

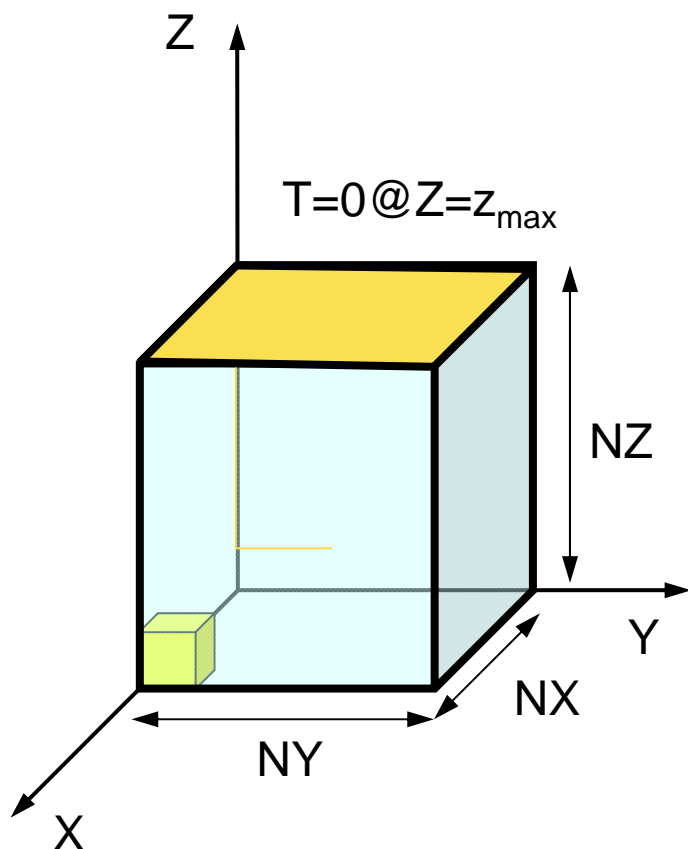
並列有限要素法による 三次元定常熱伝導解析プログラム (2/2) Fortran編

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対象とする問題：三次元定常熱伝導

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



- 定常熱伝導＋発熱
- 一様な熱伝導率 λ
- 直方体
 - 一辺長さ1の立方体（六面体）要素
 - 各方向に $NX \cdot NY \cdot NZ$ 個
- 境界条件
 - $T=0@Z=z_{\max}$
- 体積当たり発熱量は位置（メッシュの中心の座標 x_c, y_c ）に依存
 - $\dot{Q}(x, y, z) = QVOL|x_c + y_c|$

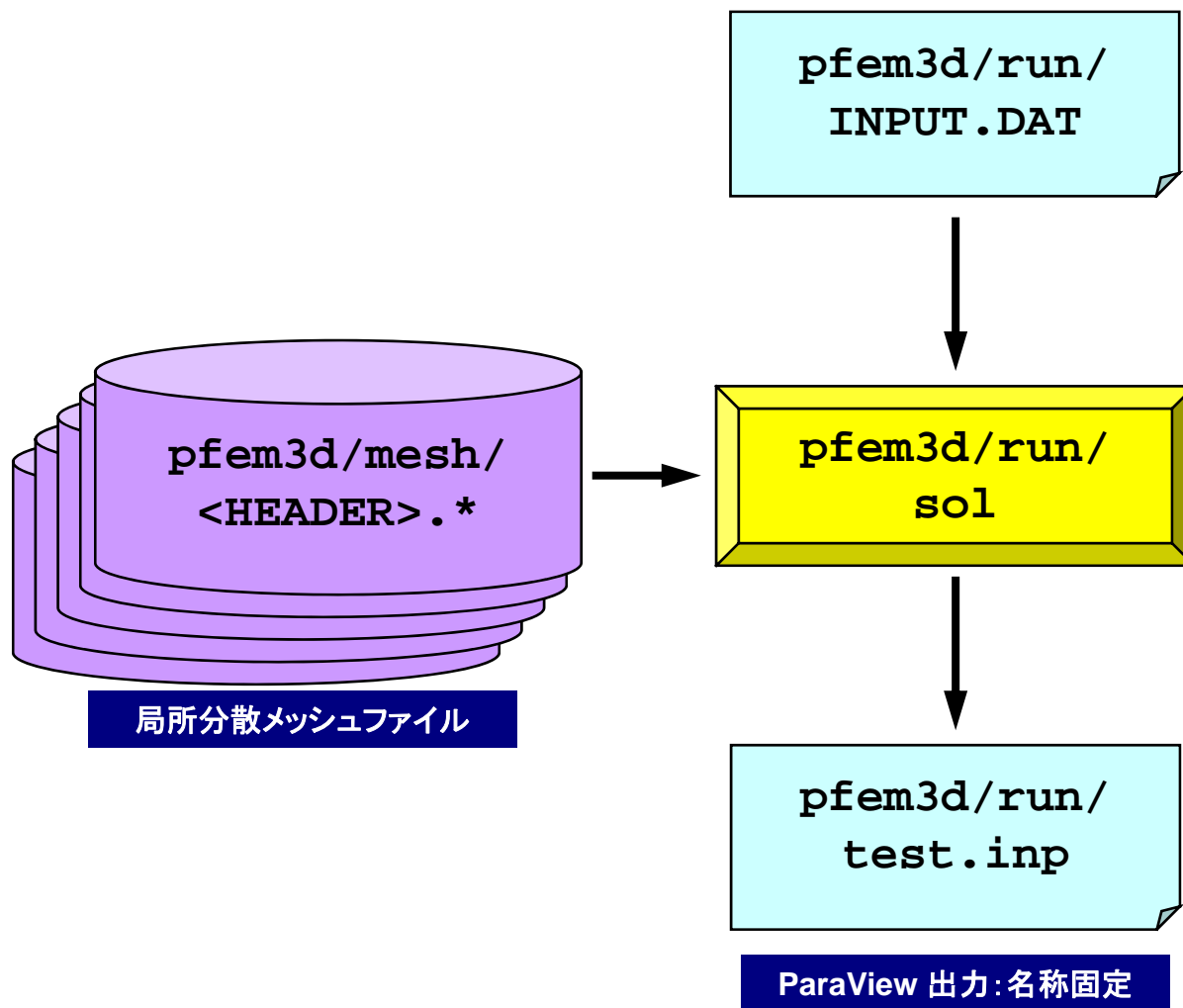
有限要素法の処理

- 支配方程式
- ガラーキン法：弱形式
- 要素単位の積分
 - 要素マトリクス生成
- 全体マトリクス生成
- 境界条件適用
- 連立一次方程式

並列有限要素法の処理：プログラム

- 初期化
 - 制御変数読み込み
 - 座標読み込み⇒要素生成 (N:節点数, NE:要素数)
 - 配列初期化 (全体マトリクス, 要素マトリクス)
 - 要素⇒全体マトリクスマッピング (Index, Item)
- マトリクス生成
 - 要素単位の処理 (do icel= 1, NE)
 - 要素マトリクス計算
 - 全体マトリクスへの重ね合わせ
 - 境界条件の処理
- 連立一次方程式
 - 共役勾配法 (CG)

並列有限要素法の手順（並列計算実行）



制御ファイル：INPUT.DAT

```

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

```

- HEADER : 局所分散ファイルヘッダ名
<HEADER>.my_rank
- ITER : 反復回数上限
- COND : 熱伝導率
- QVOL : 体積当たり発熱量係数
- RESID : 反復法の収束判定値

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

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

~/pFEM/pfem3d/run/go.sh

```
#!/bin/sh
#PJM -L "node=1"          ノード数 (≦12)
#PJM -L "elapse=00:10:00" 実行時間 (≦15分)
#PJM -L "rscgrp=school"   実行キュー名
#PJM -
#PJM -o "test.lst"        標準出力
#PJM --mpi "proc=8"      MPIプロセス数 (≦192)

mpiexec ./sol
```

