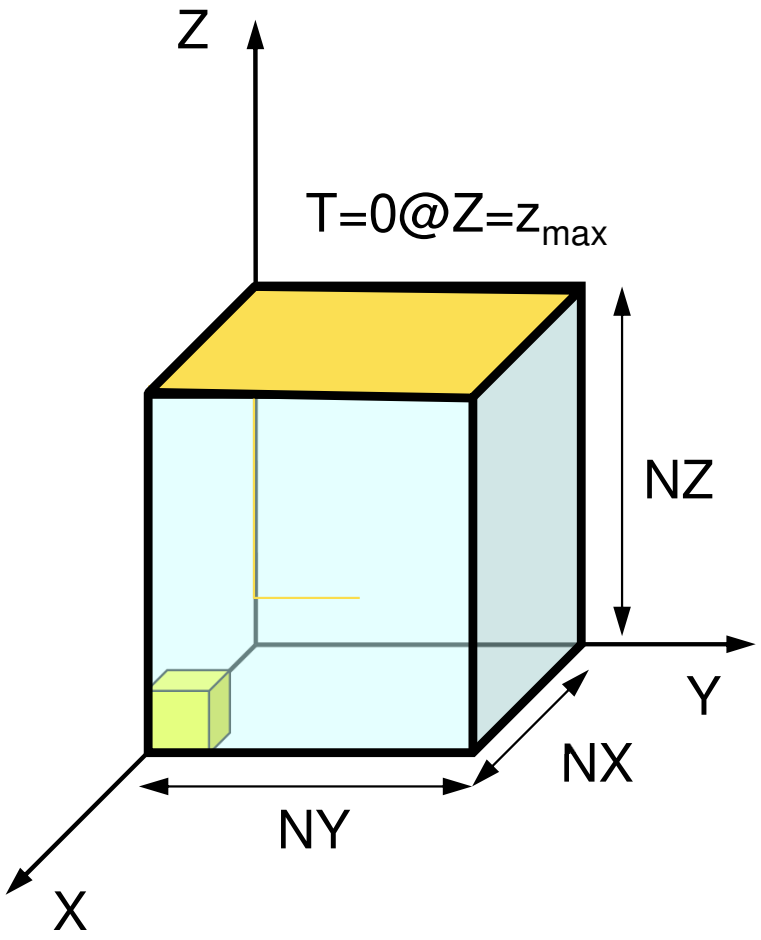
3D Parallel FEM (II)
C

Kengo Nakajima
RIKEN R-CCS

3D Steady-State Heat Conduction

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



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

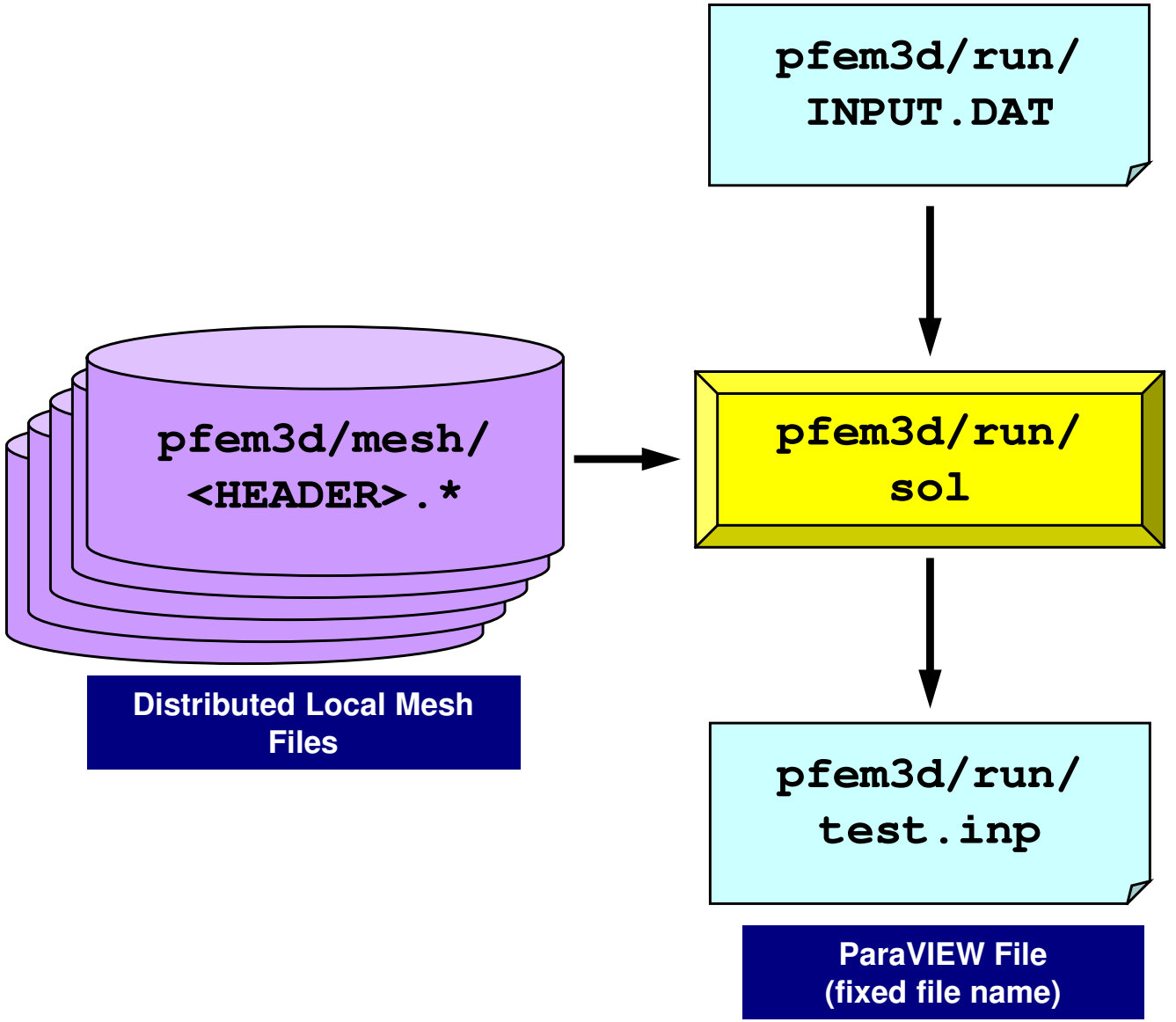
Finite-Element Procedures

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

FEM Procedures: Program

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

Procedures for Parallel FEM



Control File: INPUT.DAT

```
INPUT.DAT

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

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

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

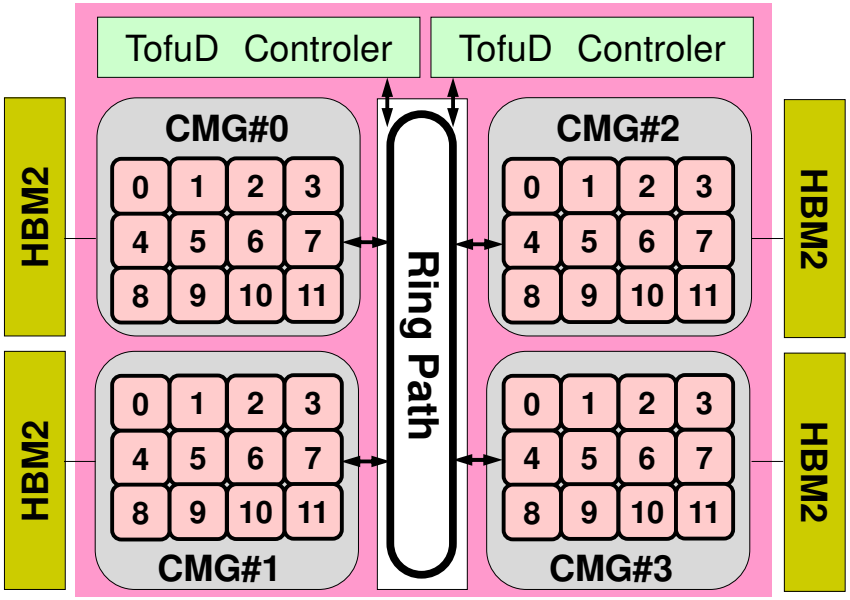
$$\dot{Q}(x,y,z)=QVOL\left|x_C+y_C\right|$$

pFEM/pfem3d/run/a08.sh

```
#!/bin/sh
#PJM -N "flat-08"                       Job Name
#PJM -L "rscgrp=small"                  Name of "Queue/Resource Group"
#PJM -L "node=8:torus"                  Node #
#PJM --mpi "max-proc-per-node=48"       MPI #/node (384/8= 48 per node)
#PJM -L elapse=00:15:00                 Computation Time
#PJM -g ra020019                        Group Name (Wallet)
#PJM -j
#PJM -e err                             Standard Error
#PJM -o a08.lst                         Standard Output


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

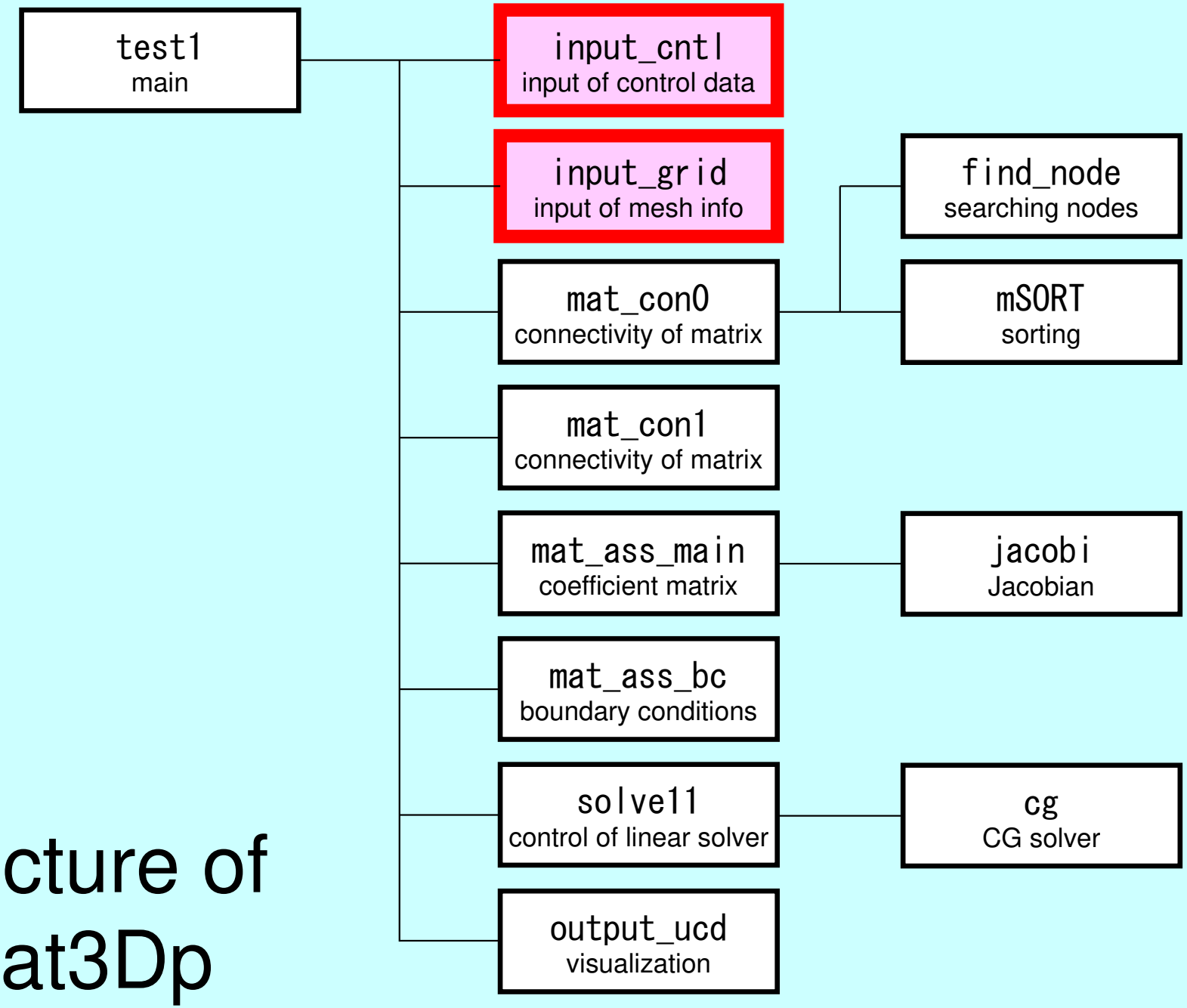
Number of Processes

```
#PJM -L "node=1";#PJM --mpi "max-proc-per-node=1"   Proc.#=  1
#PJM -L "node=1";#PJM --mpi "max-proc-per-node=4"   Proc.#=  4
#PJM -L "node=1";#PJM --mpi "max-proc-per-node=12"  Proc.#= 12
#PJM -L "node=1";#PJM --mpi "max-proc-per-node=24"  Proc.#= 24
#PJM -L "node=1";#PJM --mpi "max-proc-per-node=48"  Proc.#= 48

#PJM -L "node=4:torus";  #PJM --mpi "max-proc-per-node=48" Proc.#=192
#PJM -L "node=8:torus";  #PJM --mpi "max-proc-per-node=48" Proc.#=384
#PJM -L "node=12:torus";#PJM --mpi "max-proc-per-node=48" Proc.#=576
```



