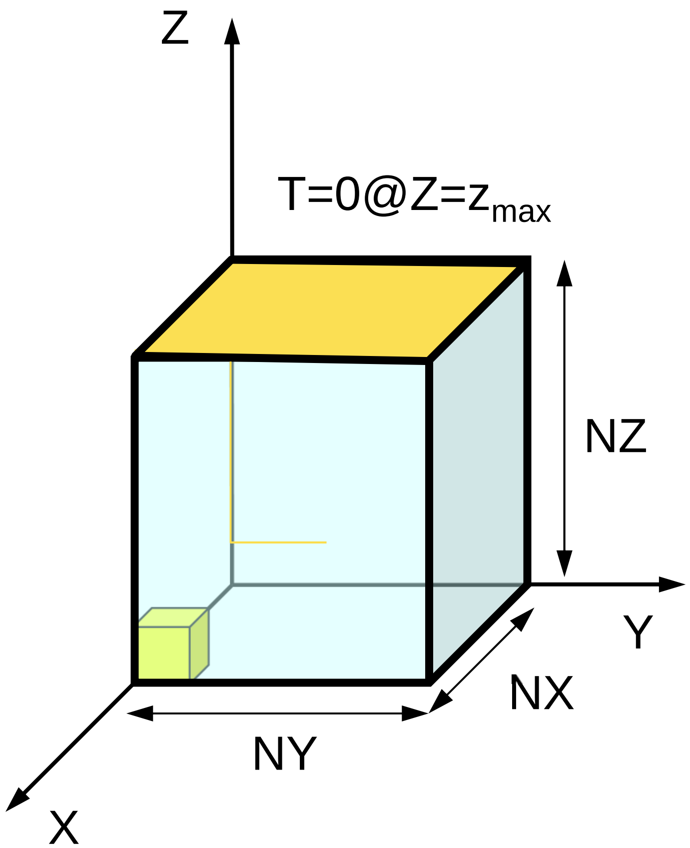
3D Parallel FEM (II)
Fortran

Kengo Nakajima
Information Technology Center
The University of Tokyo

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

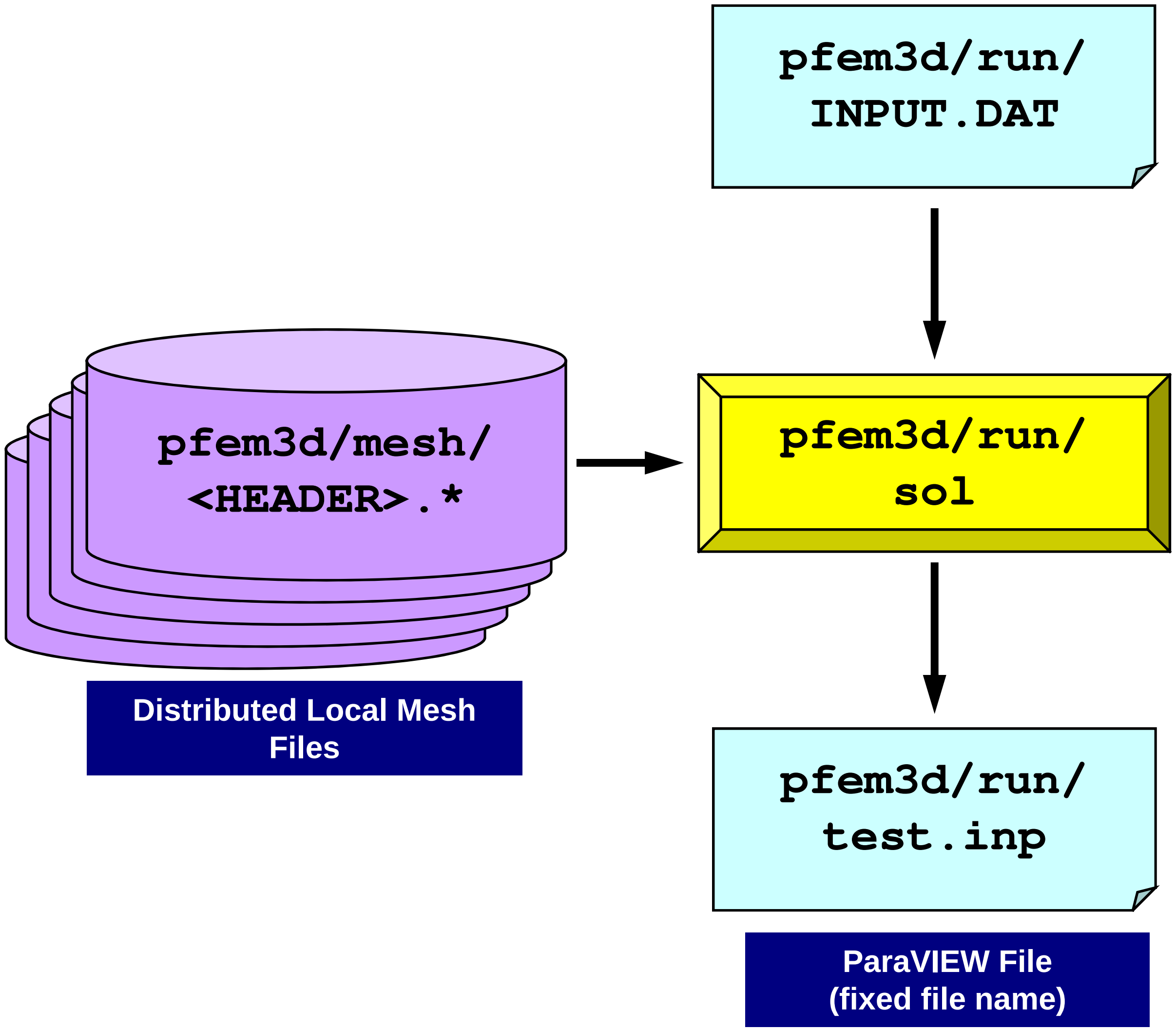
Finite-Element Procedures

- 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

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

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

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

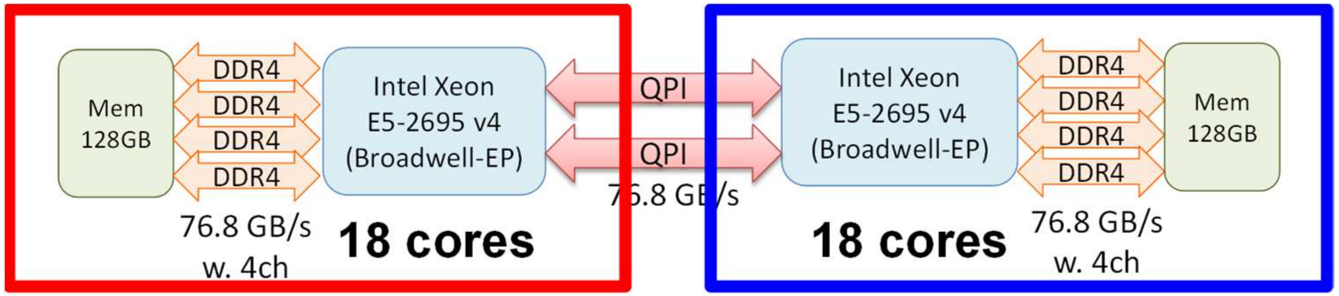
more stable with “export I_MPI_PERHOST=32”

```
#!/bin/sh
#PBS -q u-lecture8                   Name of "QUEUE"
#PBS -N flat                         Job Name
#PBS -l select=4:mpiprocs=32         node#, proc#/node
#PBS -Wgroup_list=gt18               Group Name (Wallet)
#PBS -l walltime=00:05:00            Computation Time
#PBS -e err                          Standard Error
#PBS -o test.lst                     Standard Outpt

cd $PBS_O_WORKDIR                    go to current dir
. /etc/profile.d/modules.sh          (ESSENTIAL)

export I_MPI_PIN_DOMAIN=socket       Execution on each socket
export I_MPI_PERHOST=32              MPI proc#/node (=mpiprocs)
mpirun ./impimap.sh ./sol            Exec's
```

```
#PBS -l select=1:mpiprocs=4      1-node, 4-core's
#PBS -l select=1:mpiprocs=16     1-node, 16-core's
#PBS -l select=1:mpiprocs=36     1-node, 36-core's
#PBS -l select=2:mpiprocs=32     2-nodes, 32x2=64-core's
#PBS -l select=4:mpiprocs=32     4-nodes, 32x4=128-core's
#PBS -l select=8:mpiprocs=36     8-nodes, 36x8=288-core's
```