8分割

"node=1"

"proc=8"

16分割

"node=1"

"proc=16"

32分割

"node=2"

"proc=32"

64分割

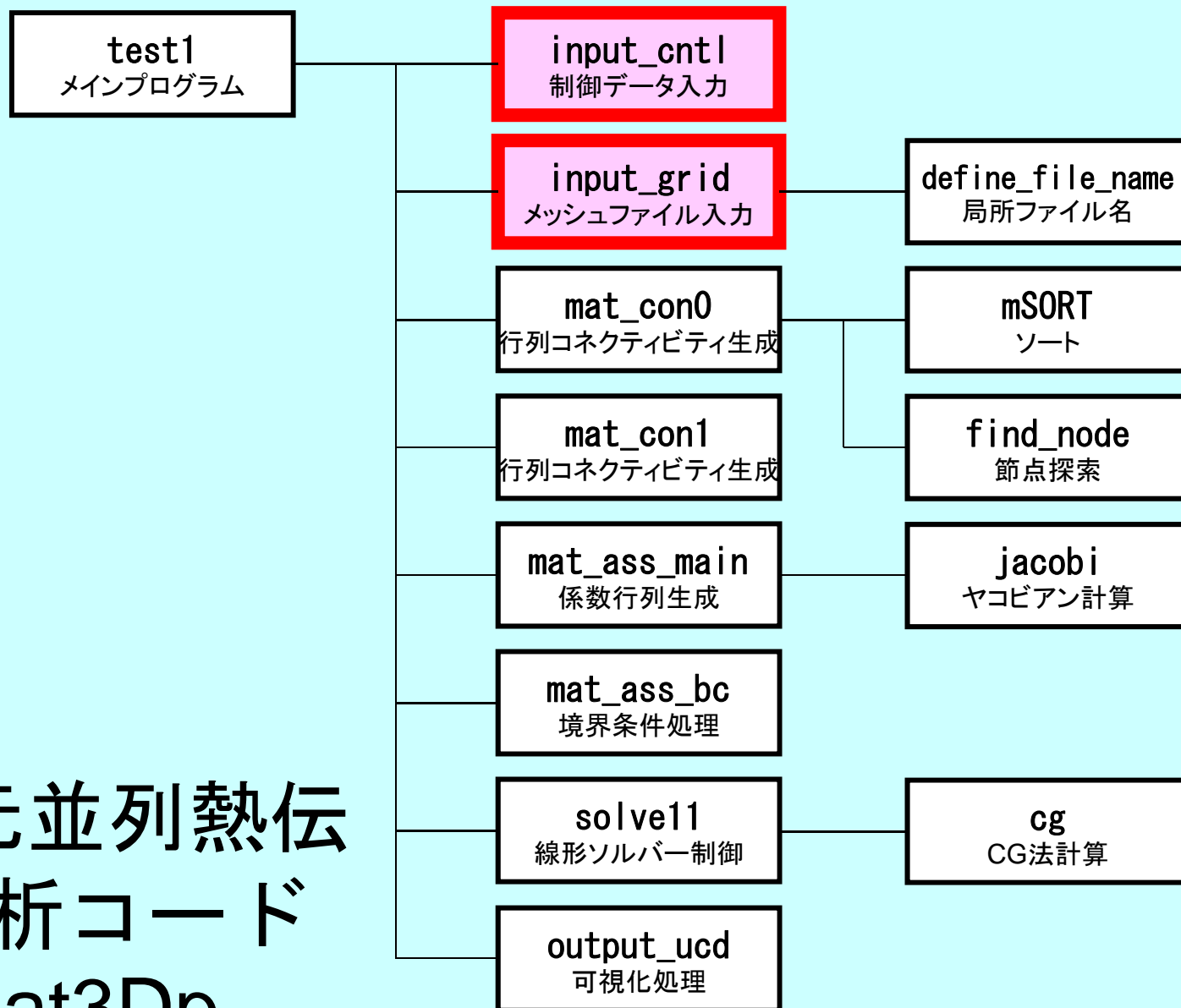
"node=4"

"proc=64"

192分割

"node=12"

"proc=192"



三次元並列熱伝 導解析コード heat3Dp

全体処理

```
program heat3Dp

use solver11
use pfem_util

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

call PFEM_INIT

call INPUT_CNTL
call INPUT_GRID

call MAT_CONO
call MAT_CON1

call MAT_ASS_MAIN
call MAT_ASS_BC

call SOLVE11

call OUTPUT_UCD

call PFEM_FINALIZE

end program heat3Dp
```

Global変数表 : pfem_util.f (1/4)

変数名	種別	サイズ	I/O	内 容
fname	C	(80)	I	メッシュファイル名
N, NP	I		I	節点数 (N : 内点, NP : 内点+外点)
ICELTOT	I		I	要素数
NODGRPtot	I		I	節点グループ数
XYZ	R	(NP, 3)	I	節点座標
ICELNOD	I	(ICELTOT, 8)	I	要素コネクティビティ
NODGRP_INDEX	I	(0:NODGRPtot)	I	各節点グループに含まれる節点数 (累積)
NODGRP_ITEM	I	(NODGRP_INDEX (NODGRPtot))	I	節点グループに含まれる節点
NODGRP_NAME	C80	(NODGRPtot)	I	節点グループ名
NLU	I		O	各節点非対角成分数
NPLU	I		O	非対角成分総数
D	R	(NP)	O	全体行列 : 対角ブロック
B, X	R	(NP)	O	右辺ベクトル, 未知数ベクトル

Global変数表 : pfem_util.f (2/4)

変数名	種別	サイズ	I/O	内 容
AMAT	R	(NPLU)	O	全体行列 : 非零非対角成分
index	I	(0:NP)	O	全体行列 : 非零非対角成分数
item	I	(NPLU)	O	全体行列 : 非零非対角成分 (列番号)
INLU	I	(NP)	O	各節点の非零非対角成分数
IALU	I	(NP, NLU)	O	各節点の非零非対角成分数 (列番号)
IWKX	I	(NP, 2)	O	ワーク用配列
ITER, ITERactual	I		I	反復回数の上限, 実際の反復回数
RESID	R		I	打ち切り誤差 (1.e-8に設定)

Global変数表 : pfem_util.f (3/4)

変数名	種別	サイズ	I/O	内 容
08th	R		I	=0.125
PNQ, PNE, PNT	R	(2, 2, 8)	O	各ガウス積分点における $\frac{\partial N_i}{\partial \xi}, \frac{\partial N_i}{\partial \eta}, \frac{\partial N_i}{\partial \zeta} (i=1\sim 8)$
POS, WEI	R	(2, 2)	O	各ガウス積分点の座標, 重み係数
NCOL1, NCOL2	I	(100)	O	ソート用ワーク配列
SHAPE	R	(2, 2, 2, 8)	O	各ガウス積分点における形状関数 $N_i (i=1\sim 8)$
PNX, PNY, PNZ	R	(2, 2, 2, 8)	O	各ガウス積分点における $\frac{\partial N_i}{\partial x}, \frac{\partial N_i}{\partial y}, \frac{\partial N_i}{\partial z} (i=1\sim 8)$
DETJ	R	(2, 2, 2)	O	各ガウス積分点におけるヤコビアン行列式
COND, QVOL	R		I	熱伝導率, 体積当たり発熱量係数

Global変数表 : pfem_util.f (4/4)

変数名	種別	サイズ	I/O	内 容
PETOT	I		O	領域数 (MPIプロセス数)
my_rank	I		O	MPIプロセス番号
errno	I		O	エラーフラグ
NEIBPETOT	I		I	隣接領域数
NEIBPE	I	(NEIBPETOT)	I	隣接領域番号
IMPORT_INDEX EXPORT_INEDX	I	(0:NEIBPETOT)	I	送信, 受信テーブルのサイズ (一次元圧縮配列)
IMPORT_ITEM	I	(Npimport)	I	受信テーブル (外点) (NPimport=IMPORT_INDEX (NEIBPETOT))
EXPORT_ITEM	I	(Npexport)	I	送信テーブル (境界点) (NPexport=EXPORT_INDEX (NEIBPETOT))
ICELTOT_INT	I		I	領域所属要素数
intELEM_list	I	(ICELTOT_INT)	I	領域所属要素のリスト: 可視化に使用