Because Fugaku is now very crowded, it is recommended to add **":torus"** after **"node=XX"** in the script for getting computational resources smoothly, **if XX is larger than 1**. Example for 512 nodes: 12x12x4 with "torus", 14x19x2 without "torus"

Structure of heat3Dp



Main Part

```
#include <stdio.h>
#include <stdlib.h>
FILE* fp_log;
#define GLOBAL_VALUE_DEFINE
#include "pfem_util.h"
extern void PFEM_INIT(int,char**);
extern void INPUT_CNTL();
extern void INPUT_GRID();
extern void MAT_CON0();
extern void MAT_CON1();
extern void MAT_ASS_MAIN();
extern void MAT_ASS_BC();
extern void SOLVE11();
extern void OUTPUT_UCD();
extern void PFEM_FINALIZE();
int main(int argc,char* argv[])
{
  double START_TIME,END_TIME;

  PFEM_INIT(argc,argv);

  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()   ;

  SOLVE11();

  OUTPUT_UCD()    ;
  PFEM_FINALIZE() ;
}
```

Global Variables: pfem_util.h (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	[NODGRPtot+1]	I	# Node in each Node Group
NODGRP_ITEM	I	[NODGRP_INDEX[NODGRPTOT+1]]	I	Node ID in each Node Group
NODGRP_NAME	C80	[NODGRP_INDEX[NODGRPTOT+1]]	I	Name of NodeGroup
NLU	I		O	# Non-Zero Off-Diagonals at each node
NPLU	I		O	# Non-Zero Off-Diagonals
D	R	[NP]	O	Diagonal Block of Global Matrix
B,X	R	[NP]	O	RHS, Unknown Vector

Global Variables: pfem_util.h (2/4)

Name	Type	Size	I/O	Definition
AMAT	R	[NPLU]	O	Non-Zero Off-Diagonal Components of Global Matrix
indexLU	I	[NP+1]	O	# Non-Zero Off-Diagonal Components
itemLU	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.h (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.h (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	[NEIBPETOT+1]	I	Size of Import/Export Arrays for Communication Table
IMPORT_ITEM	I	[NPimport]	I	Receiving Table (External Points) NPimport=IMPORT_INDEX[NEIBPETOT+1])
EXPORT_ITEM	I	[NPexport]	I	Sending Table (Boundary Points) NPexport=EXPORT_INDEX[NEIBPETOT+1])
ICELTOT_INT	**I**		**I**	**Number of Local Elements**
intELEM_list	**I**	**[ICELTOT_INT]**	**I**	**List of Local Elements**

Start/End: MPI_Init/Finalize

```
#include "pfem_util.h"
void PFEM_INIT(int argc, char* argv[])
{
        int i;
        MPI_Init(&argc,&argv);
        MPI_Comm_size(MPI_COMM_WORLD,&PETOT);
        MPI_Comm_rank(MPI_COMM_WORLD,&my_rank);

        for(i=0;i<100;i++)  pfemRarray[i]=0.0;
        for(i=0;i<100;i++)  pfemIarray[i]=0;
}
```

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

void  PFEM_FINALIZE()
{
      MPI_Finalize ();

          if( my_rank == 0 ){
                  fprintf(stdout,"* normal terminatio¥n");
                  exit(0);
          }
}
```

Reading Control File: INPUT_CNTL

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

  if( my_rank == 0 ){
    if( (fp=fopen("INPUT.DAT","r")) == NULL){
      fprintf(stdout,"input file cannot be opened!¥n");
      exit(1);
    }

    fscanf(fp,"%s",HEADER);
    fscanf(fp,"%d",&ITER);
    fscanf(fp, "%lf %lf", &COND, &QVOL);
    fscanf(fp, "%lf",     &RESID);
    fclose(fp);
  }

  MPI_Bcast(HEADER ,80,MPI_CHAR,0,MPI_COMM_WORLD);
  MPI_Bcast(&ITER   , 1,MPI_INTEGER,0,MPI_COMM_WORLD);
  MPI_Bcast(&COND   , 1,MPI_DOUBLE,0,MPI_COMM_WORLD);
  MPI_Bcast(&QVOL   , 1,MPI_DOUBLE,0,MPI_COMM_WORLD);
  MPI_Bcast(&RESID  , 1,MPI_DOUBLE,0,MPI_COMM_WORLD);

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

Reading Meshes: INPUT_GRID (1/3)

```
#include <stdio.h>
#include <stdlib.h>
#include "pfem_util.h"
#include "allocate.h"
/*** external functions **/
extern void ERROR_EXIT (int, int);
extern void DEFINE_FILE_NAME(char*,char*,int);
/** **/
void INPUT_GRID()
{
        FILE *fp;
        int i,j,k,ii,kk,kkk,nn,icel,iS,iE,ic0;
        int NTYPE,IMAT;
        int idummy;

        DEFINE_FILE_NAME(HEADER, fname, my_rank);
        if( (fp=fopen(fname,"r")) == NULL){
                fprintf(stdout,"input file cannot be opened!¥n");
                exit(1);}
/**
        NEIB-PE
**/
        fscanf(fp,"%d",&kkk);
        fscanf(fp,"%d",&NEIBPETOT);

        NEIBPE=(int*)allocate_vector(sizeof(int),NEIBPETOT);
        for(i=0;i<NEIBPETOT;i++) fscanf(fp,"%d",&NEIBPE[i]);

        for(i=0;i<NEIBPETOT;i++){
                if( NEIBPE[i] > PETOT-1 ){
                        ERROR_EXIT (202,my_rank);}
        }
```

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

```
#include <stdio.h>
#include <string.h>
void DEFINE_FILE_NAME (char HEADERo[], char filename[],int my_rank)
{
        char string[80];
        sprintf(string,".%-d",my_rank);
        strcpy(filename,HEADERo);
        strcat(filename,string);
}
```

allocate, deallocate

```
#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)

```
/**
        NODE
**/
        fscanf(fp,"%d %d",&NP,&N);

        XYZ    =(KREAL**)allocate_matrix(sizeof(KREAL),NP,3);
        NODE_ID=(KINT **)allocate_matrix(sizeof(KINT ),NP,2);

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

        for(i=0;i<NP;i++){

          fscanf(fp,"%d %d %lf %lf %lf",&NODE_ID[i][0],&NODE_ID[i][1],&XYZ[i][0],&XYZ[i][1],&XYZ[i][2]);
        }
/**
        ELEMENT
**/
        fscanf(fp,"%d %d",&ICELTOT,&ICELTOT_INT);

        ICELNOD=(KINT**)allocate_matrix(sizeof(KINT),ICELTOT,8);
        intELEM_list=(KINT*)allocate_vector(sizeof(KINT),ICELTOT);
        ELEM_ID=(KINT**)allocate_matrix(sizeof(KINT),ICELTOT,2);

        for(i=0;i<ICELTOT;i++) fscanf(fp,"%d",&NTYPE);

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

        for(ic0=0;ic0<ICELTOT_INT;ic0++) fscanf(fp,"%d",&intELEM_list[ic0]);
```

Reading Meshes: INPUT_GRID (3/3)

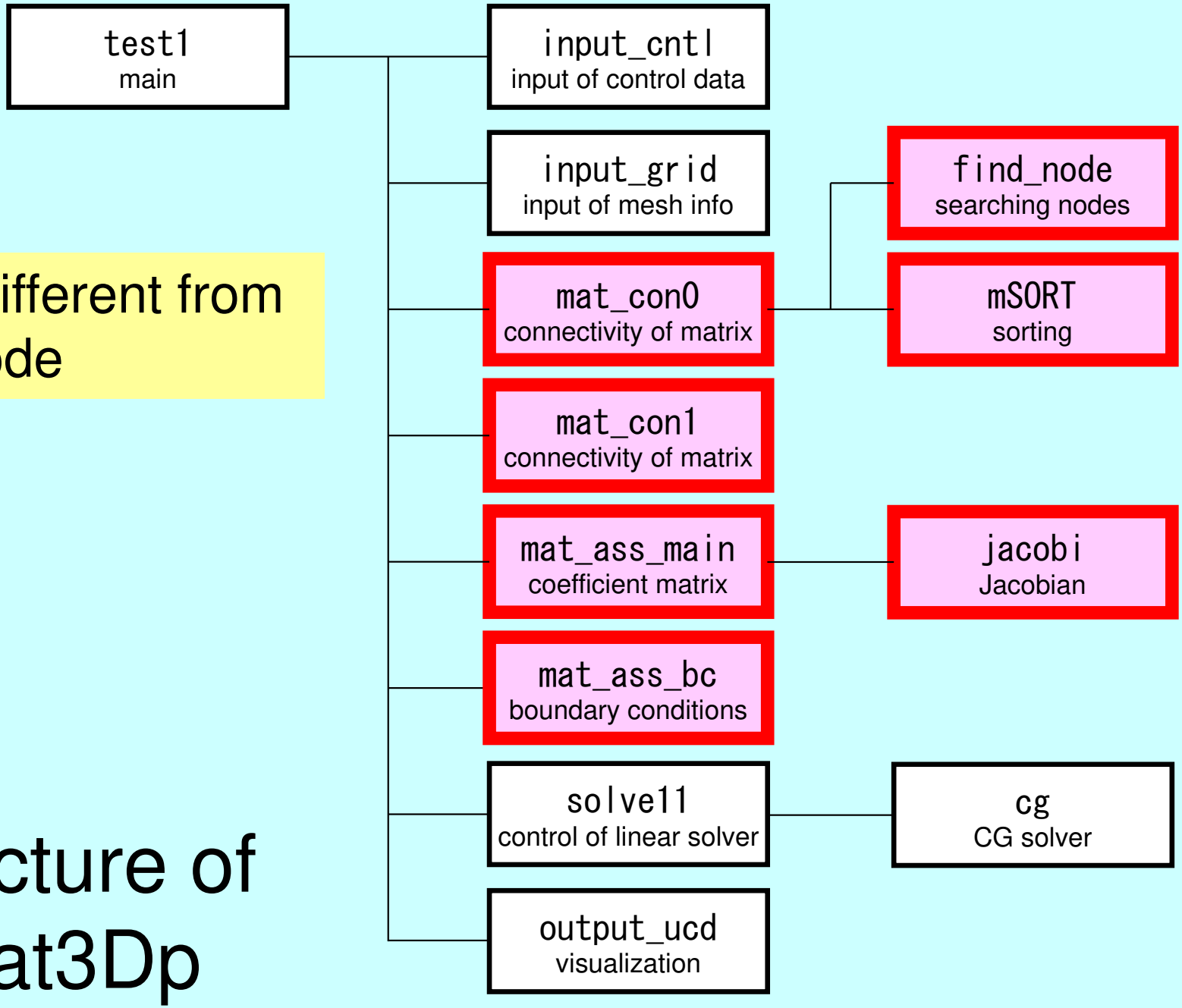
```
/**
        COMMUNICATION table
**/
        IMPORT_INDEX=(int*)allocate_vector(sizeof(int),NEIBPETOT+1);
        EXPORT_INDEX=(int*)allocate_vector(sizeof(int),NEIBPETOT+1);

        for(i=0;i<NEIBPETOT+1;++i) IMPORT_INDEX[i]=0;
        for(i=0;i<NEIBPETOT+1;++i) EXPORT_INDEX[i]=0;

        if( PETOT != 1 ) {
                for(i=1;i<=NEIBPETOT;i++) fscanf(fp,"%d",&IMPORT_INDEX[i]);
                nn=IMPORT_INDEX[NEIBPETOT];
                if( nn > 0 ) IMPORT_ITEM=(int*)allocate_vector(sizeof(int),nn);
                for(i=0;i<nn;i++) fscanf(fp,"%d %d",&IMPORT_ITEM[i],&idummy);

                for(i=1;i<=NEIBPETOT;i++) fscanf(fp,"%d",&EXPORT_INDEX[i]);
                nn=EXPORT_INDEX[NEIBPETOT];
                if( nn > 0 ) EXPORT_ITEM=(int*)allocate_vector(sizeof(int),nn);
                for(i=0;i<nn;i++) fscanf(fp,"%d",&EXPORT_ITEM[i]);}
/**
        NODE grp.  info.
**/
        fscanf(fp,"%d",&NODGRPtot);

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

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

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

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

```
#include <stdio.h>
#include <stdlib.h>
FILE* fp_log;
#define GLOBAL_VALUE_DEFINE
#include "pfem_util.h"
extern void PFEM_INIT(int,char**);
extern void INPUT_CNTL();
extern void INPUT_GRID();
extern void MAT_CON0();
extern void MAT_CON1();
extern void MAT_ASS_MAIN();
extern void MAT_ASS_BC();
extern void SOLVE11();
extern void OUTPUT_UCD();
extern void PFEM_FINALIZE();
int main(int argc,char* argv[])
{
  double START_TIME,END_TIME;

  PFEM_INIT(argc,argv);

  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()  ;

  SOLVE11();