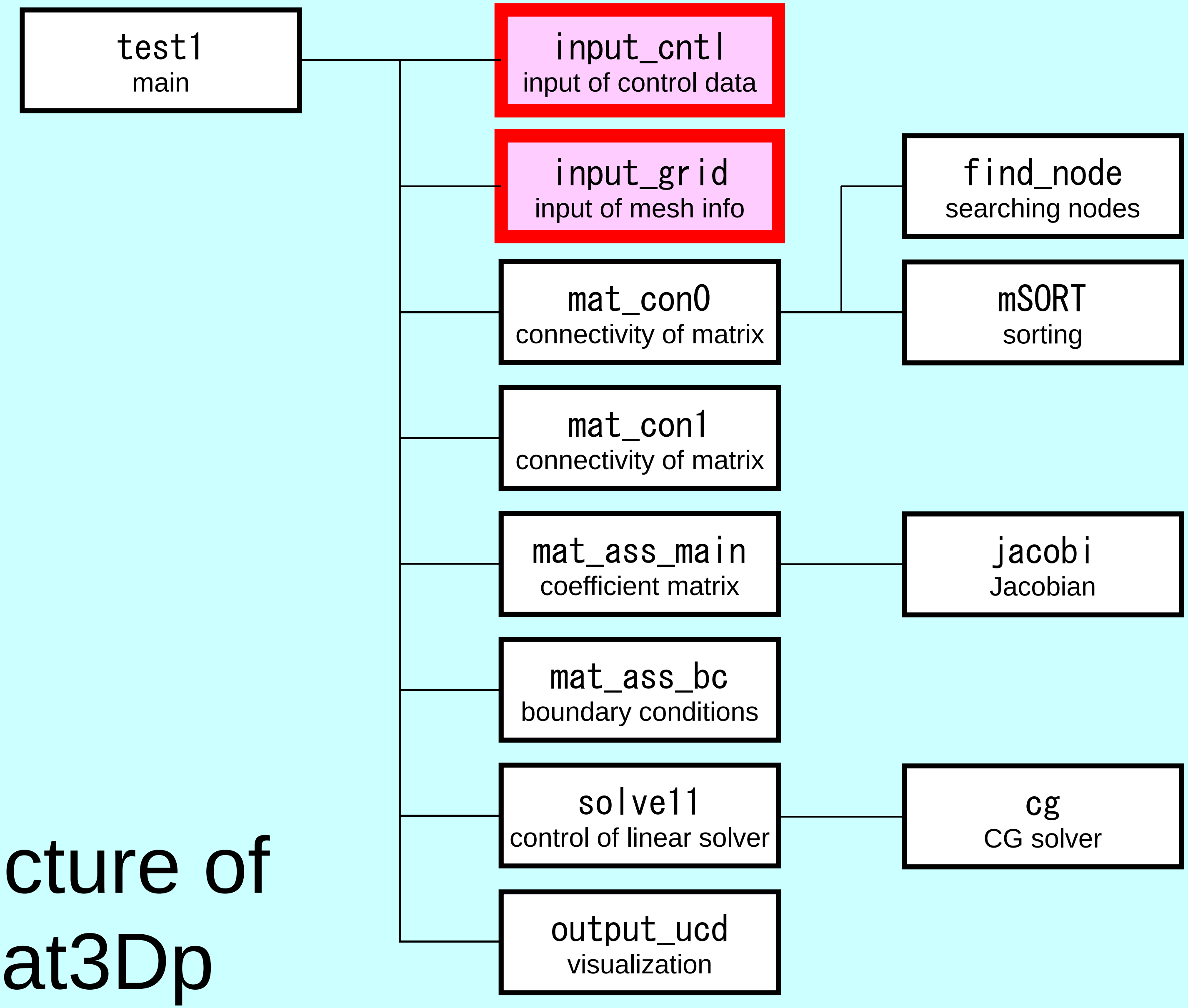
<$O-TOP>/pfem3d/run/a32.sh

```
#!/bin/sh
#PBS -q u-lecture8                   Name of "QUEUE"
#PBS -N flat                         Job Name
#PBS -l select=4:mpiprocs=32         node#, proc#/node
#PBS -Wgroup_list=gt18               Group Name (Wallet)
#PBS -l walltime=00:05:00            Computation Time
#PBS -e err                          Standard Error
#PBS -o test.lst                     Standard Outpt

cd $PBS_O_WORKDIR                    go to current dir
. /etc/profile.d/modules.sh          (ESSENTIAL)

export I_MPI_PIN_PROCESSOR_LIST=0-15,18-33
mpirun ./impimap.sh ./sol            Exec's
```



Socket #0
0^{th}-17^{th} cores

Socket #1
18^{th}-35^{th} cores



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)

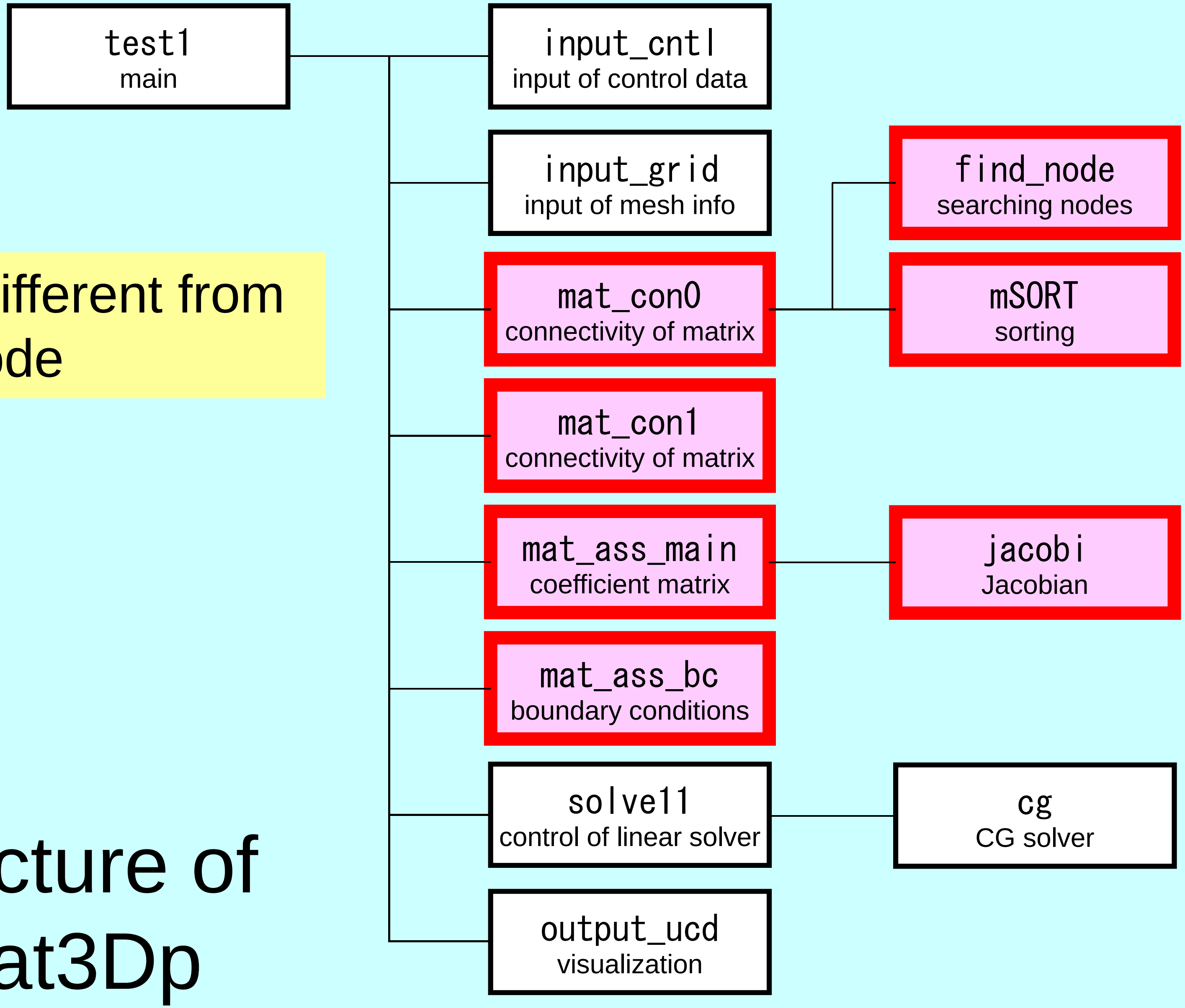
```
!C-- COMMUNICATION table
      allocate (IMPORT_INDEX(0:NEIBPETOT))
      allocate (EXPORT_INDEX(0:NEIBPETOT))

      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

NOT so different from 1-CPU code

Structure of heat3Dp



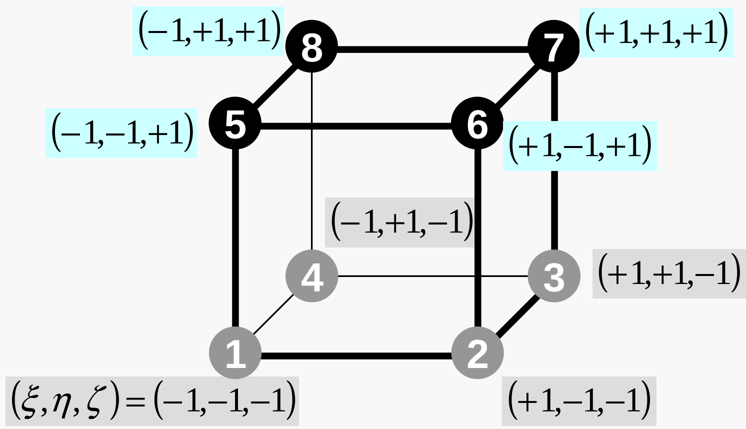
Main Part

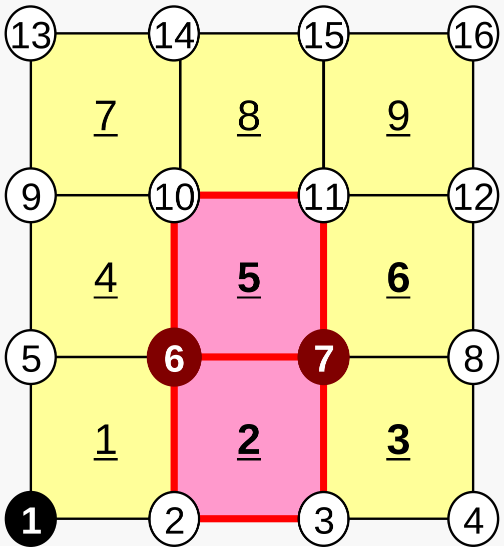
```
program heat3Dp