開始, 終了 : 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
```

制御ファイル入力 : 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
```

メッシュ入力 : 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
```


分散メッシュファイル名： DEFINE_FILE_NAME

HEADER+ランク番号，実際は 10^6 個まで可能

```
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関数 : C言語

```
#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 );
}
```

allocateをFORTRAN並みに
簡単にやるための関数

メッシュ入力 : 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)
```

メッシュ入力 : 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

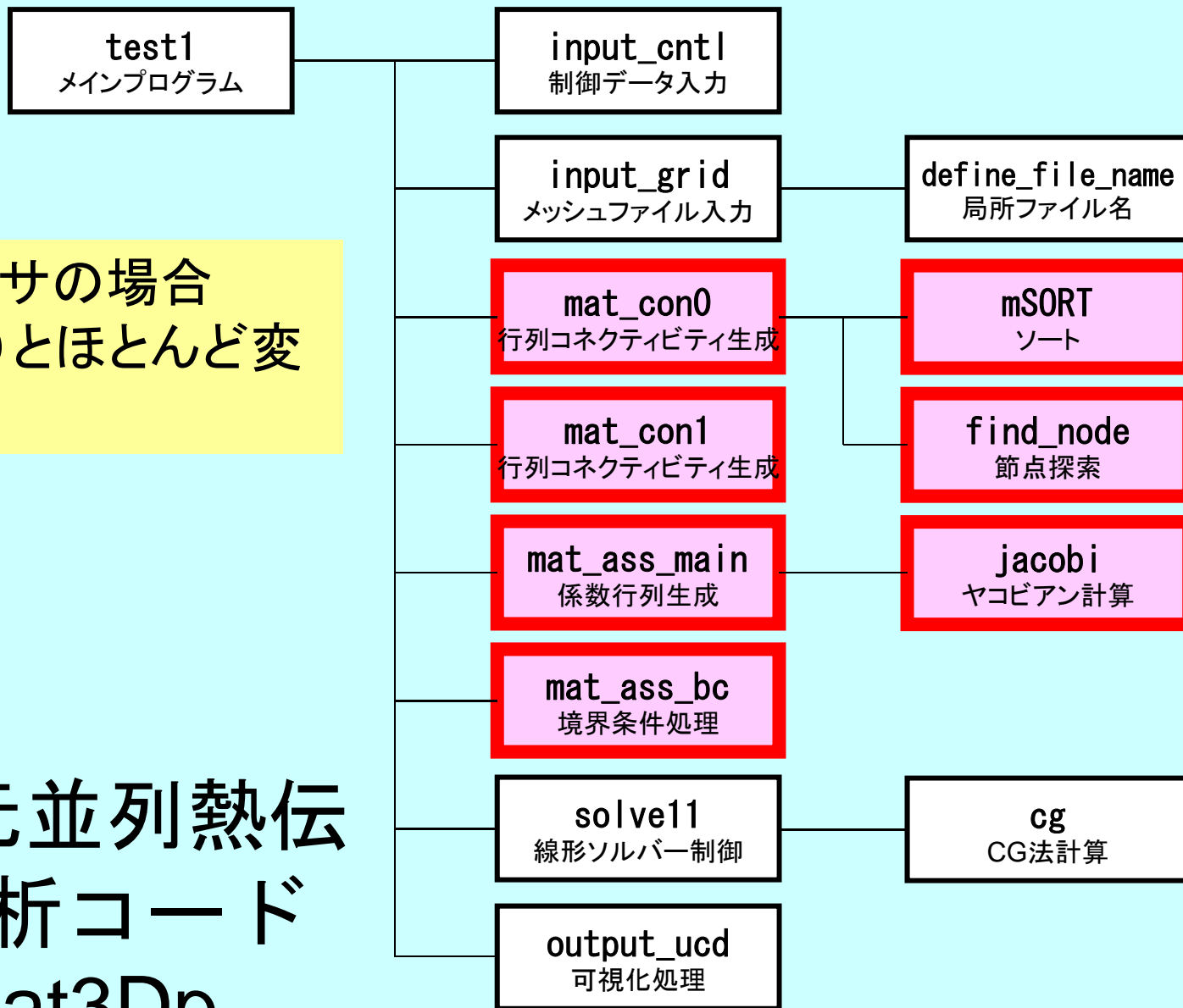
read (11,'(10i10)') (NODGRP_INDEX(i), i= 1, NODGRPtot)
nn= NODGRP_INDEX(NODGRPtot)
allocate (NODGRP_ITEM(nn))

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

```

並列有限要素法の処理：プログラム

- 初期化
 - 制御変数読み込み
 - 座標読み込み⇒要素生成 (N:節点数, NE:要素数)
 - 配列初期化 (全体マトリクス, 要素マトリクス)
 - 要素⇒全体マトリクスマッピング (Index, Item)
- マトリクス生成
 - 要素単位の処理 (do icel= 1, NE)
 - 要素マトリクス計算
 - 全体マトリクスへの重ね合わせ
 - 境界条件の処理
- 連立一次方程式
 - 共役勾配法 (CG)



1プロセッサの場合
(heat3D)とほとんど変
わらない

三次元並列熱伝 導解析コード heat3Dp

マトリクス生成まで

- 一次元の場合は, index, itemに関連した情報を簡単に作ることができた
 - 非ゼロ非対角成分の数は2
 - 番号が自分に対して : +1と-1
- 三次元の場合はもっと複雑
 - 非ゼロ非対角ブロックの数は7~26 (現在の形状)
 - 実際はもっと複雑
 - 前以て, 非ゼロ非対角ブロックの数はわからない

マトリクス生成まで

- 一次元の場合は, index, itemに関連した情報を簡単に作ることができた
 - 非ゼロ非対角成分の数は2
 - 番号が自分に対して : +1と-1
- 三次元の場合はもっと複雑
 - 非ゼロ非対角ブロックの数は7~26 (現在の形状)
 - 実際はもっと複雑
 - 前以て, 非ゼロ非対角ブロックの数はわからない
- INLU(N), IALU(N,NLU) を使って非ゼロ非対角成分数を予備的に勘定する

全体処理

```
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

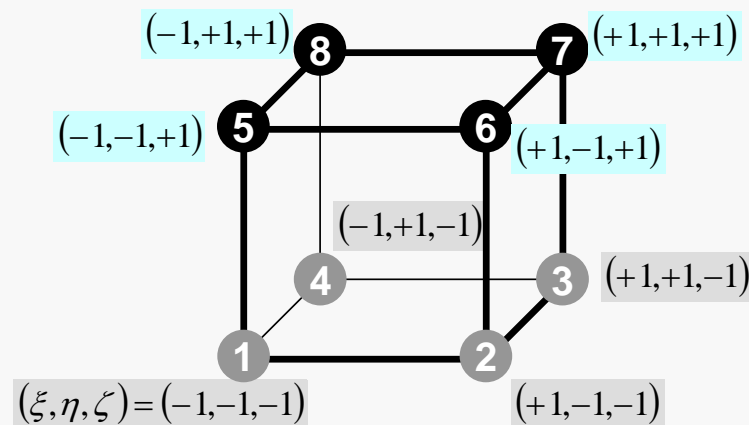
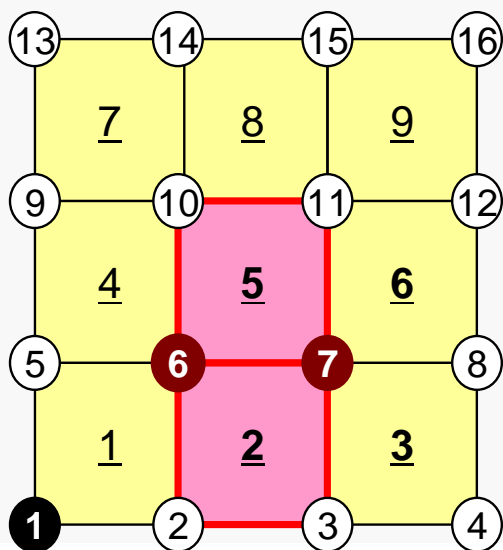
call PFEM_FINALIZE

end program heat3Dp
```