  OUTPUT_UCD()    ;
  PFEM_FINALIZE() ;
}
```

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

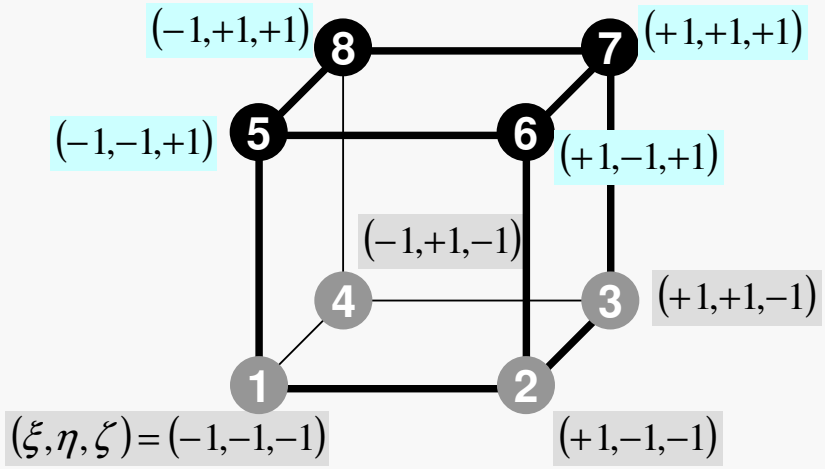
Node ID starting from “1”

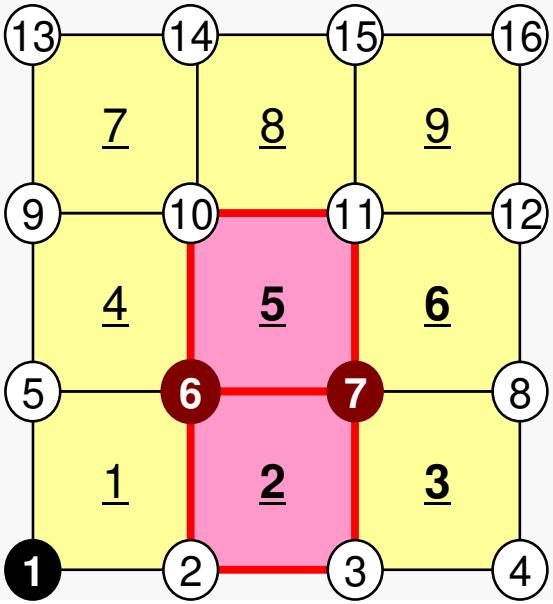
Please compare parallel/serial codes

```
$ cd /home/ra020019/<Your-UID>/pFEM/pfem3d/src

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

MAT_CON0: Overview

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





Generating Connectivity of Matrix MAT_CON0 (1/4)

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

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

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

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

  NLU= 26;

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

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

NLU:
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 NLU in this way.

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

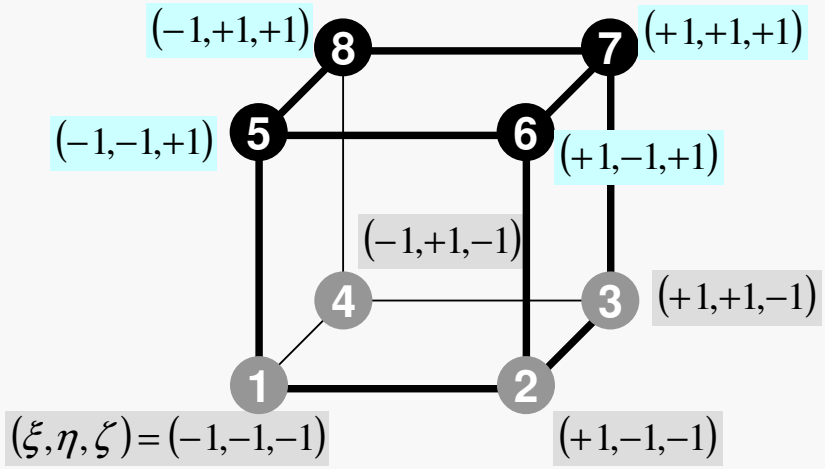
Generating Connectivity of Matrix MAT_CON0 (1/4)

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

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

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

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

  NLU= 26;

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

  for(i=0;i<NP;i++) INLU[i]=0;
  for(i=0;i<NP;i++) for(j=0;j<NLU;j++) IALU[i][j]=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): Starting from 1

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

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

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

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



FIND_TS_NODE: Search Connectivity

INLU,IALU: Automatic Search

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

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

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

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

  return;
}
```

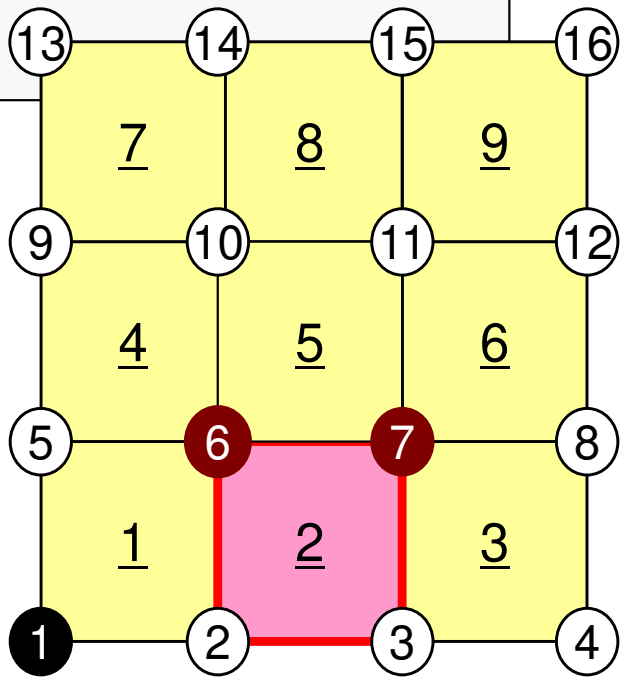
Array	Size	Description
INLU	[NP]	Number of connected nodes to each node (lower/upper)
IALU	[NP][NLU]	Corresponding connected node ID (column ID)

FIND_TS_NODE: Search Connectivity

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

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

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

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

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

  return;
}
```

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



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

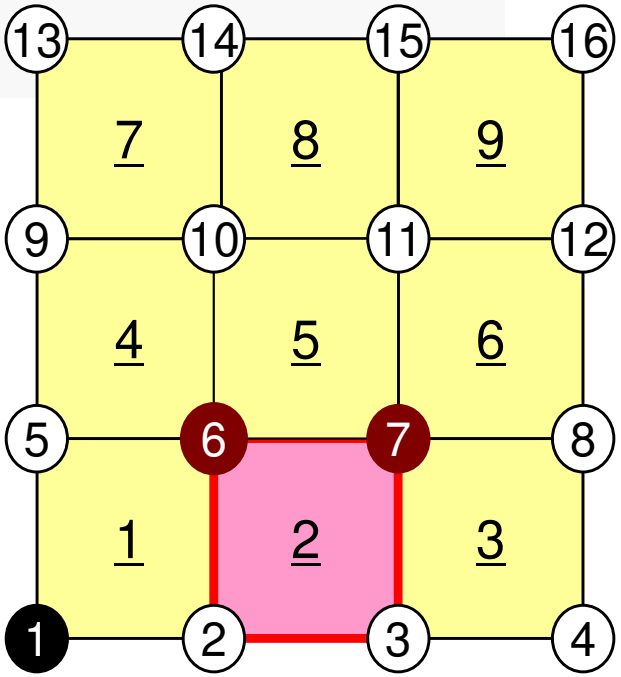
FIND_TS_NODE: Search Connectivity

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

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

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

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

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

  return;
}
```

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

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

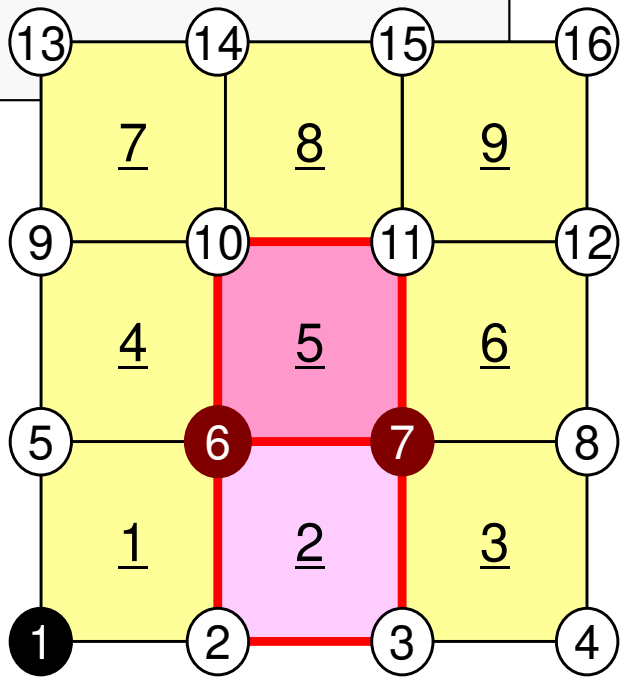


FIND_TS_NODE: Search Connectivity

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

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

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

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

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

  return;
}
```

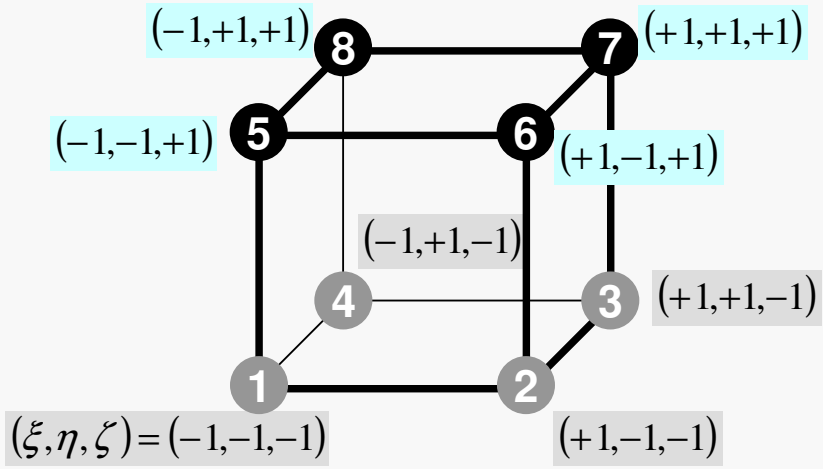
If the target node is already included in IALU, proceed to next pair of nodes



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

Generating Connectivity of Matrix MAT_CON0 (3/4)

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

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

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

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



Generating Connectivity of Matrix MAT_CON0 (4/4)

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

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

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

    mSORT(NCOL1,NCOL2,NN);

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

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

MAT_CON1: CRS format

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

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

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

  NPLU=indexLU[NP];

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

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


  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

C

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

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

FORTRAN

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

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

MAT_CON1: CRS format

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

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

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

  NPLU=indexLU[NP];

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

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


  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

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

MAT_CON1: CRS format

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

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

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

  NPLU=indexLU[NP];

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

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


  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

itemLU
store node ID starting from 0

MAT_CON1: CRS format

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

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

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

  NPLU=indexLU[NP];

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

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


  deallocate_vector(INLU);
  deallocate_vector(IALU);
}
```

Not required any more

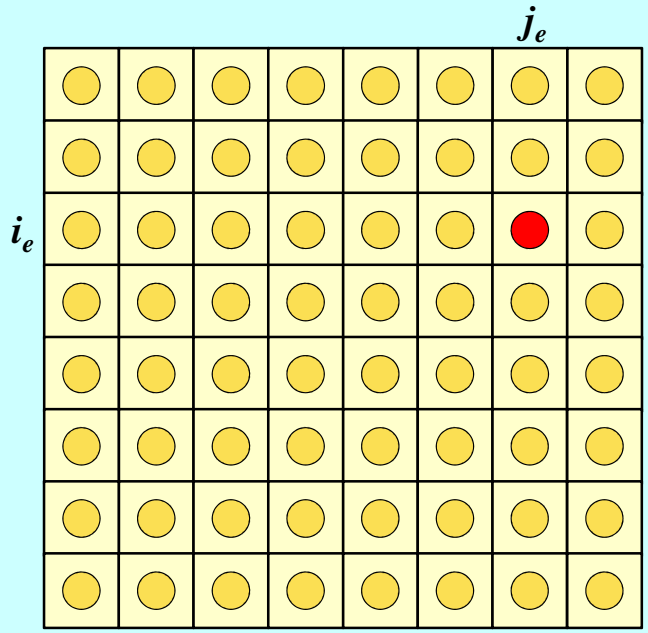
Main Part

```
#include <stdio.h>
#include <stdlib.h>
FILE* fp_log;
#define GLOBAL_VALUE_DEFINE
#include "pfem_util.h"
extern void PFEM_INIT(int,char**);
extern void INPUT_CNTL();
extern void INPUT_GRID();
extern void MAT_CON0();
extern void MAT_CON1();
extern void MAT_ASS_MAIN();
extern void MAT_ASS_BC();
extern void SOLVE11();
extern void OUTPUT_UCD();
extern void PFEM_FINALIZE();
int main(int argc,char* argv[])
{
  double START_TIME,END_TIME;

  PFEM_INIT(argc,argv);

  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()  ;

  SOLVE11();