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

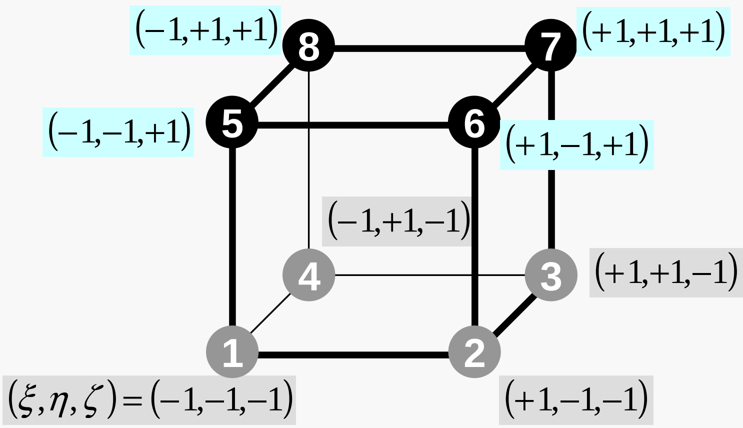
Generating Connectivity of Matrix MAT_CON0 (1/4)

```
!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
```

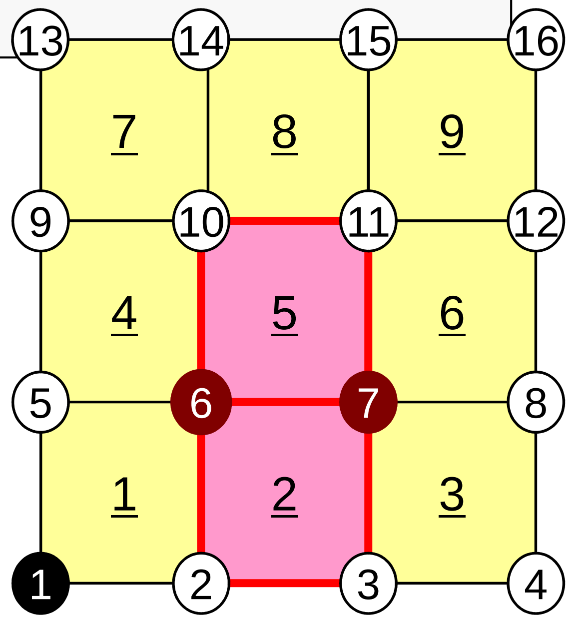
Array	Size	Description
INLU	(NP)	Number of connected nodes to each node (lower/upper)
IALU	(NP, NLU)	Corresponding connected node ID (column ID)

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

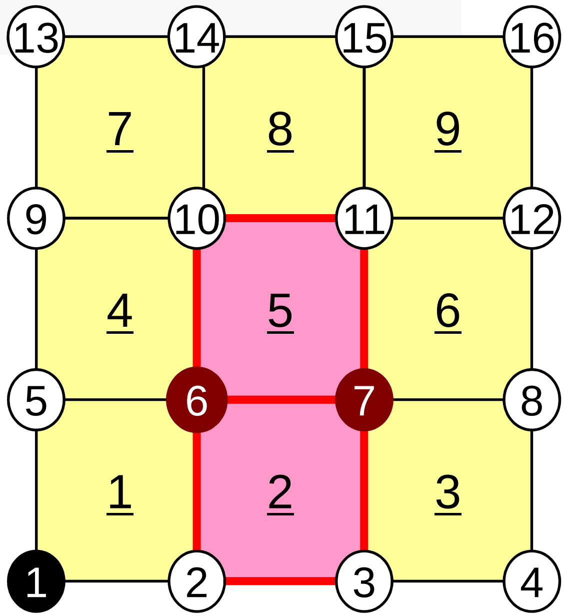


FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search

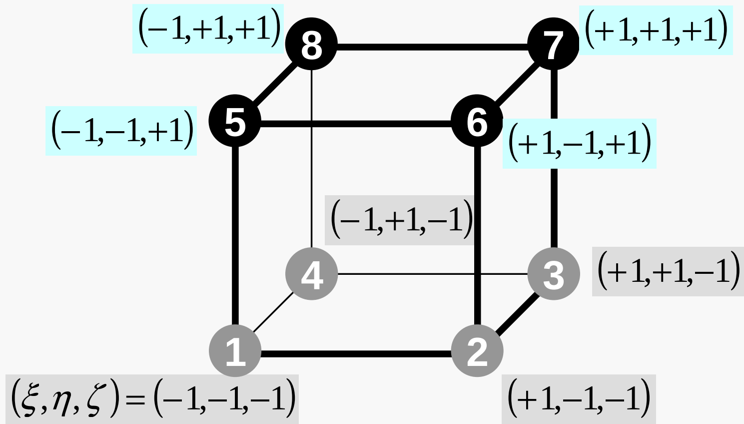
```
!C
!C***
!C*** FIND_TS_NODE
!C***
!C
       subroutine FIND_TS_NODE (ip1, ip2)

         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)

```
      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

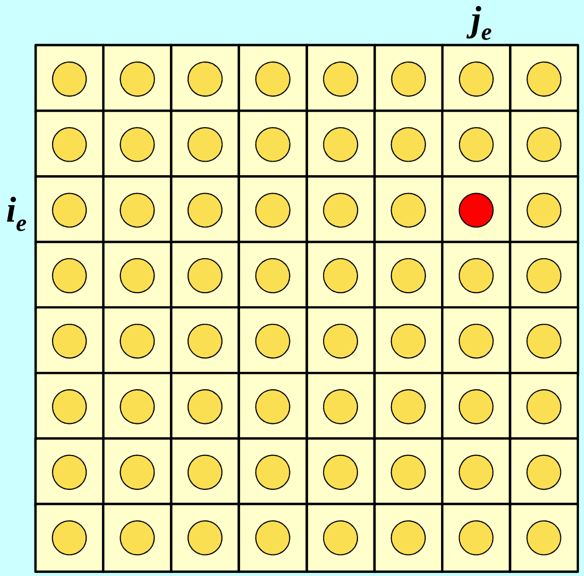
Main Part

```
      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
```