MAT_CON0: INLU, IALU生成
MAT_CON1: index, item生成

MAT_CON0 : 全体構成

```
do icel= 1, ICELTOT
  8節点相互の関係から,
  INL, INU, IAL, IAUを生成
  (FIND_NODE)
enddo
```



行列コネクティビティ生成： MAT_CONO (1/4)

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

NLU= 26

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

INLU= 0
IALU= 0
```

NLU:
各節点における
非ゼロ非対角成分
の最大数
(接続する節点数)

今の問題の場合は
わかっているので、
このようにできる

不明の場合の実装:
⇒レポート課題

行列コネクティビティ生成： MAT_CONO (1/4)

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

NLU= 26

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

INLU= 0
IALU= 0
```

変数名	サイズ	内 容
INLU	(NP)	各節点の非零非対角成分数
IALU	(NP, NLU)	各節点の非零非対角成分 (列番号)

行列コネクティビティ生成： MAT_CON0 (2/4)

```

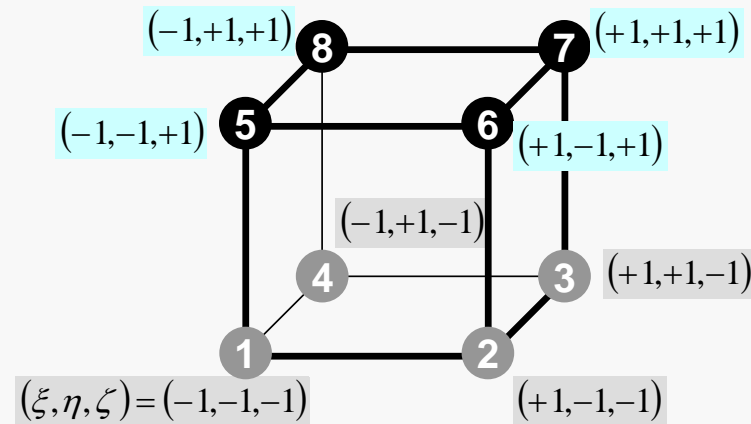
do icel= 1, ICELTOT
  in1= ICELNOD(icel, 1)
  in2= ICELNOD(icel, 2)
  in3= ICELNOD(icel, 3)
  in4= ICELNOD(icel, 4)
  in5= ICELNOD(icel, 5)
  in6= ICELNOD(icel, 6)
  in7= ICELNOD(icel, 7)
  in8= ICELNOD(icel, 8)

  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)

```



節点探索 : FIND_TS_NODE

INL,INU,IAL,IAU探索 : 一次元ではこの部分は手動

```

!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

```

変数名	サイズ	内 容
INLU	(NP)	各節点の非零非対角成分数
IALU	(NP, NLU)	各節点の非零非対角成分 (列番号)

節点探索 : FIND_TS_NODE

一次元ではこの部分は手動

```

!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

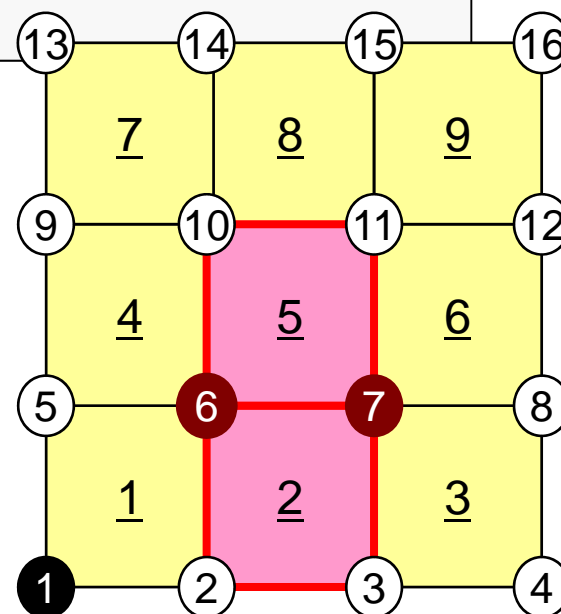
        icou= INLU(ip1) + 1
        IALU(ip1, icou)= ip2
        INLU(ip1      )= icou

        return

      end subroutine FIND_TS_NODE

```

既にIALUに含まれている
場合は、次のペアへ



行列コネクティビティ生成： 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)

```

```

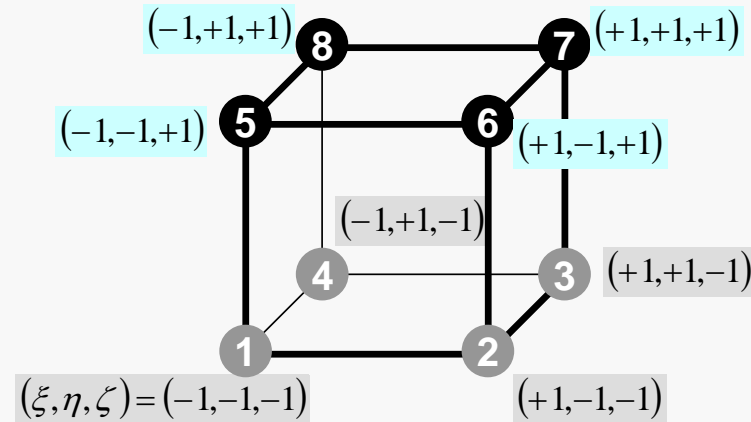
call FIND_TS_NODE (in6, in1)
call FIND_TS_NODE (in6, in2)
call FIND_TS_NODE (in6, in3)
call FIND_TS_NODE (in6, in4)
call FIND_TS_NODE (in6, in5)
call FIND_TS_NODE (in6, in7)
call FIND_TS_NODE (in6, in8)

```

```

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)

```



行列コネクティビティ生成： 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
```

各節点において, IALU[i][k]が
小さい番号から大きい番号に
並ぶようにソート(単純なバブルソート)
せいぜい100程度のものをソートする

CRS形式への変換 : MAT_CON1

```

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

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

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

  NPLU= index(NP)

  allocate (item(NPLU))

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

  deallocate (INLU, IALU)

  end subroutine MAT_CON1

```

C

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

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

FORTRAN

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

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

CRS形式への変換 : MAT_CON1

```
!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=index(NP)
itemのサイズ
非ゼロ非対角成分総数

CRS形式への変換 : MAT_CON1

```
!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
```

itemに1から始まる
節点番号を記憶

CRS形式への変換 : MAT_CON1

```
!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
```

これらはもはや不要

全体処理

```
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 : 全体構成

```

do kpn= 1, 2      ガウス積分点番号 (ζ方向)
  do jpn= 1, 2    ガウス積分点番号 (η方向)
    do ipn= 1, 2  ガウス積分点番号 (ξ方向)
      ガウス積分点 (8個) における形状関数,
      およびその「自然座標系」における微分の算出
    enddo
  enddo
enddo

```

```

do icel= 1, ICELTOT  要素ループ
  8節点の座標から, ガウス積分点における, 形状関数の「全体座標系」における微分,
  およびヤコビアンを算出 (JACOBI)