  OUTPUT_UCD()    ;
  PFEM_FINALIZE() ;
}
```

MAT_ASS_MAIN: Overview

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

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

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

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

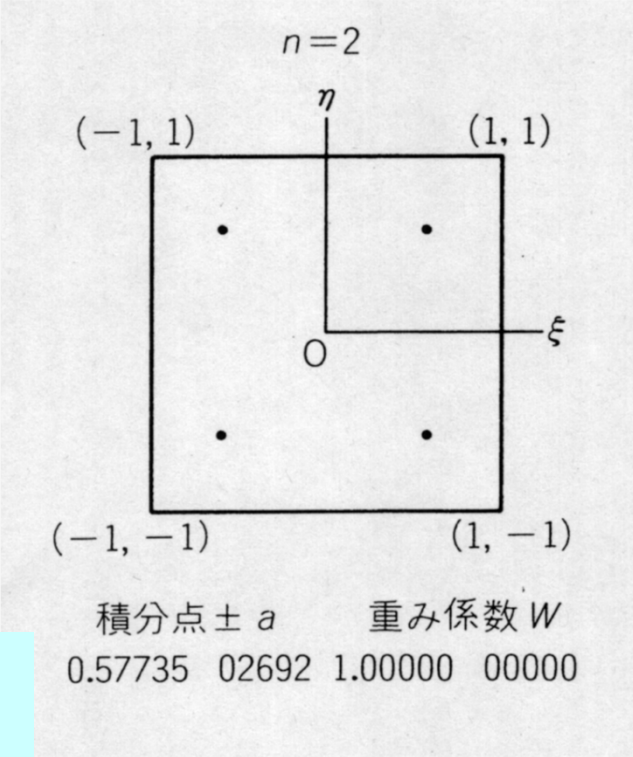


MAT_ASS_MAIN (1/6)

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

  KINT nodLOCAL[8];

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

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

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

MAT_ASS_MAIN (1/6)

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

  KINT nodLOCAL[8];

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

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

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



POS: Quad. Point

WEI: Weighting Factor

係数行列：MAT_ASS_MAIN（2/6）

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

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

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

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

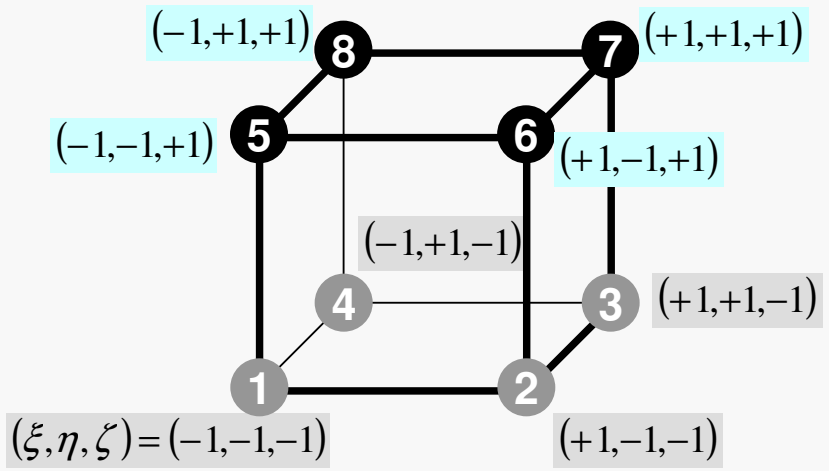
MAT_ASS_MAIN (2/6)

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

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

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

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

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

MAT_ASS_MAIN (2/6)

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

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

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

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



MAT_ASS_MAIN (2/6)

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

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

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

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

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

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

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

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

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

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

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

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

MAT_ASS_MAIN (2/6)

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

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

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

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

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

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

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

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

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

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

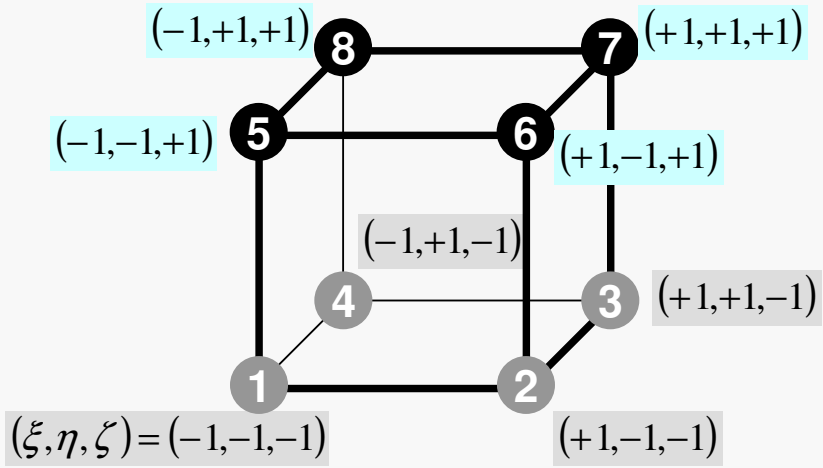
$$\frac{\partial N_3}{\partial \xi}(\xi_i,\eta_j,\zeta_k)=+\frac{1}{8}(1+\eta_j)(1-\zeta_k)$$

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

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

MAT_ASS_MAIN (3/6)

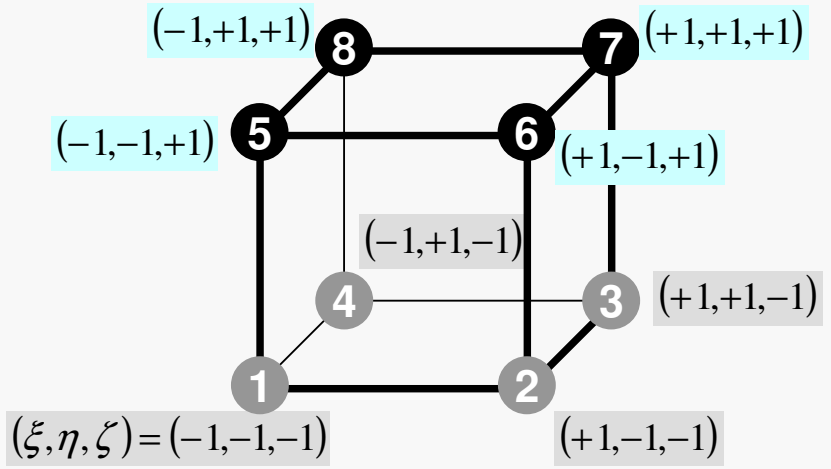
```
        PNQ[jp][kp][0]= - 08th * EM1 * TM1;
        PNQ[jp][kp][1]= + 08th * EM1 * TM1;
        PNQ[jp][kp][2]= + 08th * EP1 * TM1;
        PNQ[jp][kp][3]= - 08th * EP1 * TM1;
        PNQ[jp][kp][4]= - 08th * EM1 * TP1;
        PNQ[jp][kp][5]= + 08th * EM1 * TP1;
        PNQ[jp][kp][6]= + 08th *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

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

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

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

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



MAT_ASS_MAIN (4/6)

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

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

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

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

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

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

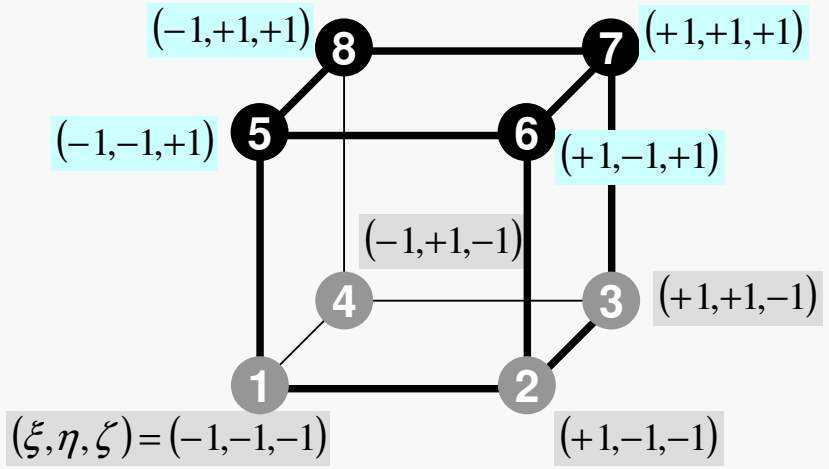
Node ID (Global)



MAT_ASS_MAIN (4/6)

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

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

X-Coordinates of 8 nodes




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

Y-Coordinates of 8 nodes

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

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

Z-Coordinates of 8 nodes

Coordinates: Node ID - 1

```
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);
```

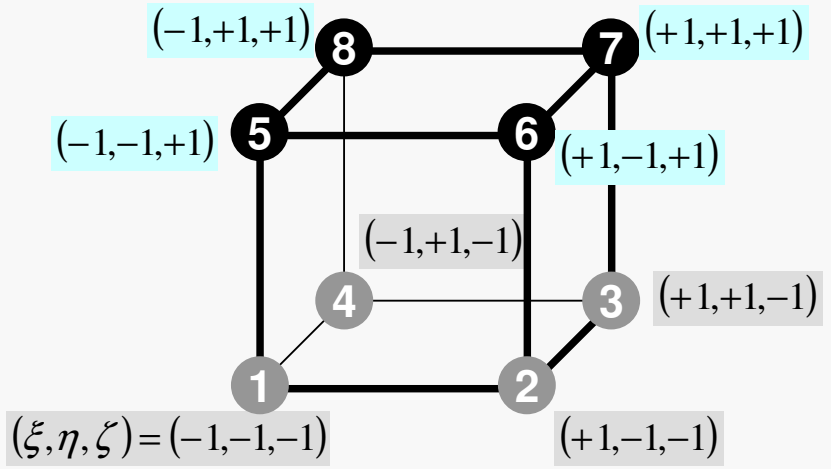
MAT_ASS_MAIN (4/6)

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

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

X-Coordinates of 8 nodes

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

Y-Coordinates of 8 nodes



Coordinates: Node ID - 1

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

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

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

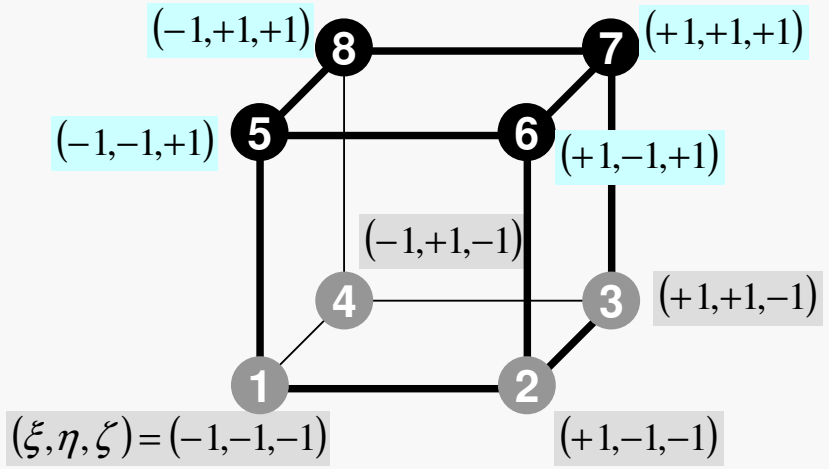
$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\dot{Q}(x,y,z)=0$$

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

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

係数行列：MAT_ASS_MAIN（4/6）

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

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

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

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

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

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



Coordinates:
Node ID - 1

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

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

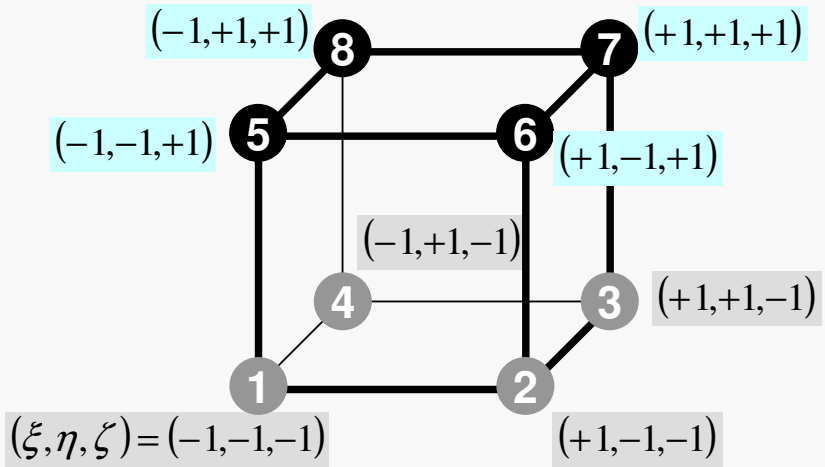
$$QVC=\left|x_C+y_C\right|$$

MAT_ASS_MAIN (4/6)

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

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

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

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

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

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

MAT_ASS_MAIN (5/6)