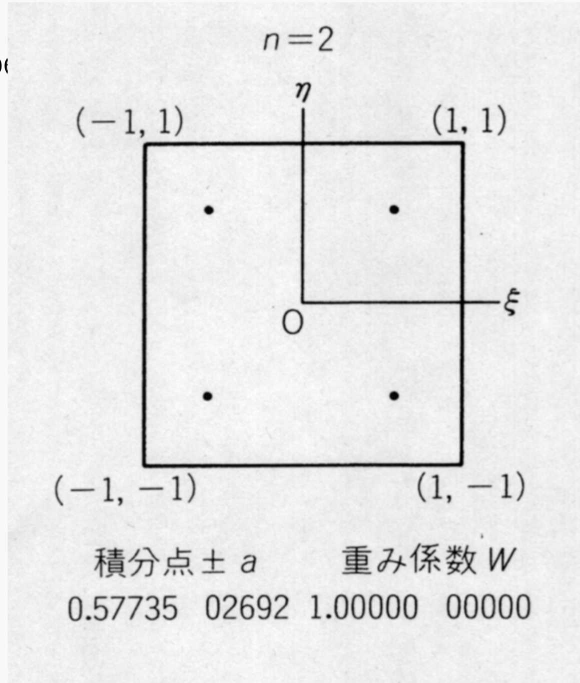
MAT_ASS_MAIN (1/6)

```
!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 * QP1 * EP1 * TP1
```

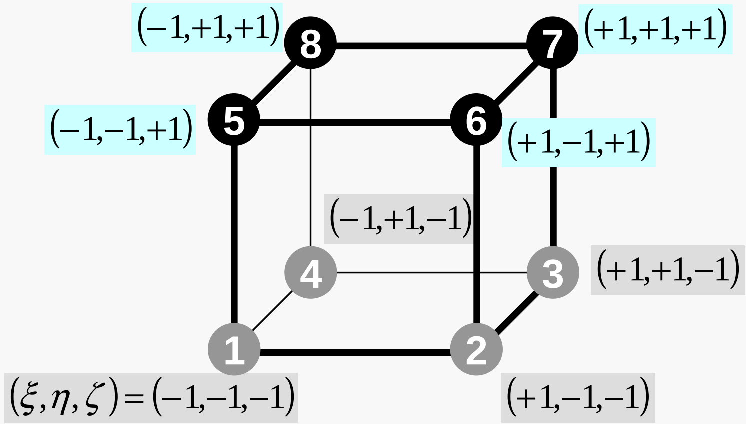
$$\mathrm{QP1}(\mathrm{i}) = (1+\xi_i), \quad \mathrm{QM1}(\mathrm{i}) = (1-\xi_i)$$

$$\mathrm{EP1}(\mathrm{j}) = (1+\eta_j), \quad \mathrm{EM1}(\mathrm{j}) = (1-\eta_i)$$

$$\mathrm{TP1}(\mathrm{k}) = (1+\zeta_k), \quad \mathrm{TM1}(\mathrm{k}) = (1-\zeta_k)$$

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 * QM1 * 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
```

$$N_1(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1-\eta)(1-\zeta)$$
$$N_2(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1-\eta)(1-\zeta)$$
$$N_3(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1+\eta)(1-\zeta)$$
$$N_4(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1+\eta)(1-\zeta)$$

$$N_5(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1-\eta)(1+\zeta)$$
$$N_6(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1-\eta)(1+\zeta)$$
$$N_7(\xi,\eta,\zeta)=\frac{1}{8}(1+\xi)(1+\eta)(1+\zeta)$$
$$N_8(\xi,\eta,\zeta)=\frac{1}{8}(1-\xi)(1+\eta)(1+\zeta)$$

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)
```

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

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

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

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

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

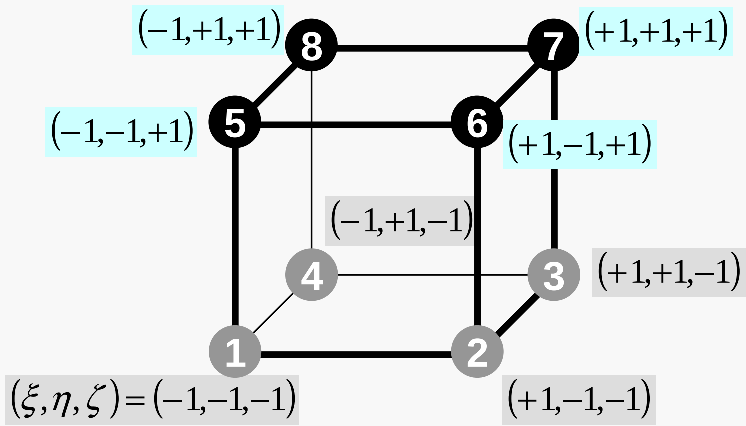
$$\frac{\partial N_3}{\partial \xi}(\xi_i, \eta_j, \zeta_k) = +\frac{1}{8}(1+\eta_j)(1-\zeta_k)$$

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

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

MAT_ASS_MAIN (3/6)

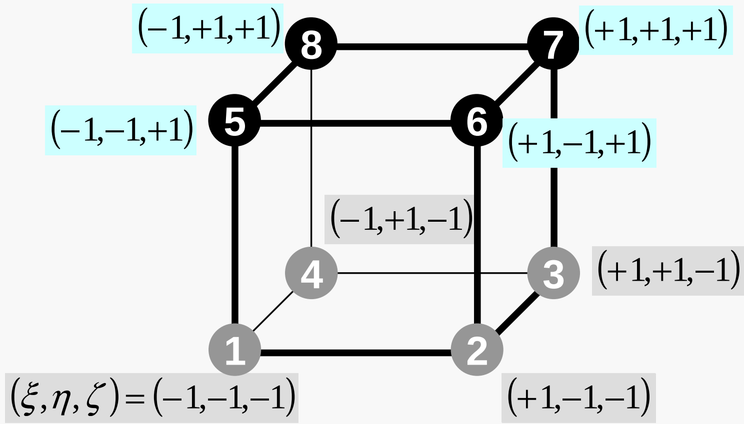
```
      PNQ(jp,kp,1)= - O8th * EM1 * TM1
      PNQ(jp,kp,2)= + O8th * EM1 * TM1
      PNQ(jp,kp,3)= + O8th * EP1 * TM1
      PNQ(jp,kp,4)= - O8th * EP1 * TM1
      PNQ(jp,kp,5)= - O8th * EM1 * TP1
      PNQ(jp,kp,6)= + O8th * EM1 * TP1
      PNQ(jp,kp,7)= + O8th * EP1 * TP1
      PNQ(jp,kp,8)= - O8th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



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)



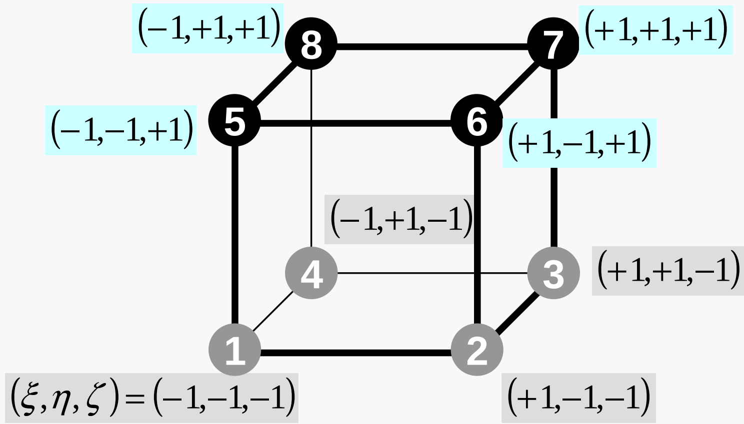
MAT_ASS_MAIN (4/6)