```

```

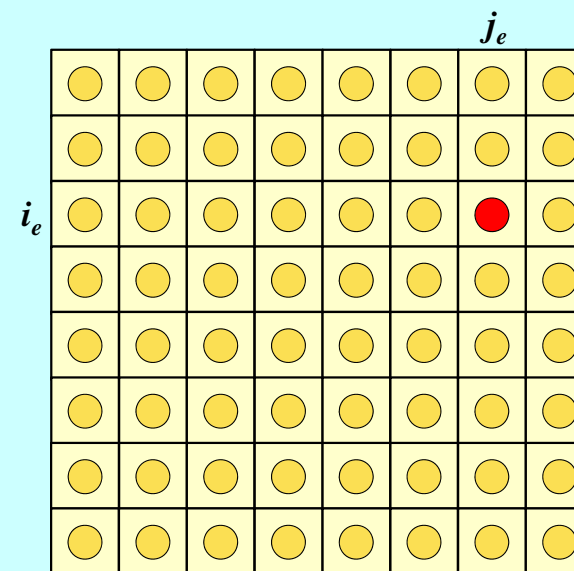
do ie= 1, 8          局所節点番号
  do je= 1, 8        局所節点番号
    全体節点番号 : ip, jp
    Aip, jp の itemLUI におけるアドレス : kk

```

```

do kpn= 1, 2      ガウス積分点番号 (ζ方向)
  do jpn= 1, 2    ガウス積分点番号 (η方向)
    do ipn= 1, 2  ガウス積分点番号 (ξ方向)
      要素積分⇒要素行列成分計算, 全体行列への足しこみ
    enddo
  enddo
enddo
enddo
enddo
enddo

```



係数行列 : MAT_ASS_MAIN (1/6)

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

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

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

  WEI (1)= +1. 0000000000D+00
  WEI (2)= +1. 0000000000D+00

  POS (1)= -0. 5773502692D+00
  POS (2)= +0. 5773502692D+00
```

係数行列 (非零非対角成分)
右辺ベクトル
未知数ベクトル
係数行列 (対角成分)

係数行列 : MAT_ASS_MAIN (1/6)

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

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

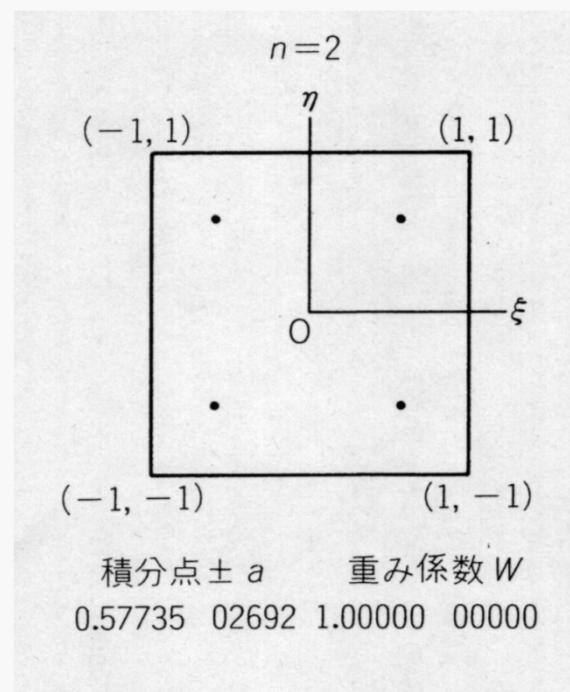
AMAT= 0. d0
B= 0. d0
X= 0. d0
D= 0. d0
```

係数行列 (非零非対角成分)
 右辺ベクトル
 未知数ベクトル
 係数行列 (対角成分)

WEI (1) = +1. 0000000000D+00
WEI (2) = +1. 0000000000D+00

POS (1) = -0. 5773502692D+00
POS (2) = +0. 5773502692D+00

POS: 積分点座標
WEI: 重み係数



系数行列：MAT_ASS_MAIN (2/6)

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

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

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

```
SHAPE(ip, jp, kp, 1) = 08th * QM1 * EM1 * TM1
SHAPE(ip, jp, kp, 2) = 08th * QP1 * EM1 * TM1
SHAPE(ip, jp, kp, 3) = 08th * QP1 * EP1 * TM1
SHAPE(ip, jp, kp, 4) = 08th * QM1 * EP1 * TM1
SHAPE(ip, jp, kp, 5) = 08th * QM1 * EM1 * TP1
SHAPE(ip, jp, kp, 6) = 08th * QP1 * EM1 * TP1
SHAPE(ip, jp, kp, 7) = 08th * QP1 * EP1 * TP1
```

系数行列：MAT_ASS_MAIN (2/6)

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

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

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

```
SHAPE(ip, jp, kp, 1) = 08th * QM1 * EM1 * TM1
SHAPE(ip, jp, kp, 2) = 08th * QP1 * EM1 * TM1
SHAPE(ip, jp, kp, 3) = 08th * QP1 * EP1 * TM1
SHAPE(ip, jp, kp, 4) = 08th * QM1 * EP1 * TM1
SHAPE(ip, jp, kp, 5) = 08th * QM1 * EM1 * TP1
SHAPE(ip, jp, kp, 6) = 08th * QP1 * EM1 * TP1
SHAPE(ip, jp, kp, 7) = 08th * QP1 * EP1 * TP1
```

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

$$EP1(j) = (1 + \eta_j), \quad EM1(j) = (1 - \eta_j)$$

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

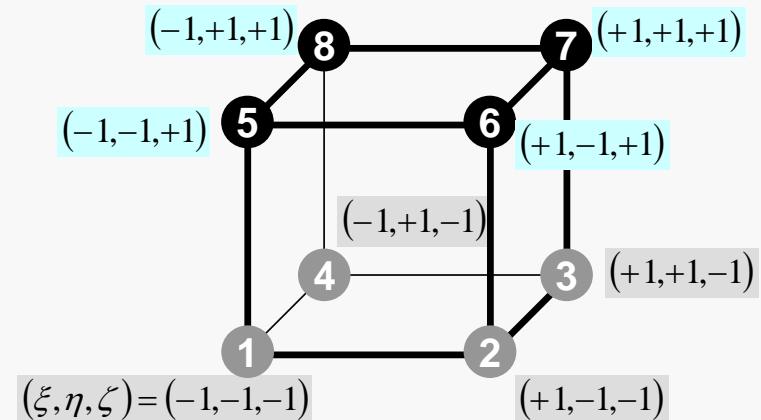
系数行列：MAT_ASS_MAIN (2/6)

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

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

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

```
SHAPE(ip, jp, kp, 1) = 08th * QM1 * EM1 * TM1
SHAPE(ip, jp, kp, 2) = 08th * QP1 * EM1 * TM1
SHAPE(ip, jp, kp, 3) = 08th * QP1 * EP1 * TM1
SHAPE(ip, jp, kp, 4) = 08th * QM1 * EP1 * TM1
SHAPE(ip, jp, kp, 5) = 08th * QM1 * EM1 * TP1
SHAPE(ip, jp, kp, 6) = 08th * QP1 * EM1 * TP1
SHAPE(ip, jp, kp, 7) = 08th * QP1 * EP1 * TP1
```



系数行列：MAT_ASS_MAIN (2/6)

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

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

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

```
SHAPE (ip, jp, kp, 1) = 08th * QM1 * EM1 * TM1
SHAPE (ip, jp, kp, 2) = 08th * QP1 * EM1 * TM1
SHAPE (ip, jp, kp, 3) = 08th * QP1 * EP1 * TM1
SHAPE (ip, jp, kp, 4) = 08th * QM1 * EP1 * TM1
SHAPE (ip, jp, kp, 5) = 08th * QM1 * EM1 * TP1
SHAPE (ip, jp, kp, 6) = 08th * QP1 * EM1 * TP1
SHAPE (ip, jp, kp, 7) = 08th * QP1 * EP1 * TP1
```

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

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

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

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

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

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

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

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

係数行列 : MAT_ASS_MAIN (3/6)

```

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