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

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

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

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



Non-Zero Off-Diagonal Block in Global Matrix

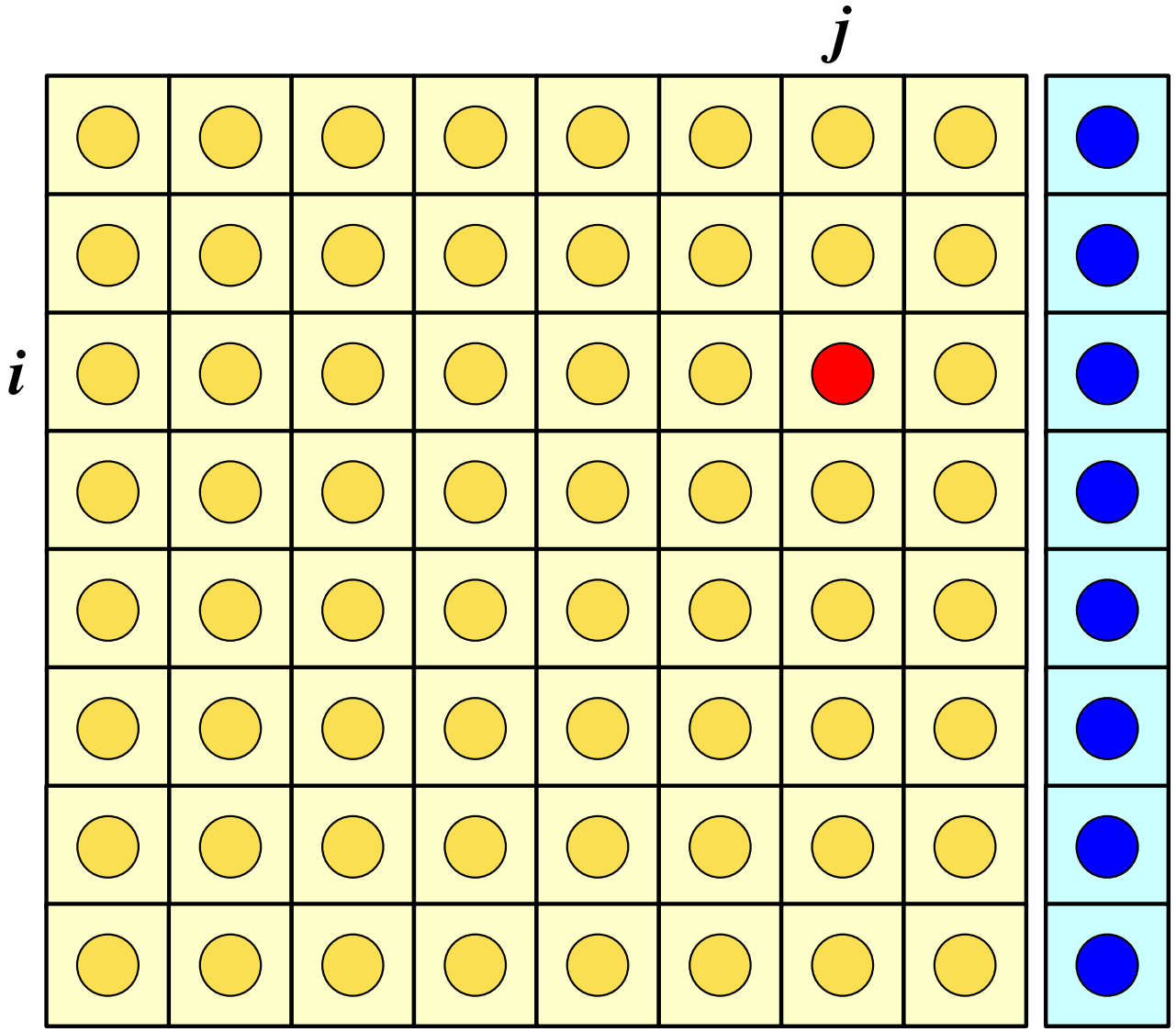
$A_{ip,jp}$

kk: address in “itemLU”

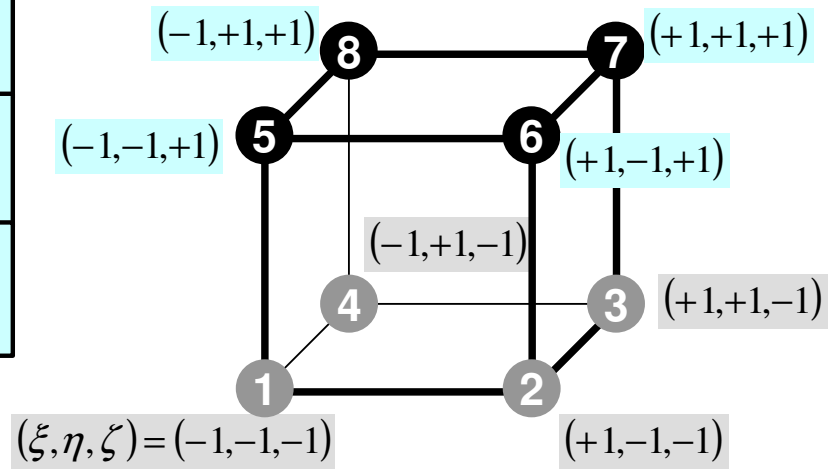
ip= nodLOCAL[ie]
jp= nodLOCAL[je]

Node ID (ip,jp) starting from 1

Element Matrix: 8x8



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



MAT_ASS_MAIN (5/6)

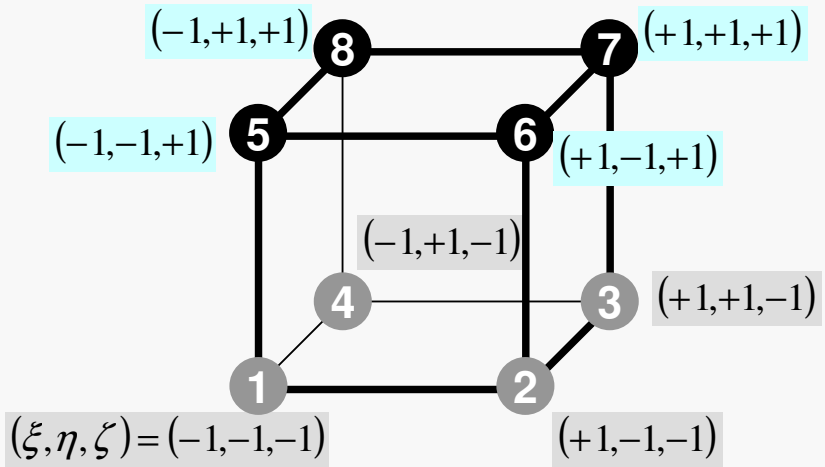
```
/**
   CONSTRUCT the GLOBAL MATRIX
**/

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

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

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

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

kk : address in "itemLU" starting from "0"

k: starting from "0"

ip,jp: starting from "1"



MAT_ASS_MAIN (6/6)

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

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

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

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

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

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

            }
          }
        }

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

      }
    }
  }
}
```

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

MAT_ASS_MAIN (6/6)

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

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

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

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

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

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

            }
          }
        }

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

      }
    }
  }
}
```

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

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

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

MAT_ASS_MAIN (6/6)

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

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

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


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

    }
  }
}
```

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

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

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

MAT_ASS_MAIN (6/6)

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

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

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

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

    }
  }
}
```

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

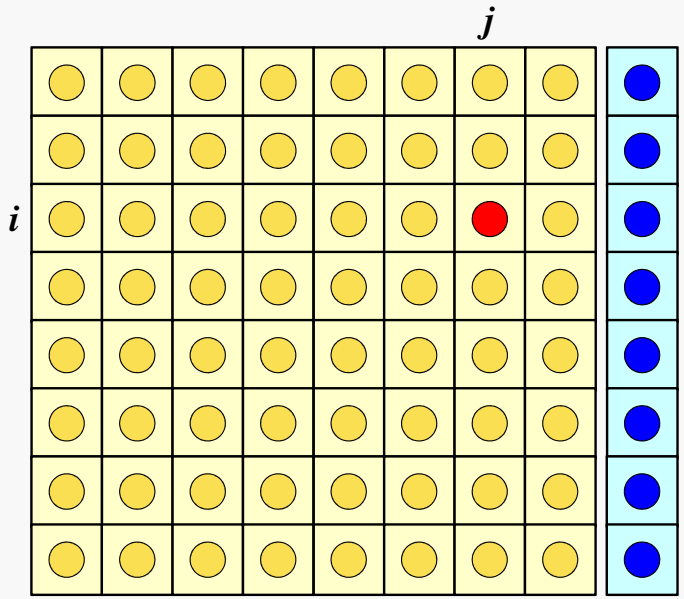
$$I = \int_{-1}^{+1}\int_{-1}^{+1}\int_{-1}^{+1} f(\xi,\eta,\zeta)\, d\xi d\eta d\zeta = \sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{N} W_i \cdot W_j \cdot W_k \cdot f(\xi_i,\eta_j,\zeta_k)$$

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

MAT_ASS_MAIN (6/6)

```
        QVO= 0.e0;
        COEFij= 0.e0;

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

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

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

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

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

            }
          }
        }

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

      }
    }
  }
}
```

$$[k_{ij}] \quad (i,j=1\ldots8)$$



MAT_ASS_MAIN (6/6)

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

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

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

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

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

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

            }
          }
        }

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

      }
    }
  }
}
```

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

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

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

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

MAT_ASS_MAIN (6/6)

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

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

        }
    }
}
```

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

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

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

MAT_ASS_MAIN (6/6)

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

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

        }
    }
}
```

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

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

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

MAT_ASS_MAIN (6/6)

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

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

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

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

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

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

            }
          }
        }

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

      }
    }
  }
}
```

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

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

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

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

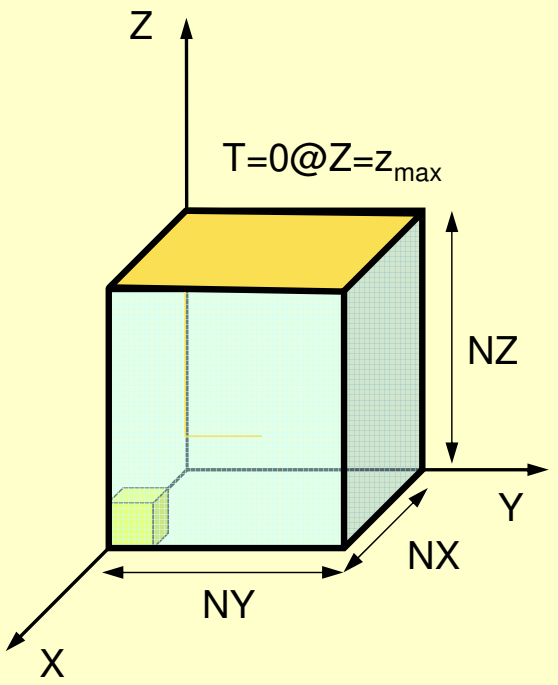
$$QVC = \left|x_C + y_C\right|$$

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

MAT_ASS_BC: Overview

```
do i= 1, 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= indexLU(i-1)+1, indexLU(i)   Non-Zero Off-Diagonal Nodes
       corresponding comp. of non-zero off-diagonal
       components (AMAT) are corrected
    enddo
  endif
enddo

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



MAT_ASS_BC (1/2)

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

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

/**
   Z=Zmax
**/

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

  ib0=-1;

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

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

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

IWKX[in-1][0]= 1

MAT_ASS_BC (2/2)

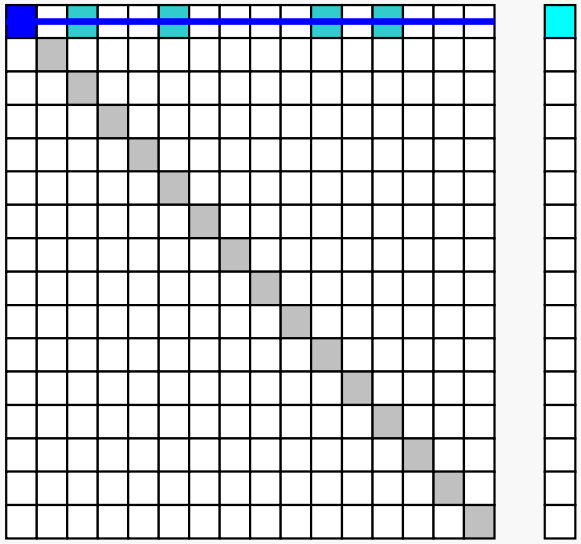
```
 for(in=0;in<NP;in++){
    if( IWKX[in][0] == 1 ){
      B[in]= 0.e0;
      D[in]= 1.e0;
      for(k=indexLU[in];k<indexLU[in+1];k++){
        AMAT[k]= 0.e0;
      }
    }
  }

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

MAT_ASS_BC (2/2)

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

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

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

Erase !!

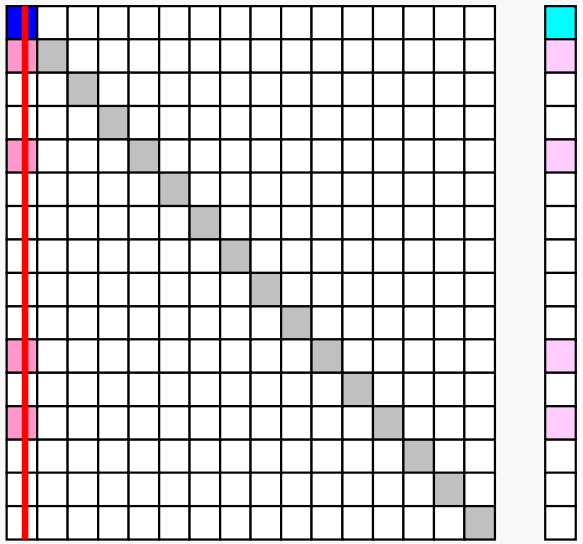


Same as 1CPU case

MAT_ASS_BC (2/2)

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

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

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



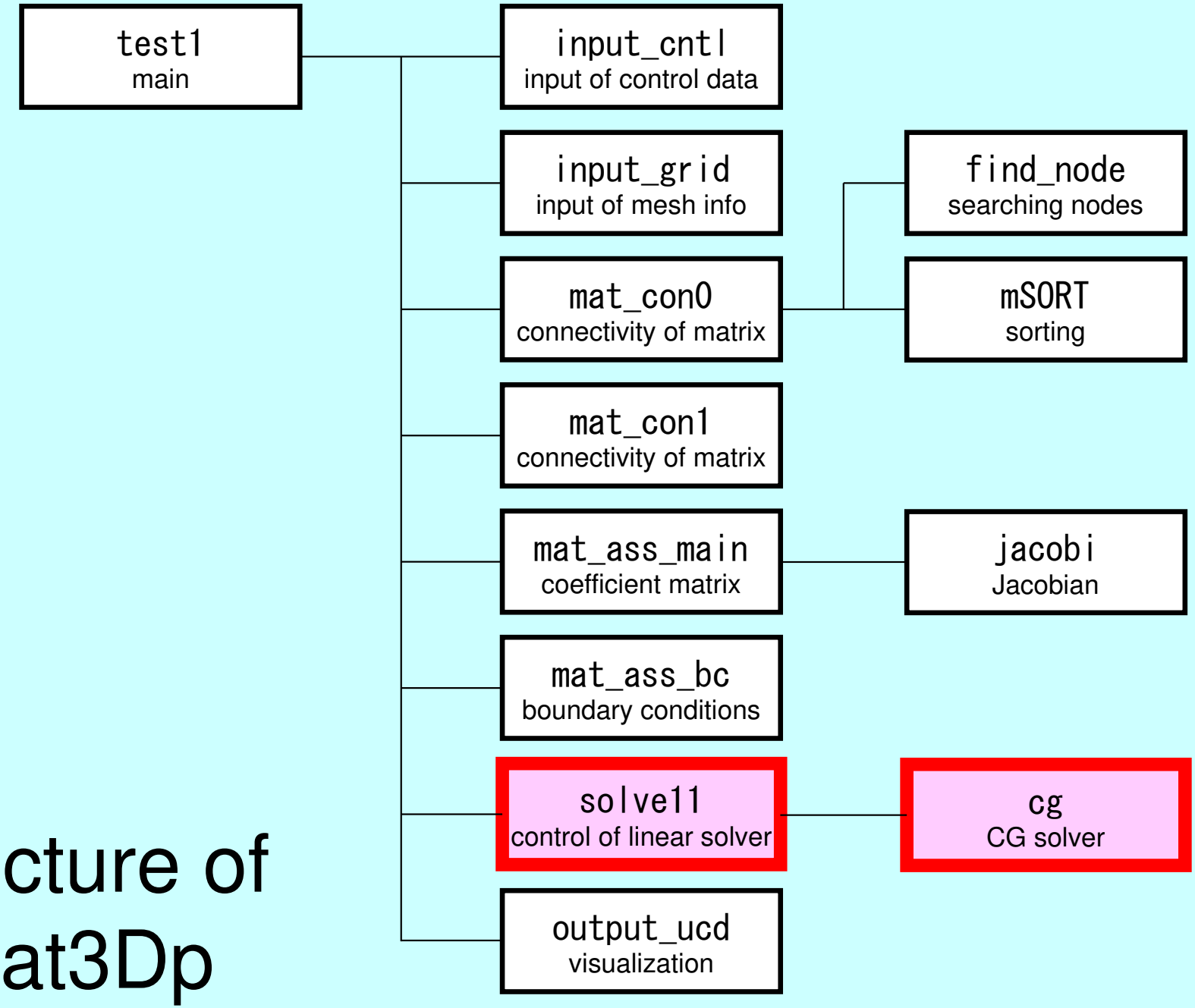
Elimination and Erase

Same as 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