```
      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

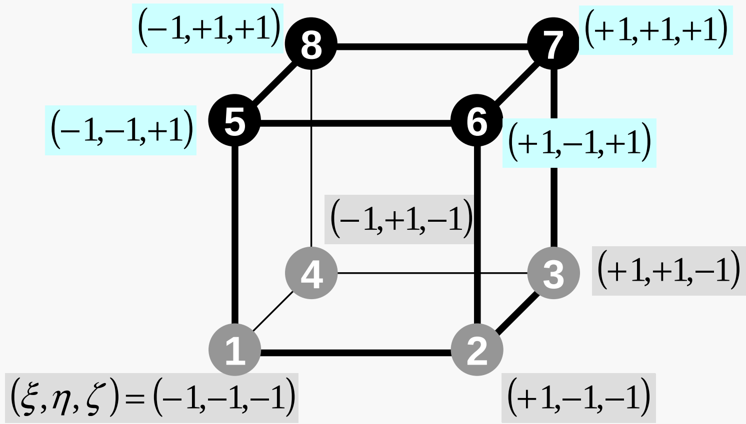


MAT_ASS_MAIN (4/6)

```
      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



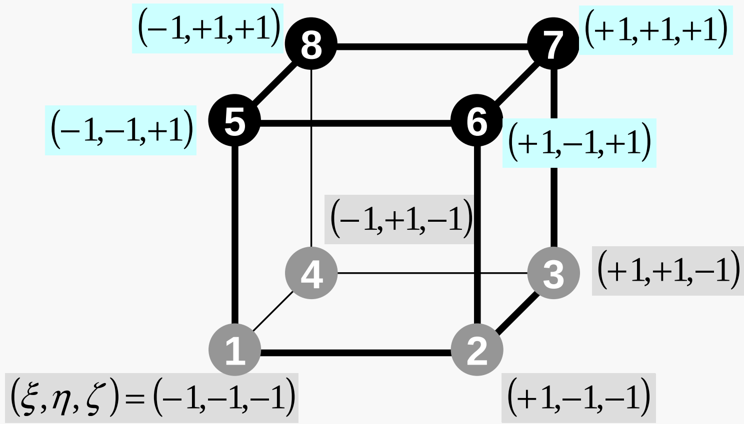
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\dot{Q}(x,y,z)=0$$

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

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 )
```



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

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

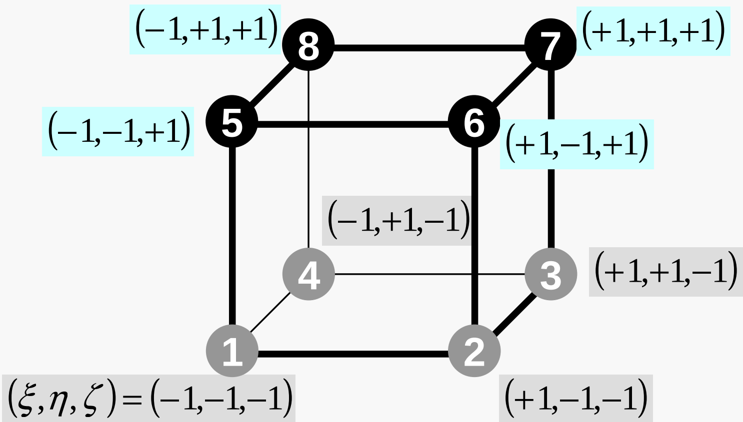
$$QVC=|x_C+y_C|$$

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= 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

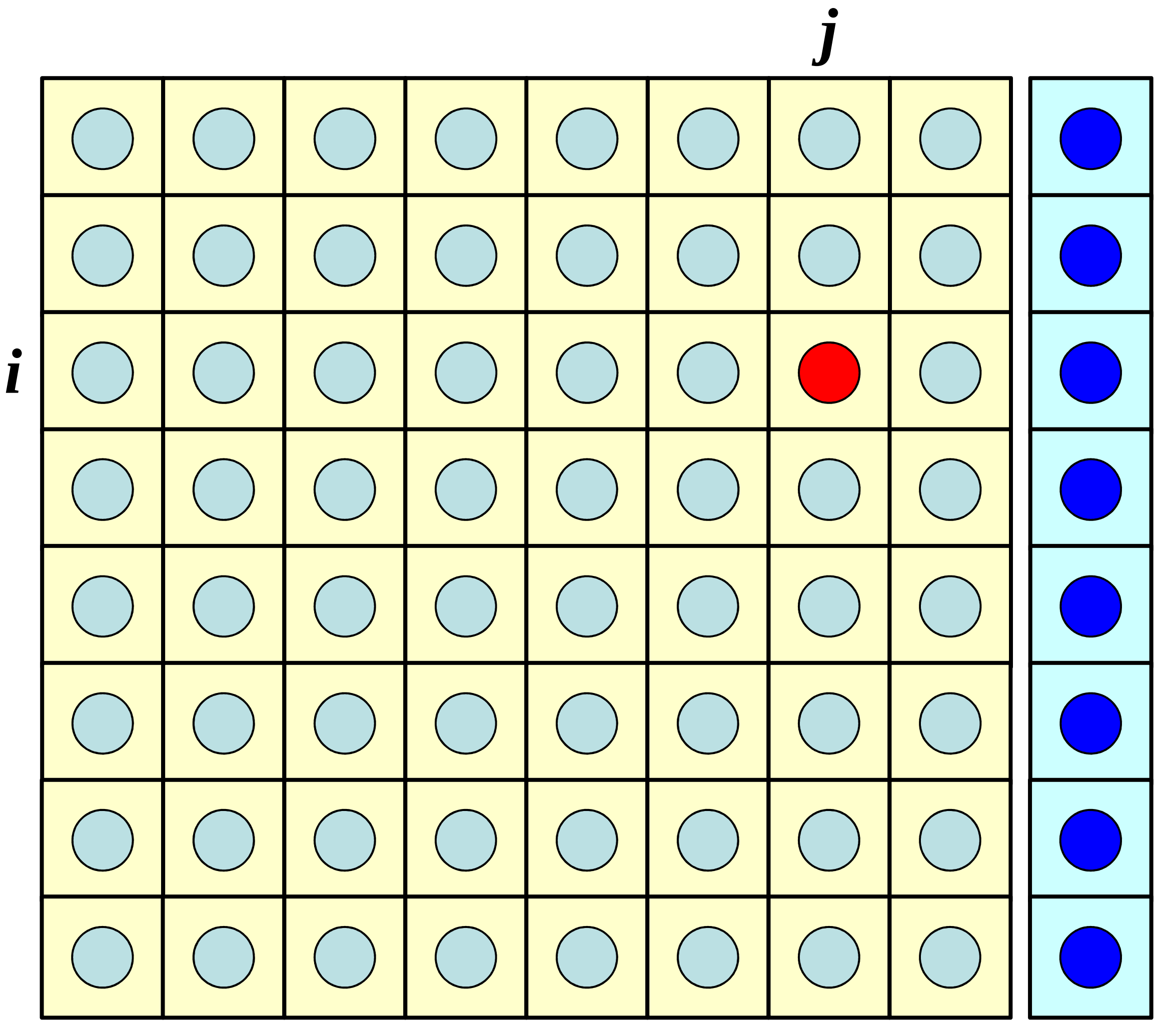
$$A_{ip,jp}$$

kk: address in “item”

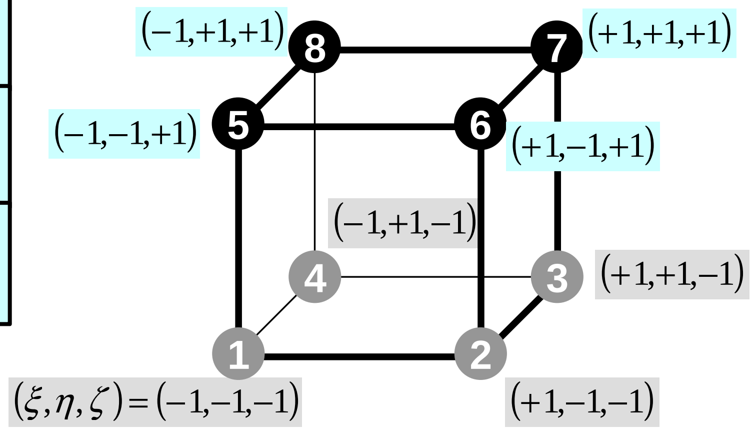
ip= nodLOCAL(ie)
jp= nodLOCAL(je)

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)