```

```

enddo
enddo
enddo

```

```

do icel= 1, ICELTOT
  CONDO= COND

```

```

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

```

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

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

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

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

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

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

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

(ξ_i, η_j, ζ_k) における形状関数の一階微分

系数行列：MAT_ASS_MAIN (3/6)

```

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

```

```

endo
endo
endo

```

```

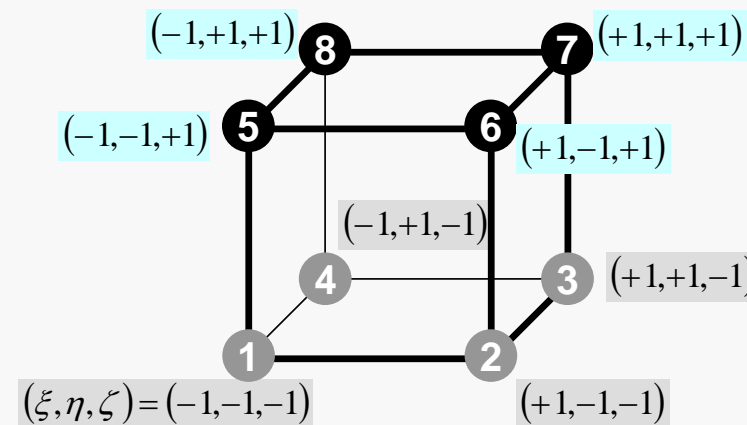
do icel= 1, ICELTOT
  CONDO= COND

```

```

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

```



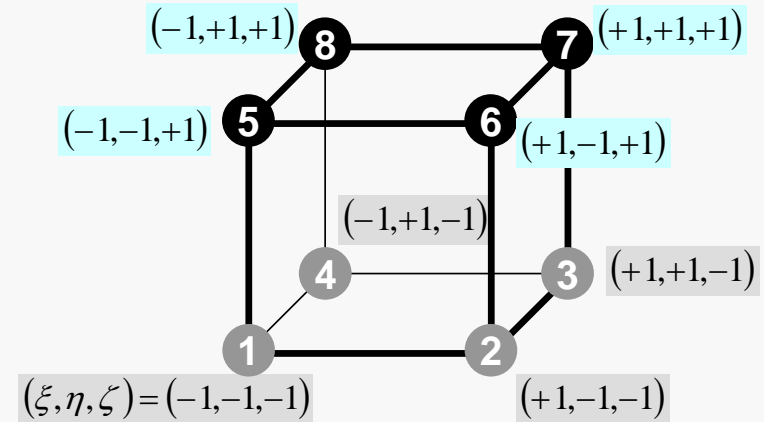
係数行列 : MAT_ASS_MAIN (4/6)

```

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

```

8節点の節点番号



```

X1= XYZ (in1, 1)
X2= XYZ (in2, 1)
X3= XYZ (in3, 1)
X4= XYZ (in4, 1)
X5= XYZ (in5, 1)
X6= XYZ (in6, 1)
X7= XYZ (in7, 1)
X8= XYZ (in8, 1)
Y1= XYZ (in1, 2)
Y2= XYZ (in2, 2)
Y3= XYZ (in3, 2)
Y4= XYZ (in4, 2)
Y5= XYZ (in5, 2)
Y6= XYZ (in6, 2)
Y7= XYZ (in7, 2)
Y8= XYZ (in8, 2)
QVC= 08th * (X1+X2+X3+X4+X5+X6+X7+X8+
& Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)

```

```

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

```

```

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

```

```

&
&
&

```

係数行列 : 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)

```

8節点のX座標

```

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)

```

8節点のY座標

```

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

```

```

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

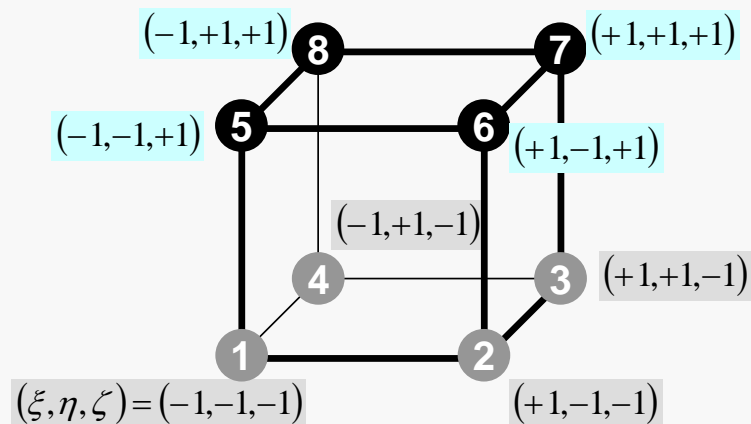
```

8節点のZ座標

```

& 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 )

```



係数行列 : MAT_ASS_MAIN (4/6)

```

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

```

```

X1= XYZ(in1, 1)
X2= XYZ(in2, 1)
X3= XYZ(in3, 1)
X4= XYZ(in4, 1)
X5= XYZ(in5, 1)
X6= XYZ(in6, 1)
X7= XYZ(in7, 1)
X8= XYZ(in8, 1)
Y1= XYZ(in1, 2)
Y2= XYZ(in2, 2)
Y3= XYZ(in3, 2)
Y4= XYZ(in4, 2)
Y5= XYZ(in5, 2)
Y6= XYZ(in6, 2)
Y7= XYZ(in7, 2)
Y8= XYZ(in8, 2)

```

```

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

```

```

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

```

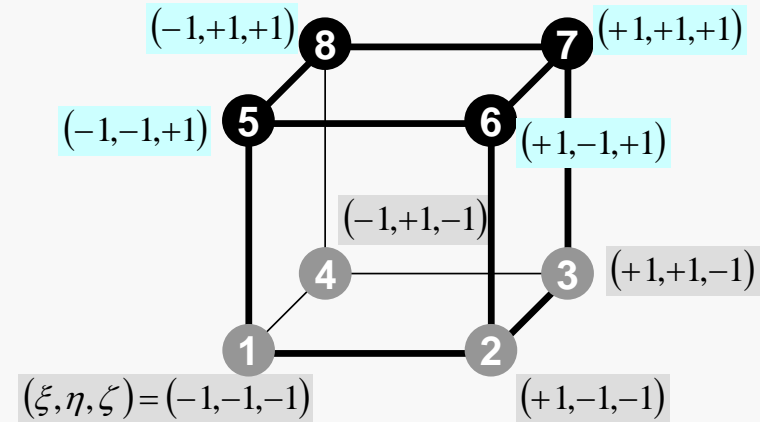
```

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

```

8節点のX座標

8節点のY座標



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

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

体積当たり発熱量は位置（メッシュの中心の座標 x_c, y_c ）に依存

系数行列：MAT_ASS_MAIN (4/6)

```

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

```

```

X1= XYZ (in1, 1)
X2= XYZ (in2, 1)
X3= XYZ (in3, 1)
X4= XYZ (in4, 1)
X5= XYZ (in5, 1)
X6= XYZ (in6, 1)
X7= XYZ (in7, 1)
X8= XYZ (in8, 1)
Y1= XYZ (in1, 2)
Y2= XYZ (in2, 2)
Y3= XYZ (in3, 2)
Y4= XYZ (in4, 2)
Y5= XYZ (in5, 2)
Y6= XYZ (in6, 2)
Y7= XYZ (in7, 2)
Y8= XYZ (in8, 2)

```