```
#include <stdio.h>
#include <stdlib.h>
FILE* fp_log;
#define GLOBAL_VALUE_DEFINE
#include "pfem_util.h"
extern void PFEM_INIT(int,char**);
extern void INPUT_CNTL();
extern void INPUT_GRID();
extern void MAT_CON0();
extern void MAT_CON1();
extern void MAT_ASS_MAIN();
extern void MAT_ASS_BC();
extern void SOLVE11();
extern void OUTPUT_UCD();
extern void PFEM_FINALIZE();
int main(int argc,char* argv[])
{
  double START_TIME,END_TIME;

  PFEM_INIT(argc,argv);

  INPUT_CNTL();
  INPUT_GRID();

  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()   ;

  SOLVE11();

  OUTPUT_UCD()    ;
  PFEM_FINALIZE() ;
}
```

SOLVE11

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

  int  ERROR, ICFLAG=0;
  CHAR_LENGTH BUF;

/**
   +------------+
   | PARAMETERs |
   +------------+
**/
  ITER      = pfemIarray[0];        Number of Iterations for CG
  RESID     = pfemRarray[0];        Convergence Criteria for CG
/**
   +-----------------+
   | ITERATIVE solver |
   +-----------------+
**/
   CG   ( N, NP, NPLU, D, AMAT, indexLU, itemLU,
          B, X,  RESID, ITER, &ERROR, my_rank,
          NEIBPETOT,NEIBPE,IMPORT_INDEX,IMPORT_ITEM,
          EXPORT_INDEX,EXPORT_ITEM);}
```

Preconditioned CG Solver

Diagonal Scaling/Point Jacobi Preconditioning

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    solve [M]z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi  = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) – αiq(i)
    check convergence |r|
end
```

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

Diagonal Scaling, Point-Jacobi

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

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

CG Solver (1/6)

```
#include <stdio.h>
#include <math.h>
#include "mpi.h"
#include "precision.h"
#include "allocate.h "

extern FILE *fp_log;

extern void SOLVER_SEND_RECV ();

/***
    CG solves the linear system Ax = b using the Conjugate Gradient
    iterative method with the following preconditioners
***/

void  CG  (
           KINT N,KINT NP,KINT NPLU, KREAL D[],
           KREAL AMAT[],KINT indexLU[], KINT itemLU[],
           KREAL B[],KREAL X[],KREAL RESID,KINT ITER, KINT *ERROR,int my_rank,
           int NEIBPETOT,int NEIBPE[],
           int IMPORT_INDEX[], int IMPORT_ITEM[],
           int EXPORT_INDEX[], int EXPORT_ITEM[])
{
  int i,j,k;
  int ieL,isL,ieU,isU;
  double WVAL;
  double BNRM20,BNRM2,DNRM20,DNRM2;
  double S1_TIME,E1_TIME;
  double ALPHA,BETA;
  double C1,C10,RHO,RHO0,RHO1;
  int    iterPRE;
  KREAL *WS,*WR;                  Sending/Receiving Buffer
  KREAL **WW;

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

  double COMPtime,COMMtime,R1;
  double START_TIME,END_TIME;
```

Variables/Arrays in CG Solver (1/2)

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

Variables/Arrays in CG Solver (2/2)

Name	Type	Size	I/O	Definition
PETOT	I		I	Number of PE's
my_rank	I		I	Process ID of MPI
NEIBPETOT	I		I	Number of Neighbors
NEIBPE	I	[NEIBPETOT]	I	ID of Neighbor
IMPORT_INDEX **EXPORT_INEDX**	I	[NEIBPETOT+1]	I	Size of Import/Export Arrays for Communication Table
IMPORT_ITEM	I	[NPimport]	I	Receiving Table (External Points) NPimport=IMPORT_INDEX[NEIBPETOT+1])
EXPORT_ITEM	I	[NPexport]	I	Sending Table (Boundary Points) NPexport=EXPORT_INDEX[NEIBPETOT+1])
WR, WS	R	[NP]		Receiving/Sending Buffer for Point-to-Point Communications

CG Solver (2/6)

```
  ERROR= 0;

  WW=(KREAL**) allocate_matrix(sizeof(KREAL),4,NP);
  WS=(KREAL* ) allocate_vector(sizeof(KREAL),  NP);
  WR=(KREAL* ) allocate_vector(sizeof(KREAL),  NP);

  MAXIT  = ITER;
  TOL    = RESID;

  for(i=0;i<NP;i++) X [i]=0.0;
  for(i=0;i<NP;i++) for(j=0;j<4;j++) WW[j][i]=0.0;
  for(i=0;i<NP;i++) WS[i]=0.0;
  for(i=0;i<NP;i++) WR[i]=0.0;

/**
   +----------------------+
   | {r0}= {b} - [A]{xini} |
   +----------------------+
**/

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

  for(j=0;j<N;j++){
    WW[DD][j]= 1.0/D[j];
    WVAL= B[j] - D[j]*X[j];

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

  BNRM20= 0.e0;
  for(i=0;i<N;i++){
    BNRM20+= B[i]*B[i];}

  MPI_Allreduce (&BNRM20, &BNRM2, 1, MPI_DOUBLE,MPI_SUM, MPI_COMM_WORLD);
```

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)

```
#include <stdio.h>
#include <math.h>
#include "mpi.h"
#include "precision.h"
#include "allocate.h"
static MPI_Status  *sta1,*sta2;
static MPI_Request *req1,*req2;
static KINT NFLAG=0;
extern FILE *fp_log;
void SOLVER_SEND_RECV( int N, int NEIBPETOT,
        int NEIBPE[], int IMPORT_INDEX[], int IMPORT_ITEM[],
        int EXPORT_INDEX[], int EXPORT_ITEM[],
        KREAL WS[], KREAL WR[], KREAL X[], int my_rank)
{
        int  ii,k,neib,istart,inum;
/***
        INIT.
***/
        if( NFLAG == 0 ){
                sta1=(MPI_Status*)allocate_vector(sizeof(MPI_Status),NEIBPETOT);
                sta2=(MPI_Status*)allocate_vector(sizeof(MPI_Status),NEIBPETOT);
                req1=(MPI_Request*)allocate_vector(sizeof(MPI_Request),NEIBPETOT);
                req2=(MPI_Request*)allocate_vector(sizeof(MPI_Request),NEIBPETOT);
                NFLAG=1;}
/***
        SEND
***/

 for( neib=1;neib<=NEIBPETOT;neib++){
    istart=EXPORT_INDEX[neib-1];
    inum  =EXPORT_INDEX[neib]-istart;
    for( k=istart;k<istart+inum;k++){
      ii= EXPORT_ITEM[k];
     WS[k]= X[ii-1];
    }

    MPI_Isend(&WS[istart],inum,MPI_DOUBLE,
              NEIBPE[neib-1],0,MPI_COMM_WORLD,&req1[neib-1]);
  }
```

SOLVER_SEND_RECV (2/2)

```
/***
        RECEIVE
***/

 for( neib=1;neib<=NEIBPETOT;neib++){
    istart=IMPORT_INDEX[neib-1];
    inum  =IMPORT_INDEX[neib]-istart;
    MPI_Irecv(&WR[istart],inum,MPI_DOUBLE,
              NEIBPE[neib-1],0,MPI_COMM_WORLD,&req2[neib-1]);
  }

  MPI_Waitall (NEIBPETOT, req2, sta2);

  for( neib=1;neib<=NEIBPETOT;neib++){
    istart=IMPORT_INDEX[neib-1];
    inum  =IMPORT_INDEX[neib]-istart;
    for( k=istart;k<istart+inum;k++){
      ii   = IMPORT_ITEM[k];
      X[ii-1]= WR[k];
    }
  }

  MPI_Waitall (NEIBPETOT, req1, sta1);

}
```

CG Solver (3/6)

```
 for( ITER=1;ITER<= MAXIT;ITER++){

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

/**
   +---------------+
   | {RHO}= {r}{z} |
   +---------------+
**/
    RHO0= 0.e0;

    for(i=0;i<N;i++){
      RHO0+= WW[R][i]*WW[Z][i];
    }
    MPI_Allreduce (&RHO0, &RHO, 1, MPI_DOUBLE,MPI_SUM,
                   MPI_COMM_WORLD);

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

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

for **i= 1, 2, …**

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

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

if i=1

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

else

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

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

endif

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

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

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

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

check convergence $|r|$

end

CG Solver (4/6)

```
/**
   +-------------+
   | {q}= [A]{p} |
   +-------------+
**/

    SOLVER_SEND_RECV
      ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,
        EXPORT_INDEX, EXPORT_ITEM, WS, WR, WW[P], my_rank);

    for( j=0;j<N;j++){
      WVAL= D[j] * WW[P][j];
      for(k=indexLU[j];k<indexLU[j+1];k++){
        i=itemLU[k];
        WVAL+= AMAT[k] * WW[P][i];
      }
      WW[Q][j]=WVAL;
    }

/**
   +---------------------+
   | ALPHA= RHO / {p}{q} |
   +---------------------+
**/
    C10= 0.e0;
    for(i=0;i<N;i++){
      C10+=WW[P][i]*WW[Q][i];
    }

    MPI_Allreduce (&C10,&C1, 1, MPI_DOUBLE,MPI_SUM,
                   MPI_COMM_WORLD);

    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)

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

    DNRM20= 0.e0;
    for(i=0;i<N;i++){
      DNRM20+=WW[R][i]*WW[R][i];
    }
    MPI_Allreduce (&DNRM20,&DNRM2, 1, MPI_DOUBLE,MPI_SUM,
                   MPI_COMM_WORLD);

    RESID= sqrt(DNRM2/BNRM2);

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

    RHO1 = RHO ;
}


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

  free ( (KREAL**)WW);
  deallocate_vector ( (KREAL**)WR);
  deallocate_vector( (KREAL**)WS);
}
```

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

for i= 1, 2, …

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

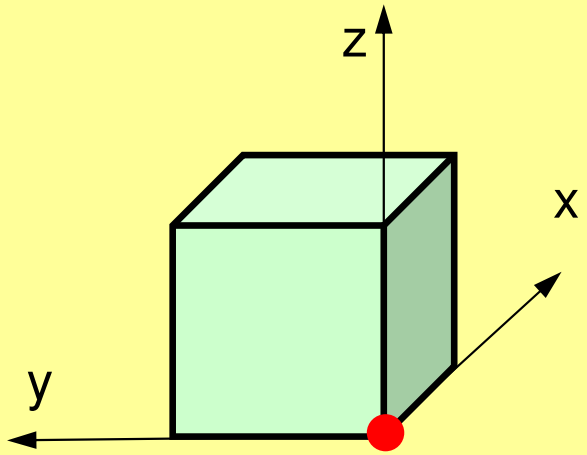
end

CG Solver (6/6)