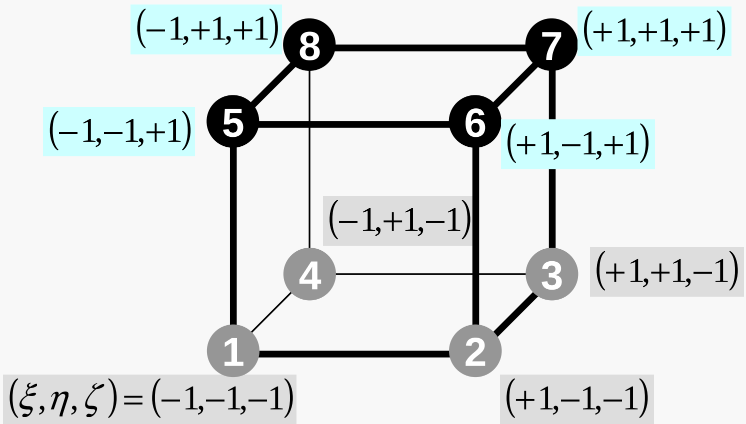
```
!C
!C== CONSTRUCT the GLOBAL MATRIX

        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 $(i_e \sim j_e)$: 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)

```
        QVO   = 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)
          QVO= QVO + SHi * QVOL * coef
        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= 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 * COND0 *
     &                   (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)

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

```
        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 * COND0 *
     &                     (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
```

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

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

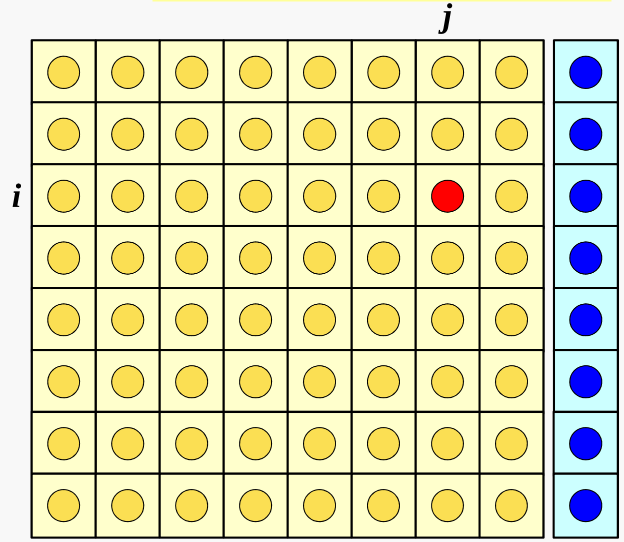
$$= \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N}\left[W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)\right]$$

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

MAT_ASS_MAIN (6/6)

```
QVO   = 0.d0
          COEFij= 0.d0
          do kpn= 1, 2
          do jpn= 1, 2
          do ipn= 1, 2
            coef= 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 * COND0 *
    &                       (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)

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

```
      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 * COND0 *
     &                  (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
```

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

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

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

$$QVC = |x_C + y_C|$$

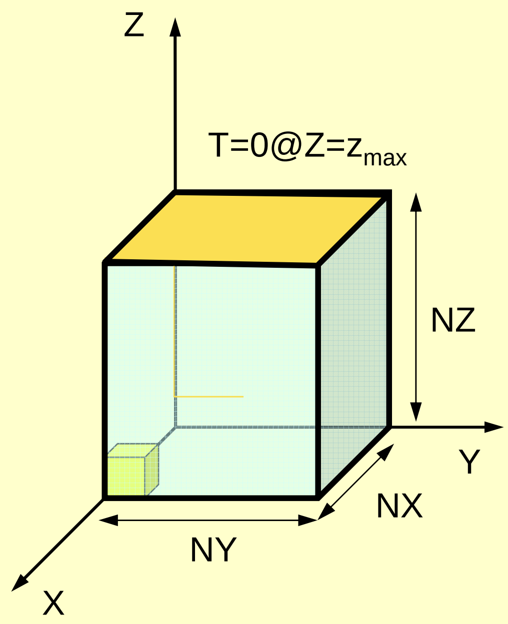
$$QV0 = \int_V QVOL[N]^T dV$$

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

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)

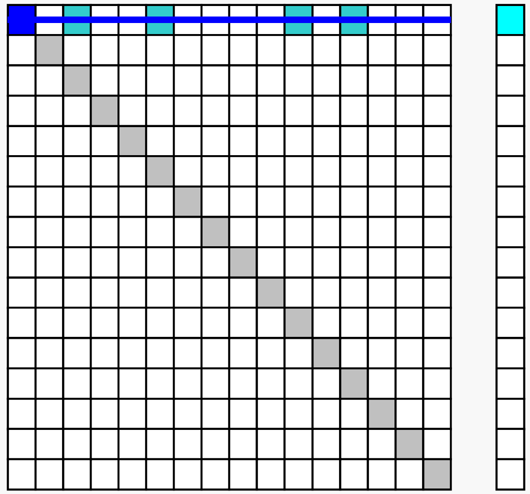
```
      do in= 1, NP
        if (IWKX(in,1).eq.1) then
          B(in)= 0.d0
          D(in)= 1.d0

          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 !!

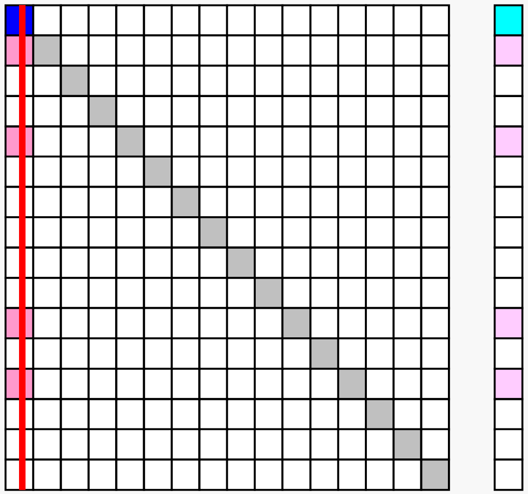


Same as 1CPU case

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

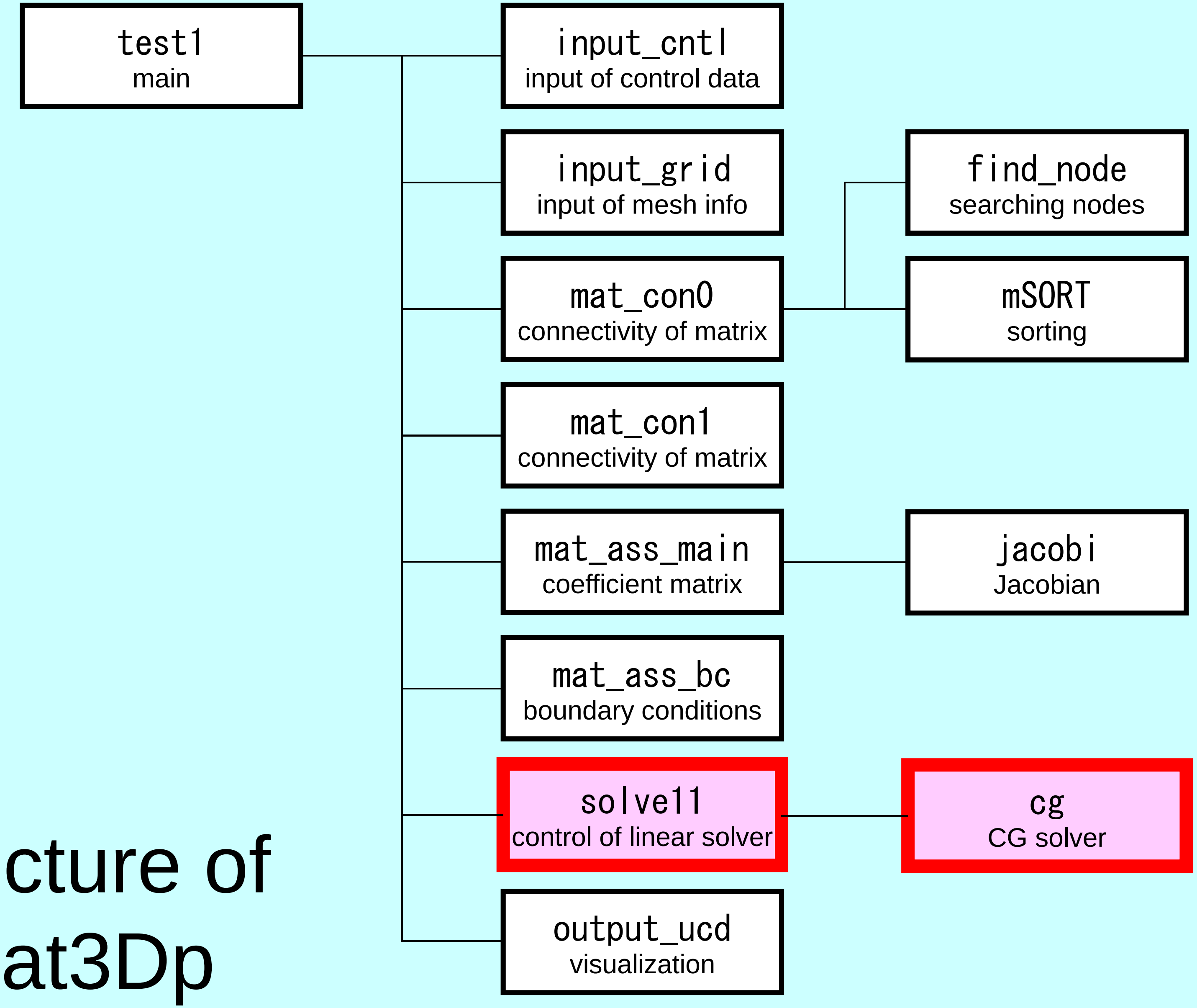


Elimination and Erase

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
```

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

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
```