```

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

```

```

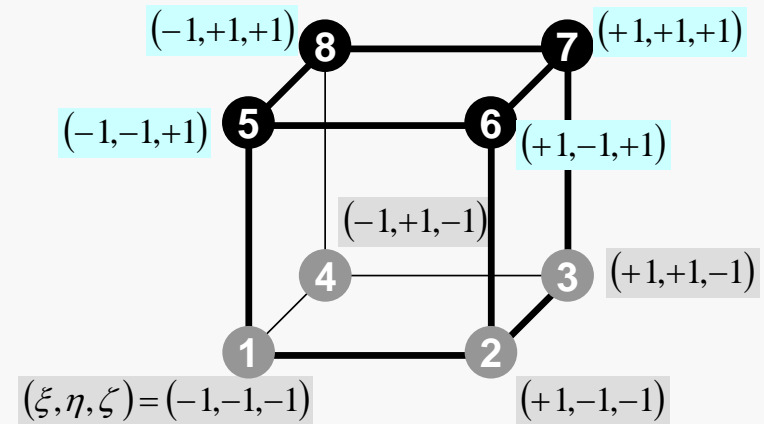
Z1= XYZ (in1, 3)
Z2= XYZ (in2, 3)
Z3= XYZ (in3, 3)
Z4= XYZ (in4, 3)
Z5= XYZ (in5, 3)
Z6= XYZ (in6, 3)
Z7= XYZ (in7, 3)
Z8= XYZ (in8, 3)

```

```

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

```



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

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

$$QVC = |x_c + y_c|$$

系数行列 : MAT_ASS_MAIN (4/6)

```

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

X1= XYZ (in1, 1)
X2= XYZ (in2, 1)
X3= XYZ (in3, 1)
X4= XYZ (in4, 1)
X5= XYZ (in5, 1)
X6= XYZ (in6, 1)
X7= XYZ (in7, 1)
X8= XYZ (in8, 1)
Y1= XYZ (in1, 2)
Y2= XYZ (in2, 2)
Y3= XYZ (in3, 2)
Y4= XYZ (in4, 2)
Y5= XYZ (in5, 2)
Y6= XYZ (in6, 2)
Y7= XYZ (in7, 2)
Y8= XYZ (in8, 2)
QVC= 08th * (X1+X2+X3+X4+X5+X6+X7+X8+
&          Y1+Y2+Y3+Y4+Y5+Y6+Y7+Y8)
Z1= XYZ (in1, 3)
Z2= XYZ (in2, 3)
Z3= XYZ (in3, 3)
Z4= XYZ (in4, 3)
Z5= XYZ (in5, 3)
Z6= XYZ (in6, 3)
Z7= XYZ (in7, 3)
Z8= XYZ (in8, 3)

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

```

係数行列 : MAT_ASS_MAIN (5/6)

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

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

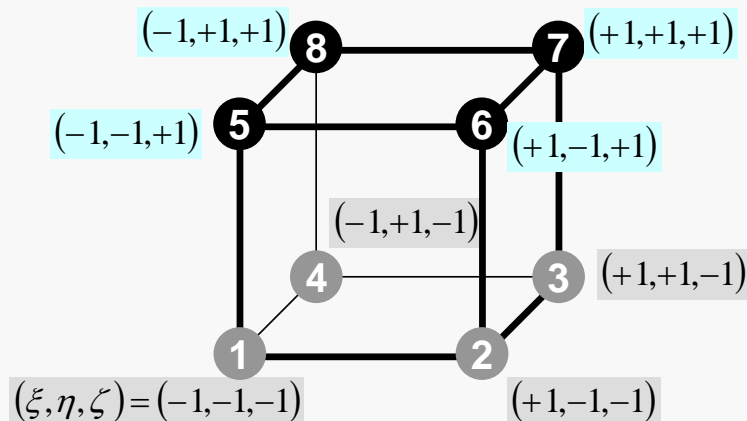
  kk= 0
  if (jp.ne. ip) then
    iiS= index(ip)-1 + 1
    iiE= index(ip )
    do k= iiS, iiE
      if ( item(k).eq. jp ) then
        kk= k
        exit
      endif
    enddo
  endif
endif
```

全体行列の非対角成分

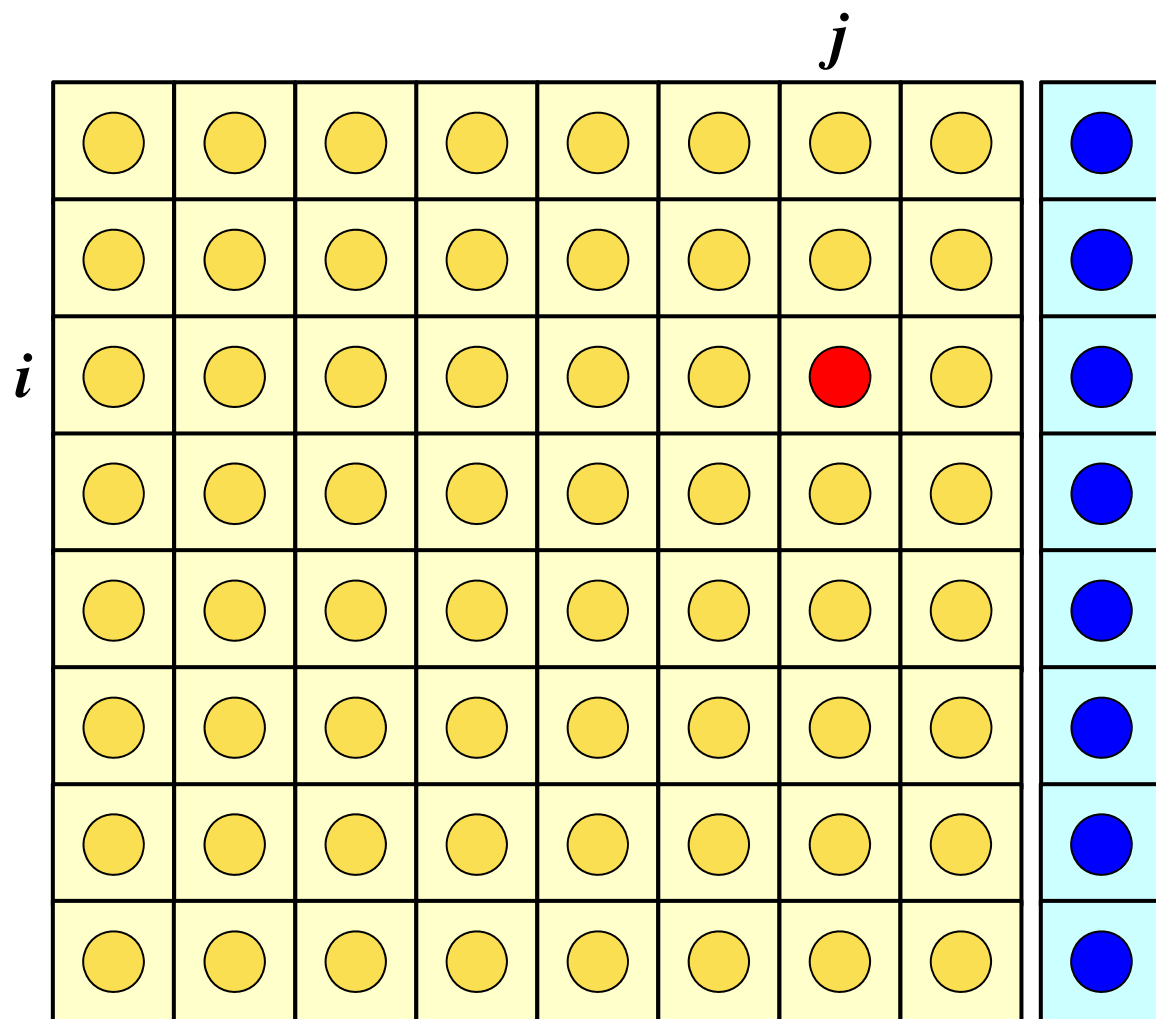
$$A_{ip, jp}$$

kk:itemにおけるアドレス

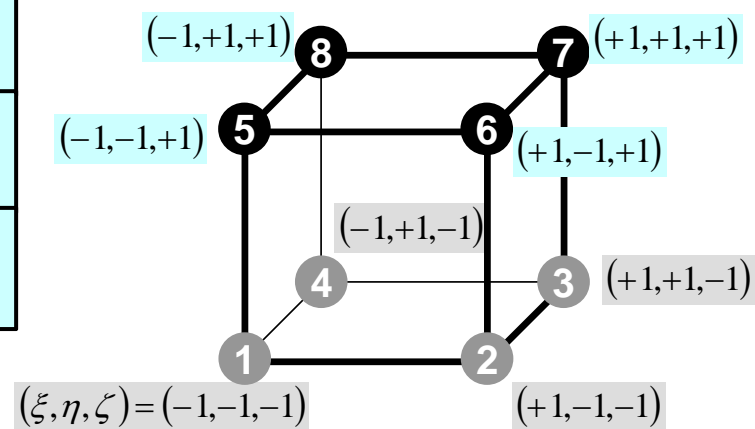
ip= nodLOCAL(ie)
jp= nodLOCAL(je)