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

    DNRM20= 0.e0;
    for(i=0;i<N;i++){
      DNRM20+=WW[R][i]*WW[R][i];
    }
    MPI_Allreduce (&DNRM20,&DNRM2, 1, MPI_DOUBLE,MPI_SUM,
                   MPI_COMM_WORLD);

    RESID= sqrt(DNRM2/BNRM2);

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

    RHO1 = RHO ;
}


  SOLVER_SEND_RECV                                          Updated temperature for external nodes
    ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,
      EXPORT_INDEX, EXPORT_ITEM, WS, WR, X, my_rank);

  free ( (KREAL**)WW);
  deallocate_vector ( (KREAL**)WR);
  deallocate_vector( (KREAL**)WS);
}
```

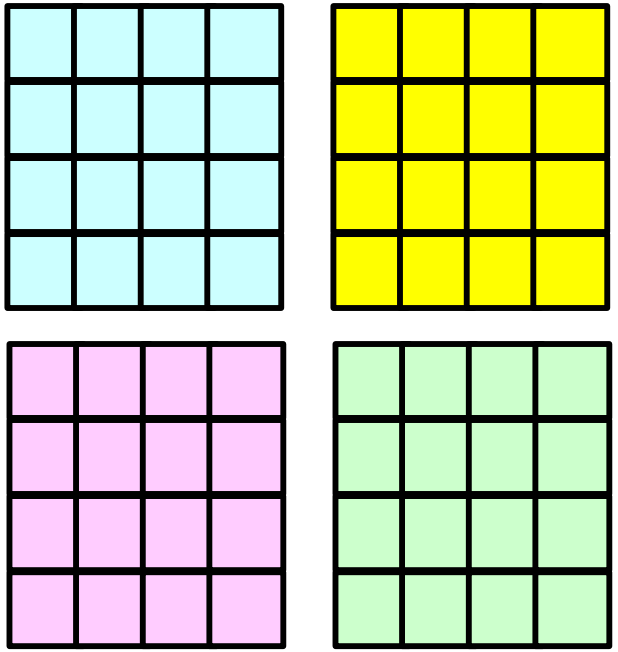
Final Output & Validation

```
  SOLVE11();

  OUTPUT_UCD()     ;

  for(i=0;i<N;i++){
    if (XYZ[i][0]==0.e0) {
    if (XYZ[i][1]==0.e0) {
    if (XYZ[i][2]==0.e0) {
      printf("%6d%8d%16.6e¥n¥n¥n", my_rank, i+1, X[i]);}
  }}}


  PFEM_FINALIZE() ;
}
```



OUTPUT_UCD for Visualization

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



Time for Computation

```
/**
   +-----------------+
   | MATRIX assemble |
   +-----------------+
**/
  START_TIME= MPI_Wtime();

    MAT_ASS_MAIN();
    MAT_ASS_BC()  ;

  END_TIME= MPI_Wtime();

  if (my_rank == 0) {
    fprintf(stdout,"*** matrix ass.  %e sec.¥n",END_TIME-START_TIME);
  }

/**
   +--------+
   | SOLVER |
   +--------+
**/
  START_TIME= MPI_Wtime();

    SOLVE11();

  END_TIME= MPI_Wtime();

  if (my_rank == 0) {
    fprintf(stdout,"*** real COMP.  %e sec.¥n",END_TIME-START_TIME);
  }
```

Example

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

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

```
>$ cd /home/ra020019/<Your-UID>/pFEM/pfem3d/mesh

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

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

inp_mg

```
255 255 191
```

inp_kmetis

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

255x255x191 elements
256x256x192 nodes
48x8= 384 partitions

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

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

>$ pjsub a08k.sh
```

INPUT.DAT

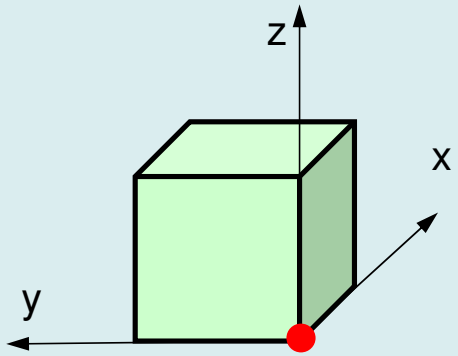
```
../mesh/aaa
2000
1.0 1.0
1.0e-08
```

a08k.sh

```
#!/bin/sh
#PJM -N "flat-08"
#PJM -L rscgrp=small
#PJM -L node=8:torus
#PJM --mpi "max-proc-per-node=48"
#PJM -L elapse=00:15:00
#PJM -g ra020019
#PJM -j
#PJM -e err
#PJM -o a08k.lst


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

a08k.lst

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

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

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



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

```
>$ cd /home/ra020019/<Your-UID>/pFEM/pfem3d/pmesh

<modify mesh.inp, mg.sh>

>$ pjsub mg.sh
```

mesh.inp

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

255x255x191 elements
256x256x192 nodes
48x8= 384 partitions

mg.sh

```
#!/bin/sh
#PJM -N "pmg"
#PJM -L "rscgrp=small"
#PJM -L "node=8:torus"
#PJM --mpi "max-proc-per-node=48"
#PJM -L elapse=00:10:00
#PJM -g ra020019
#PJM -j
#PJM -e err
#PJM -o pmg.lst

mpiexec ./pmesh
rm wk.*
```

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

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

>$ pjsub a08.sh
```

INPUT.DAT

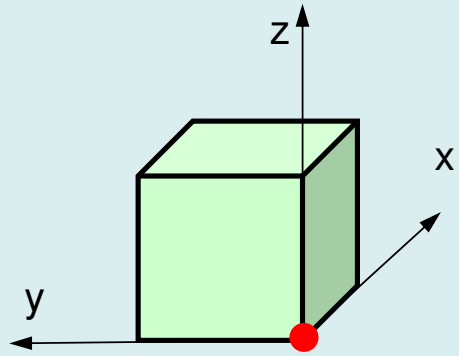
```
../pmesh/pcube
2000
1.0 1.0
1.0e-08
```

a08.sh

```
#!/bin/sh
#PJM -N "flat-08"
#PJM -L "rscgrp=small"
#PJM -L "node=8:torus"
#PJM --mpi "max-peoc-per-node=48"
#PJM -L elapse=00:15:00
#PJM -g ra020019
#PJM -j
#PJM -e err
#PJM -o a08.lst