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, …

 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 +----------------------+
      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
- $q^{(i)}= [A]p^{(i)}$
- $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
- $\mathbf{x}^{(i)}= \mathbf{x}^{(i-1)} + \alpha_i \mathbf{p}^{(i)}$
- $\mathbf{r}^{(i)}= \mathbf{r}^{(i-1)} - \alpha_i \mathbf{q}^{(i)}$
- **check convergence** $|r|$

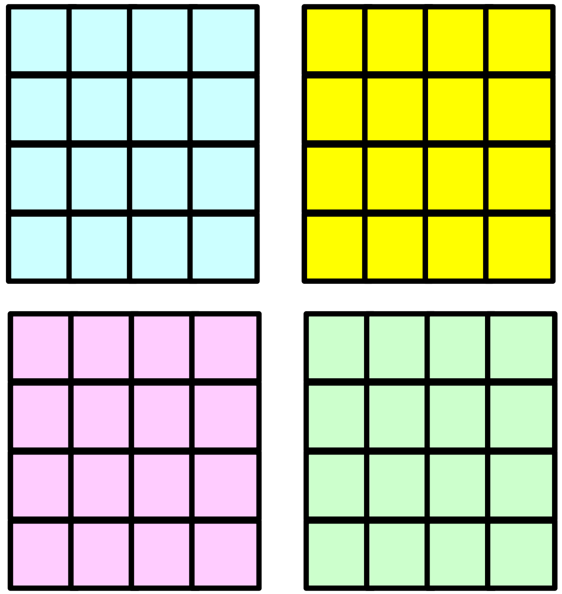
end

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
```

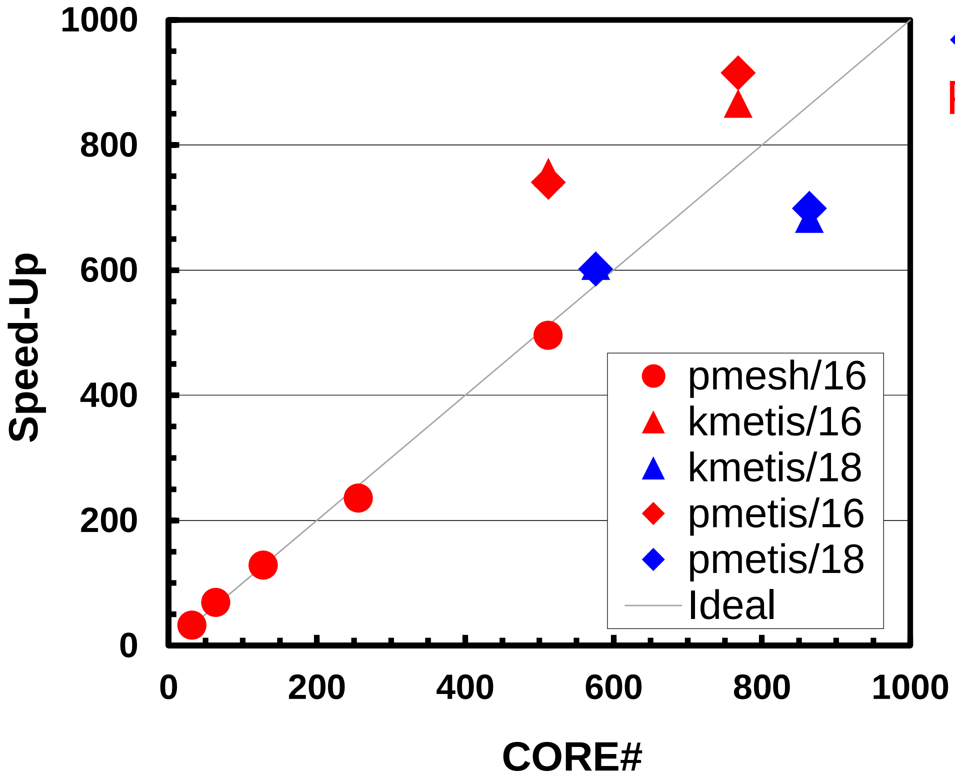
OUTPUT_UCD for Visualization

- 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

- 256×128×128 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
```

