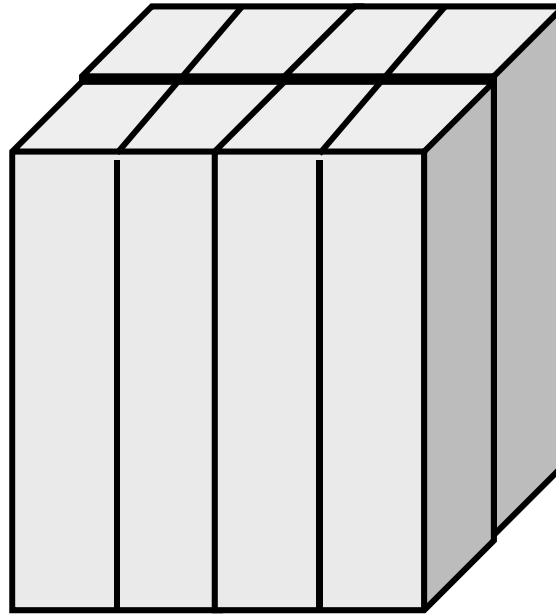
1D-3D Decomposition

mesh.inp



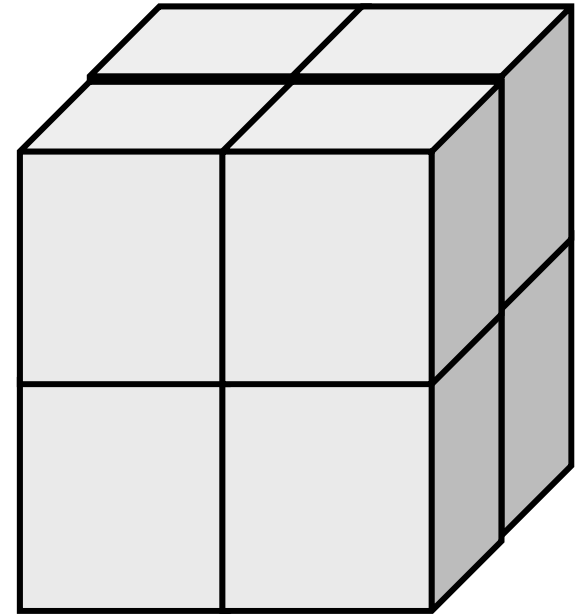
1D

```
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

```

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= STACK_EXPORT(neib-1)
        inum   = STACK_EXPORT(neib) - istart
        do k= istart+1, istart+inum
          WS(k)= X(NOD_EXPORT(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= STACK_IMPORT(neib-1)
        inum   = STACK_IMPORT(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= STACK_IMPORT(neib-1)
        inum   = STACK_IMPORT(neib) - istart
        do k= istart+1, istart+inum
          X(NOD_IMPORT(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= STACK_EXPORT(neib-1)
        inum   = STACK_EXPORT(neib) - istart
        do k= istart+1, istart+inum
          WS(k)= X(NOD_EXPORT(k))
        enddo
      enddo

      do neib= 1, NEIBPETOT
        istart= STACK_EXPORT(neib-1)
        inum   = STACK_EXPORT(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   = STACK_IMPORT(neib) - STACK_IMPORT(neib-1)
        istart= NOD_IMPORT(STACK_IMPORT(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

```

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

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

      do neib= 1, NEIBPETOT
        istart= STACK_EXPORT(neib-1)
        inum   = STACK_EXPORT(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   = STACK_IMPORT(neib) - STACK_IMPORT(neib-1)
        istart= STACK_IMPORT(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)

```

N0: 内点総数

Report P1

- Do Exercises (1/2) and (2/2)
- Deadline: 17:00 October 22nd (Sun), 2017.
 - Send files via e-mail at **nakajima (at) cc.u-tokyo.ac.jp**
- Report
 - Cover Page: Name, ID, and Problem ID (P1) must be written.
 - Less than ten pages including figures and tables (A4).
 - Strategy
 - Structure of the Program
 - Numerical Experiments, Performance Analysis
 - Remarks
 - Output list (as small as possible)