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

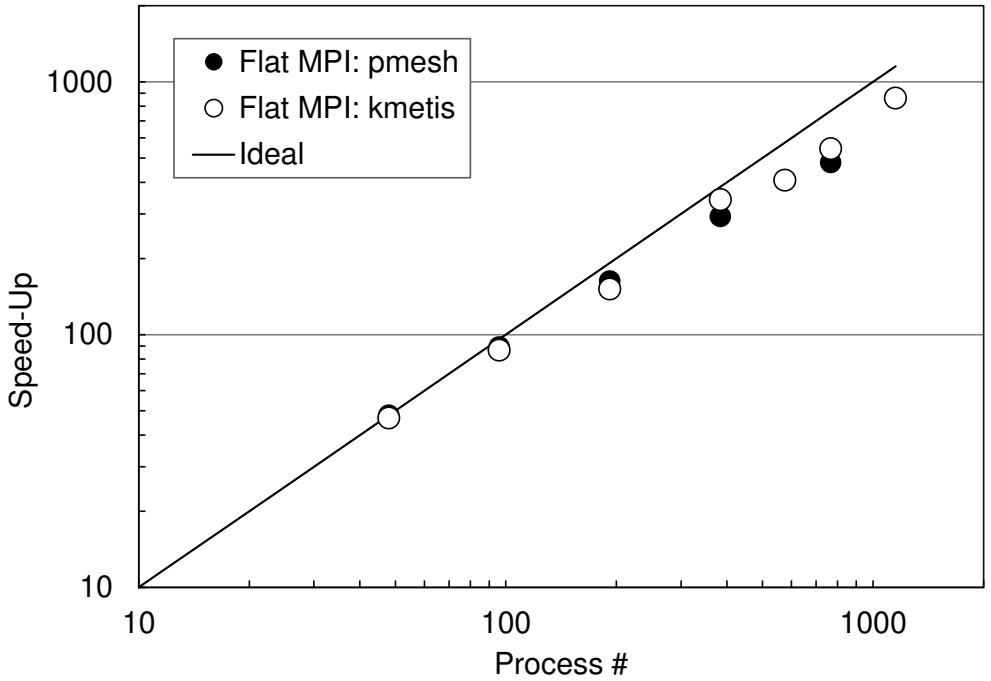
a08.lst

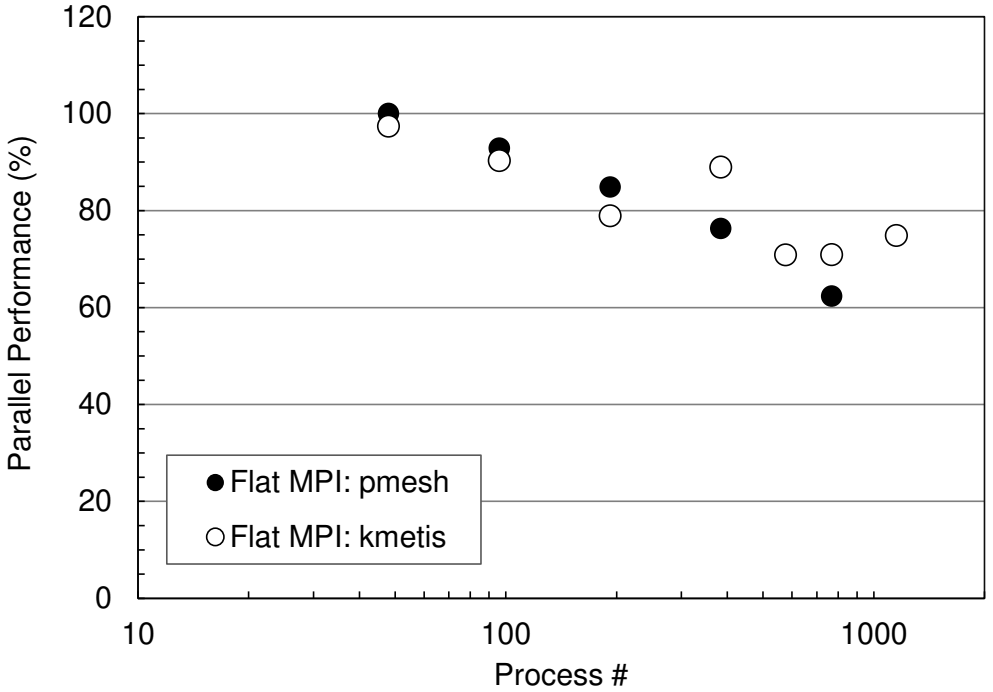
```
*** matrix conn.      3.516576E-02 sec.
*** matrix ass.       4.487921E-02 sec.

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

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



Example: Strong Scaling: C

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

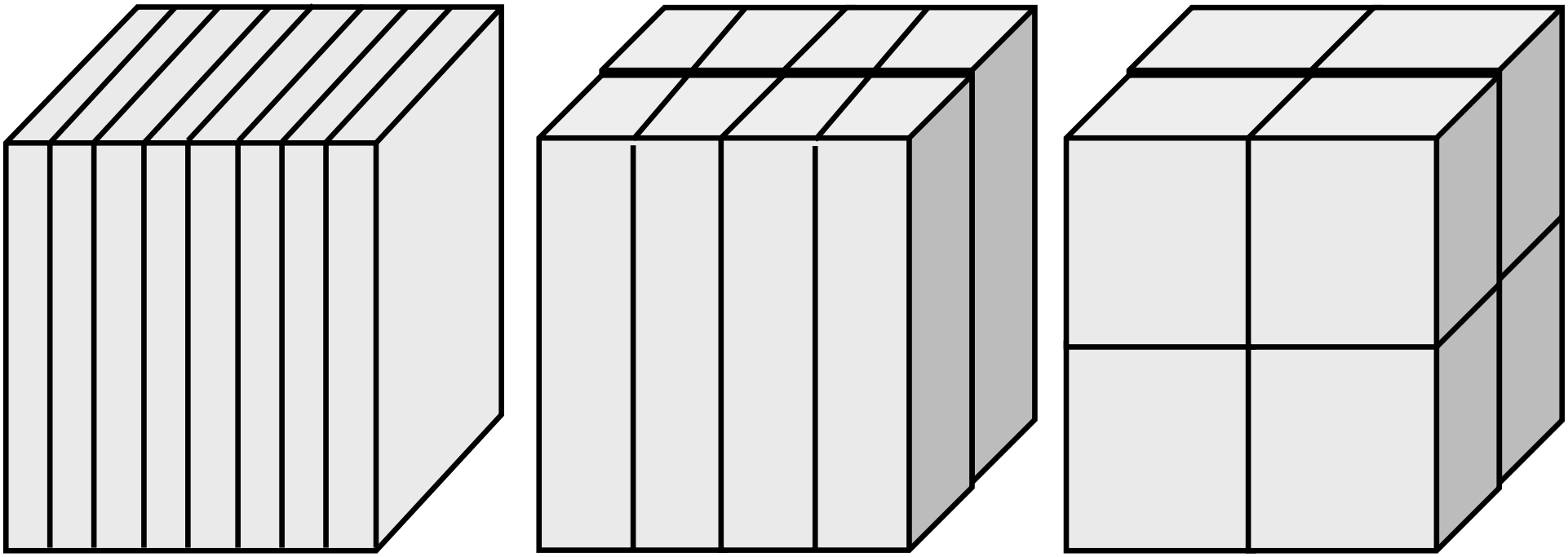




Exercise (1/2)

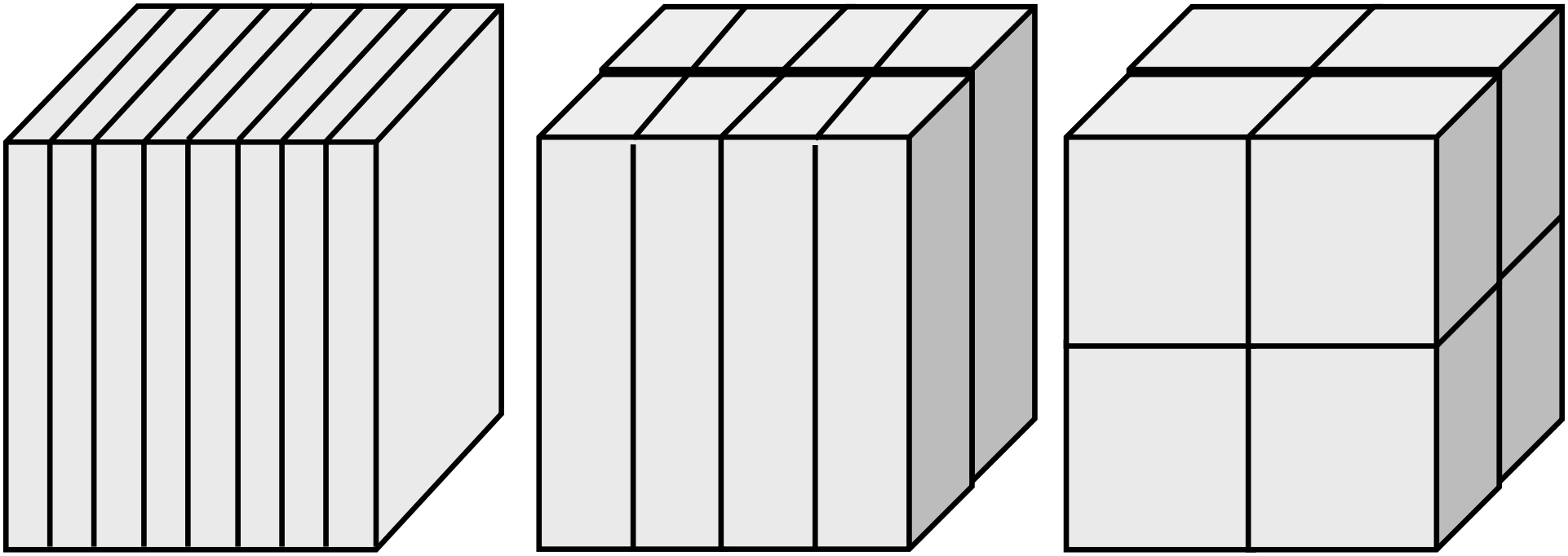
- Evaluation behavior and performance of “sol”
- Example
  - Strong Scaling
    - Fixed entire problem size
  - Weak Scaling
    - Fixed problem size/core, time for 1 iterations
  - Parameters
    - Problem size
    - Domain decomposition (1D-3D, kmetis, pmetis)
- “*.inp” may take long time.
  - delete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

1D-3D Decomposition



1D-3D Decomposition

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



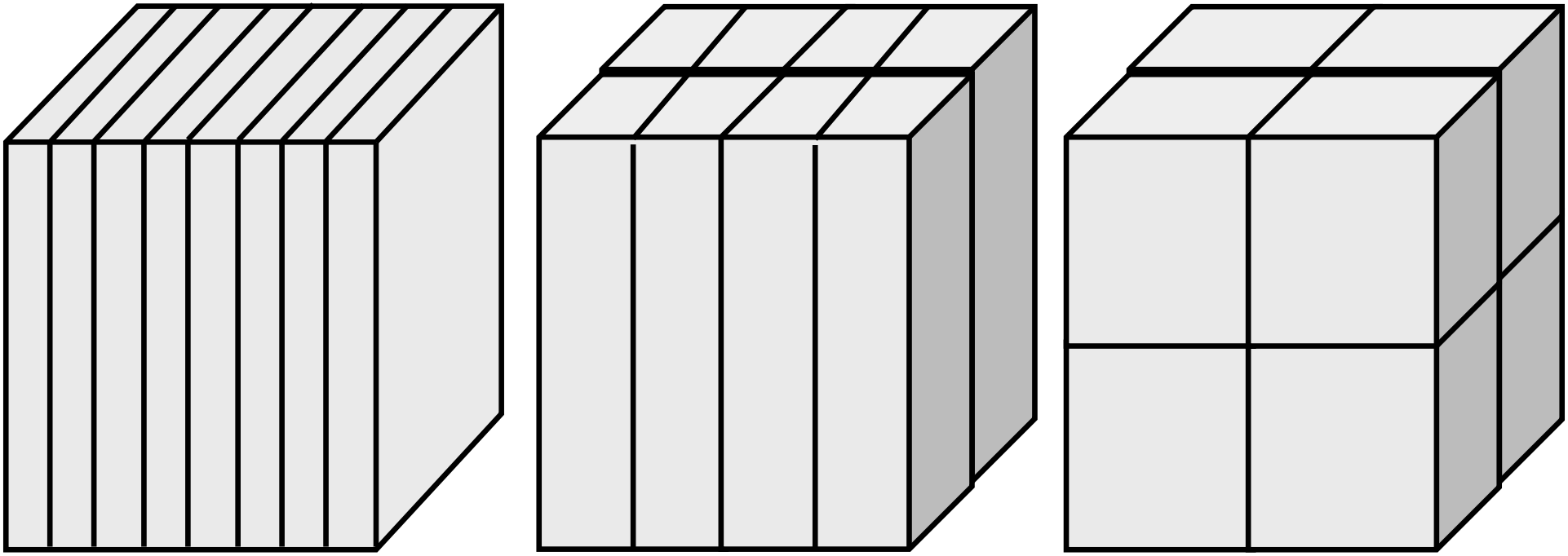
16 N^2 x 7 = 112 N^2

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)

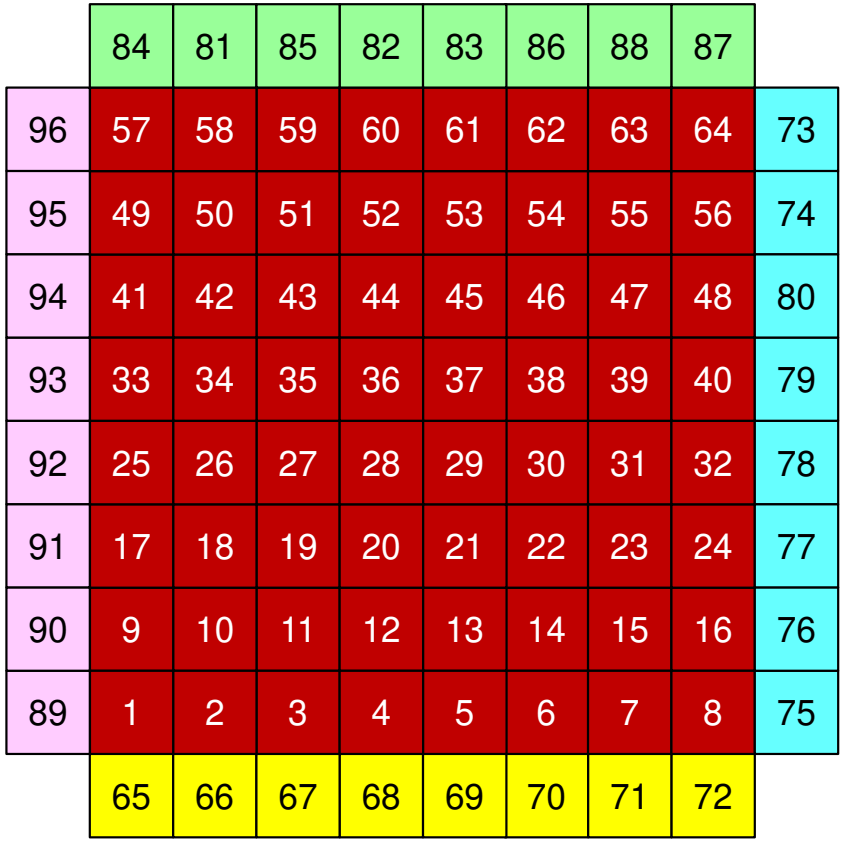
- Improve PE-to-PE communication part (solver_SR)
  - Copying to receiving buffer, Combining MPI_Wait_all
- Actually, numbering of external nodes in each neighboring domain is continuous
- You can also apply this to 1D case

```
for (neib=0; neib<NeibPETot; neib++){
   tag= 0;
   iS_i= import_index[neib];
   iE_i= import_index[neib+1];
   BUFlength_i= iE_i - iS_i

   ierr= MPI_Irecv
         (&RecvBuf[iS_i], BUFlength_i, MPI_DOUBLE, NeibPE[neib], 0,
          MPI_COMM_WORLD, &ReqRecv[neib])
}

MPI_Waitall(NeibPETot, ReqRecv, StatRecv);

for (neib=0; neib<NeibPETot;neib++){
    for (k=import_index[neib];k<import_index[neib+1];k++){
       kk= import_item[k];
       VAL[kk]= RecvBuf[k];
    }
}
```

SEND/RECV (Original)

```
sta1=(MPI_Status*)allocate_vector(sizeof(MPI_Status),NEIBPETOT);
sta2=(MPI_Status*)allocate_vector(sizeof(MPI_Status),NEIBPETOT);
req1=(MPI_Request*)allocate_vector(sizeof(MPI_Request),NEIBPETOT);
req2=(MPI_Request*)allocate_vector(sizeof(MPI_Request),NEIBPETOT);

for( neib=1;neib<=NEIBPETOT;neib++){
      istart=EXPORT_INDEX[neib-1];
      inum  =EXPORT_INDEX[neib]-istart;
      for( k=istart;k<istart+inum;k++){
                ii= EXPORT_ITEM[k];
               WS[k]= X[ii-1];}

      MPI_Isend(&WS[istart],inum,MPI_DOUBLE,
          NEIBPE[neib-1],0,MPI_COMM_WORLD,&req1[neib-1]);}


for( neib=1;neib<=NEIBPETOT;neib++){
      istart=IMPORT_INDEX[neib-1];
      inum  =IMPORT_INDEX[neib]-istart;
      MPI_Irecv(&WR[istart],inum,MPI_DOUBLE,
          NEIBPE[neib-1],0,MPI_COMM_WORLD,&req2[neib-1]);}

MPI_Waitall (NEIBPETOT, req2, sta2);

for( neib=1;neib<=NEIBPETOT;neib++){
      istart=IMPORT_INDEX[neib-1];
      inum  =IMPORT_INDEX[neib]-istart;
      for( k=istart;k<istart+inum;k++){
                ii   = IMPORT_ITEM[k];
               X[ii-1]= WR[k];}
}


MPI_Waitall (NEIBPETOT, req1, sta1);
```

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



SEND/RECV (NEW:1)

```
sta1=(MPI_Status*)allocate_vector(sizeof(MPI_Status),2*NEIBPETOT);
req1=(MPI_Request*)allocate_vector(sizeof(MPI_Request),2*NEIBPETOT);

for( neib=1;neib<=NEIBPETOT;neib++){
      istart=EXPORT_INDEX[neib-1];
      inum  =EXPORT_INDEX[neib]-istart;
      for( k=istart;k<istart+inum;k++){
                ii= EXPORT_ITEM[k];
                WS[k]= X[ii-1];}

      MPI_Isend(&WS[istart],inum,MPI_DOUBLE,
          NEIBPE[neib-1],0,MPI_COMM_WORLD,&req1[neib-1]);}


for( neib=1;neib<=NEIBPETOT;neib++){
      istart=IMPORT_ITEM[IMPORT_INDEX[neib-1]];
      inum  =IMPOERT_INDEX[neib] - IMPORT_INDEX[neib-1];;
      MPI_Irecv(&X[istart],inum,MPI_DOUBLE,
          NEIBPE[neib-1],0,MPI_COMM_WORLD,&req1[NEIBPETOT+neib-1]);}


MPI_Waitall (2*NEIBPETOT, req1, sta1);
```

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

```
sta1=(MPI_Status*)allocate_vector(sizeof(MPI_Status),2*NEIBPETOT);
req1=(MPI_Request*)allocate_vector(sizeof(MPI_Request),2*NEIBPETOT);

for( neib=1;neib<=NEIBPETOT;neib++){
      istart=EXPORT_INDEX[neib-1];
      inum  =EXPORT_INDEX[neib]-istart;
      for( k=istart;k<istart+inum;k++){
                ii= EXPORT_ITEM[k];
                WS[k]= X[ii-1];}

      MPI_Isend(&WS[istart],inum,MPI_DOUBLE,
          NEIBPE[neib-1],0,MPI_COMM_WORLD,&req1[neib-1]);}


for( neib=1;neib<=NEIBPETOT;neib++){
      istart=IMPORT_INDEX[neib-1] + N0;
      inum  =IMPORT_INDEX[neib] - IMPORT_INDEX[neib-1];
      MPI_Irecv(&X[istart],inum,MPI_DOUBLE,
          NEIBPE[neib-1],0,MPI_COMM_WORLD,&req1[NEIBPETOT+neib-1]);}


MPI_Waitall (2*NEIBPETOT, req1, sta1);
```

N0: Total Number of Internal Nodes