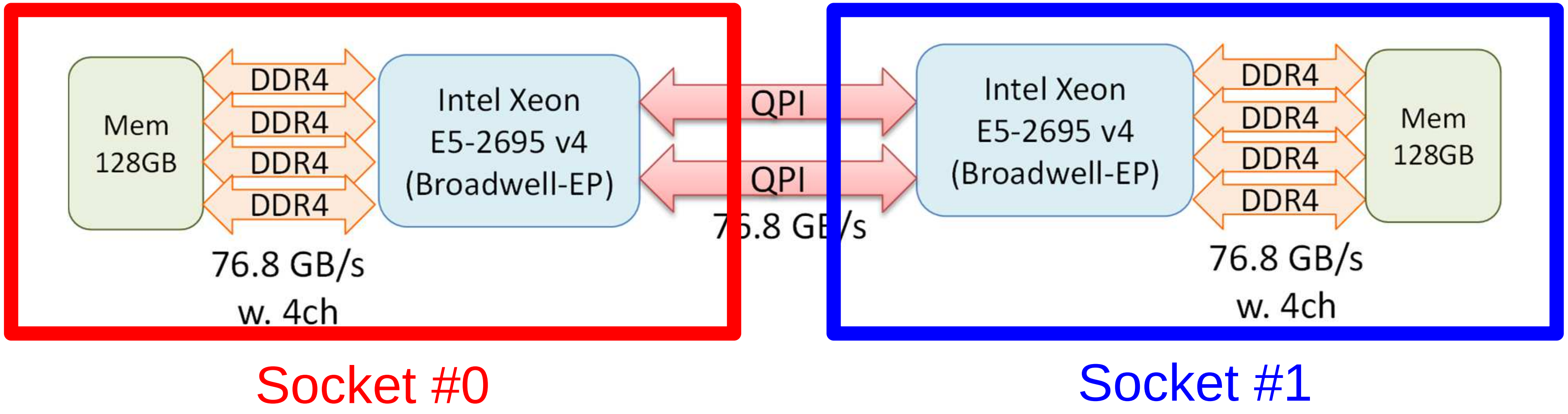
```
256 128 128
  8   4   2
pcube
```

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

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

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

1 Node = 2 Sockets (CPU's)

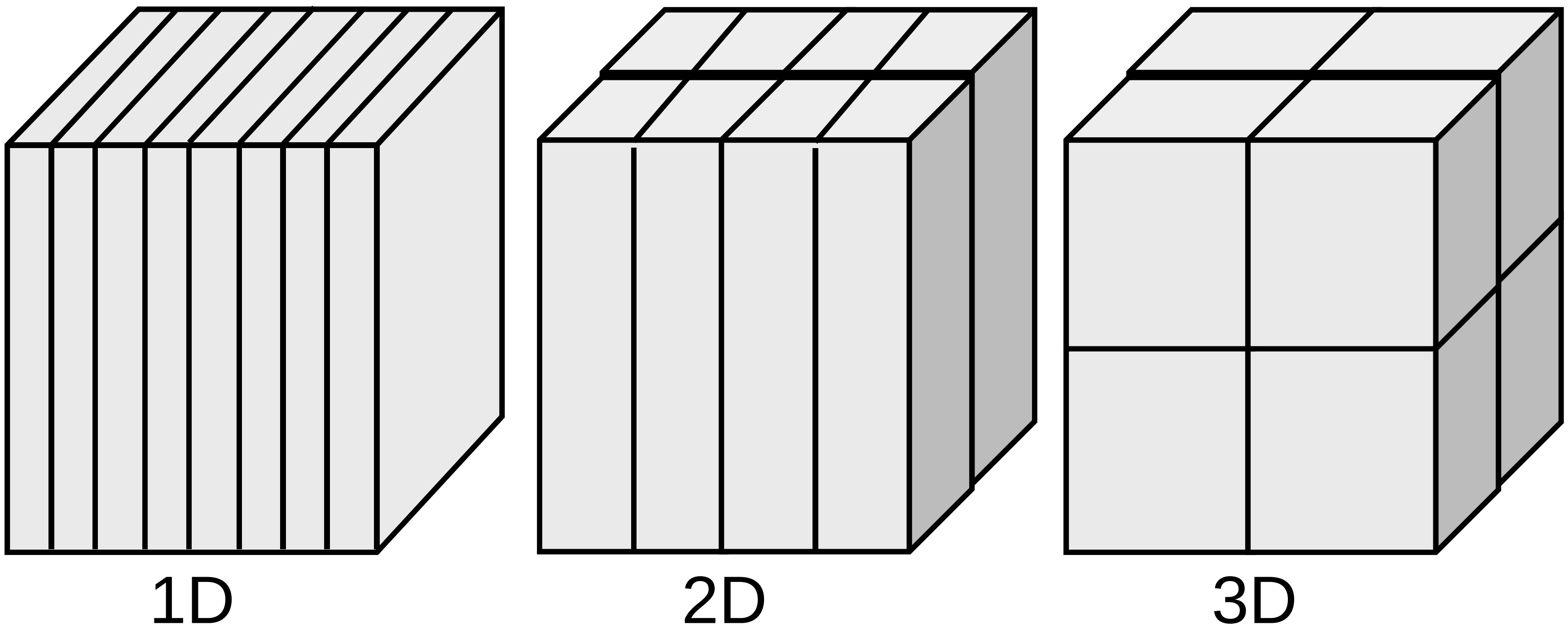


- Each Node of Reedbush-U
  - 2 Sockets (CPU's) of Intel Broadwell-EP
  - Each socket has 18 cores
- Each core of a socket can access to the memory on the other socket : NUMA (Non-Uniform Memory Access)
  - I_MPI_PIN_DOMAIN=socket, impimap.sh: local memory to be used

Exercise (1/2)

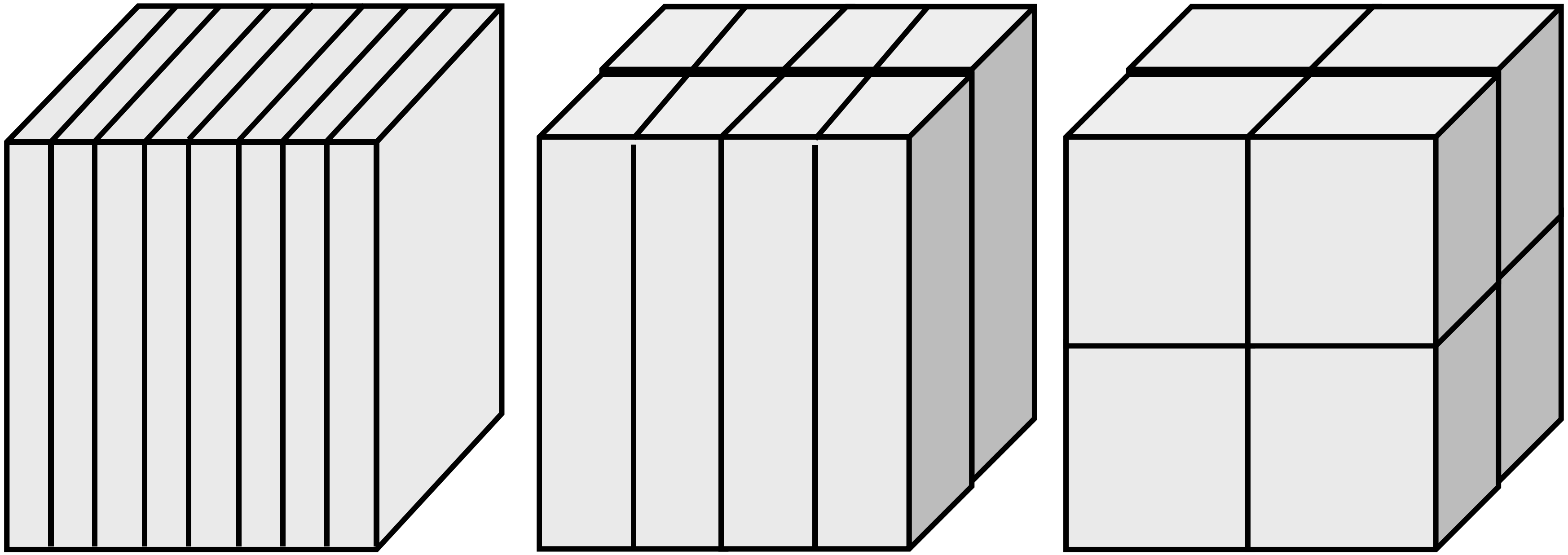
- Evaluation behavior and performance of “sol”
- Example
  - Strong Scaling
    - Fixed entire problem size
  - Weak Scaling
    - Fixed problem size/core, time for 1 iterations
  - Parameters
    - Problem size
    - Domain decomposition (1D-3D, kmetis, pmetis)
- “*.inp” may take long time.
  - delete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

1D-3D Decomposition



1D-3D Decomposition

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



1D | 2D | 3D

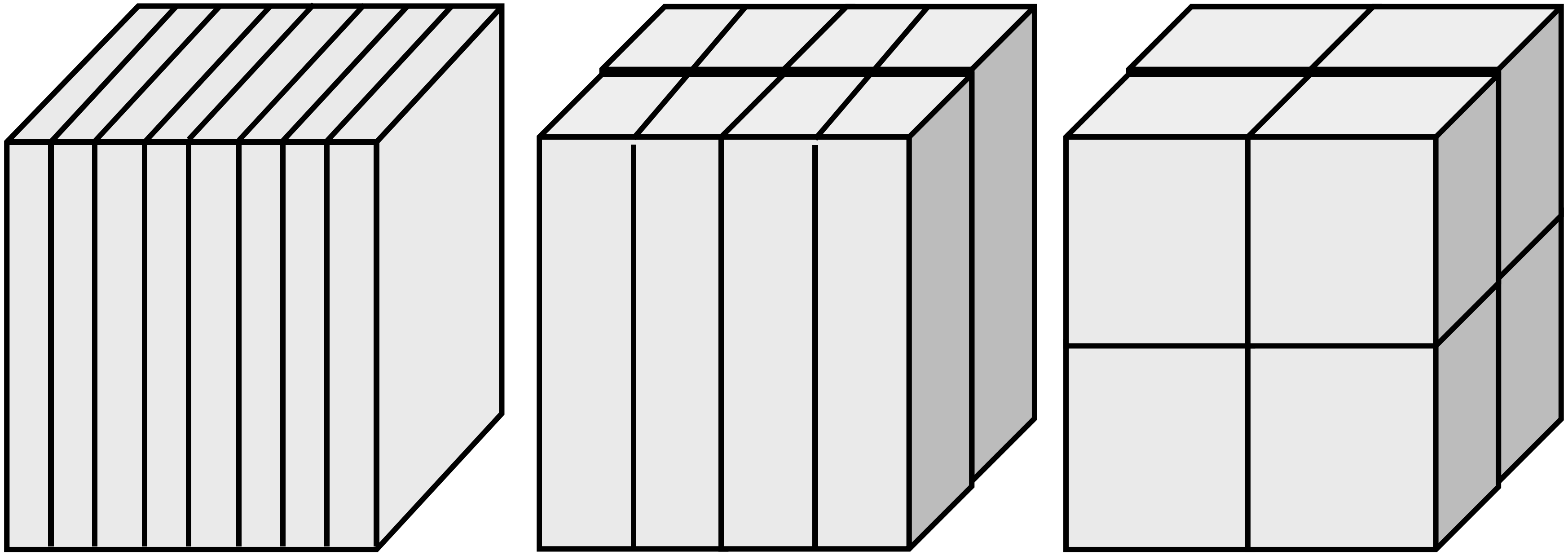
$16\ N^2$ x $7 = 112\ N^2$

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

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

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= 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 29th (Mon), 2018.
  – 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)