要素マトリクス : 8×8 行列



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



係数行列 : MAT_ASS_MAIN (5/6)

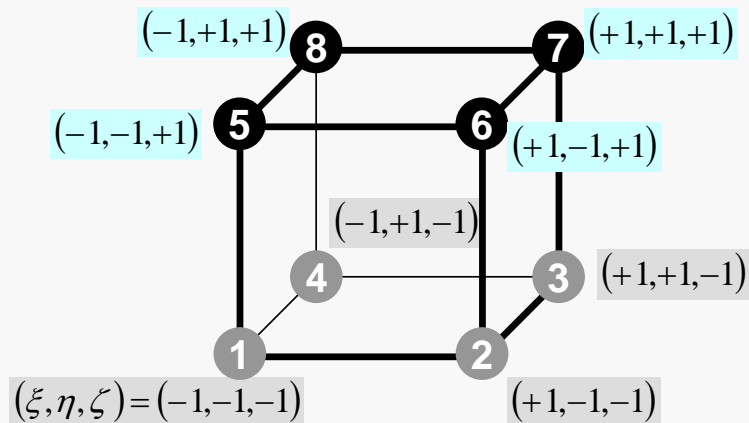
```
!C
!C== CONSTRUCT the GLOBAL MATRIX
```

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

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

要素マトリクス ($i_e \sim j_e$)
全体マトリクス ($i_p \sim j_p$) の関係

kk: itemにおけるアドレス



系数行列：MAT_ASS_MAIN (6/6)

```

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

  PNXi= PNX (ipn, jpn, kpn, ie)
  PNYi= PNY (ipn, jpn, kpn, ie)
  PNZi= PNZ (ipn, jpn, kpn, ie)

  PNXj= PNX (ipn, jpn, kpn, je)
  PNYj= PNY (ipn, jpn, kpn, je)
  PNZj= PNZ (ipn, jpn, kpn, je)

  & COEFij= COEFij + coef * CONDO *
      (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)

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

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

return
end

```

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

系数行列：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

```

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

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

系数行列：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

```

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

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

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

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

系数行列：MAT_ASS_MAIN (6/6)

```

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

  PNXi= PNX (ipn, jpn, kpn, ie)
  PNYi= PNY (ipn, jpn, kpn, ie)
  PNZi= PNZ (ipn, jpn, kpn, ie)

  PNXj= PNX (ipn, jpn, kpn, je)
  PNYj= PNY (ipn, jpn, kpn, je)
  PNZj= PNZ (ipn, jpn, kpn, je)

  & COEFij= COEFij + coef * CONDO *
      (PNXi*PNXj+PNYi*PNYj+PNZi*PNZj)

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

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

return
end

```

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

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

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

$$QVC = |x_C + y_C|$$

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

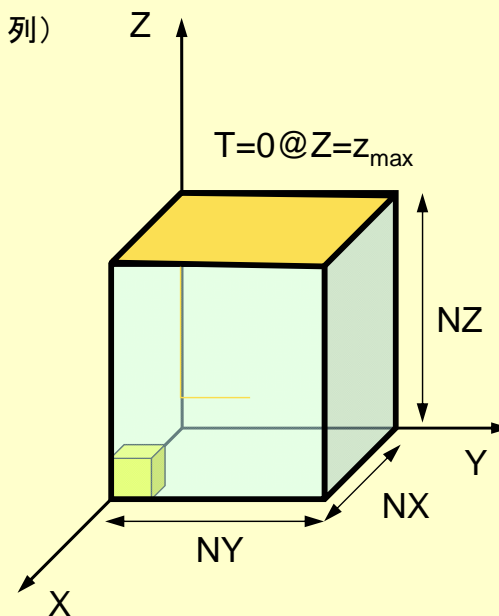
$$\{f\}^{(e)} = QV0 \cdot QVC$$

MAT_ASS_BC : 全体構成

```
do i= 1, NP  節点ループ
  (ディリクレ) 境界条件を設定する節点をマーク (IWKX)
enddo
```

```
do i= 1, NP  節点ループ
  if (IWKX(i,1).eq.1) then  マークされた節点だったら
    対応する右辺ベクトル (B) の成分, 対角成分 (D) の成分の修正 (行・列)
    do k= index(i-1)+1, index(i)
      対応する非零非対角成分 (AMAT) の成分の修正 (行)
    enddo
  endif
enddo
```

```
do i= 1, NP  節点ループ
  do k= index(i-1)+1, index(i)
    if (IWKX(item(k),1).eq.1) then  対応する非零非対角成分の
      節点がマークされていたら
      対応する右辺ベクトル, 非零非対角成分 (AMAT) の成分の修正 (列)
    endif
  enddo
enddo
```



境界条件 : 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
```

節点グループ名が「Zmax」である
節点inにおいて:

$$IWKX(in, 1) = 1$$

とする

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
```


境界条件 : MAT_ASS_BC (2/2)

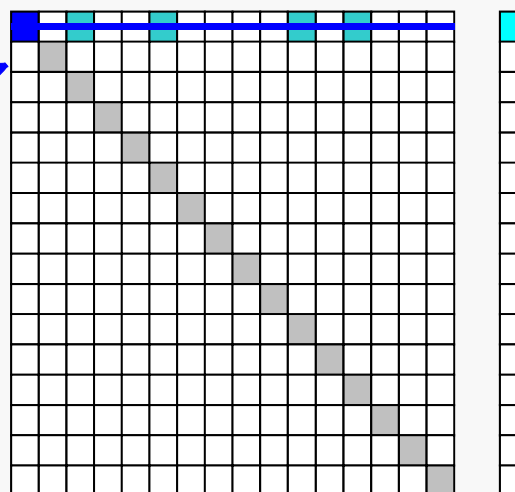
```
do in= 1, NP
  if (IWKX(in,1).eq.1) then
    B(in)= 0. d0
    D(in)= 1. d0

    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
```

IWKX(in,1)=1となる節点に対して
対角成分=1, 右辺=0, 非零対角成分=0

ゼロクリア



ここでやっていることも1CPUの時と
全く変わらない

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

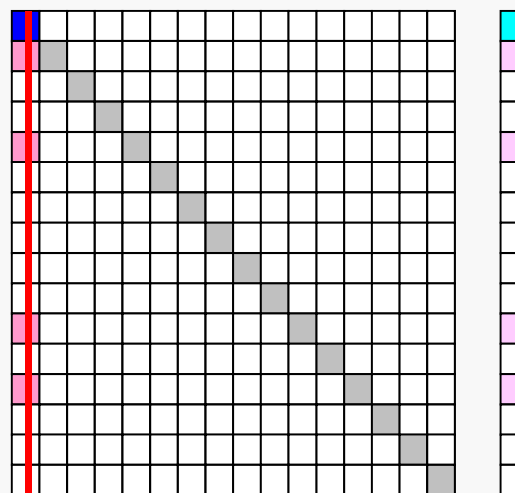
    iS= index(in-1) + 1
    iE= index(in )
    do k= iS, iE
      AMAT(k)= 0. d0
    enddo
  endif
enddo

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

```

IWKX(in,1)=1となる節点を非零非対角成分として有している節点に対して、右辺へ移項, 当該非零非対角成分=0

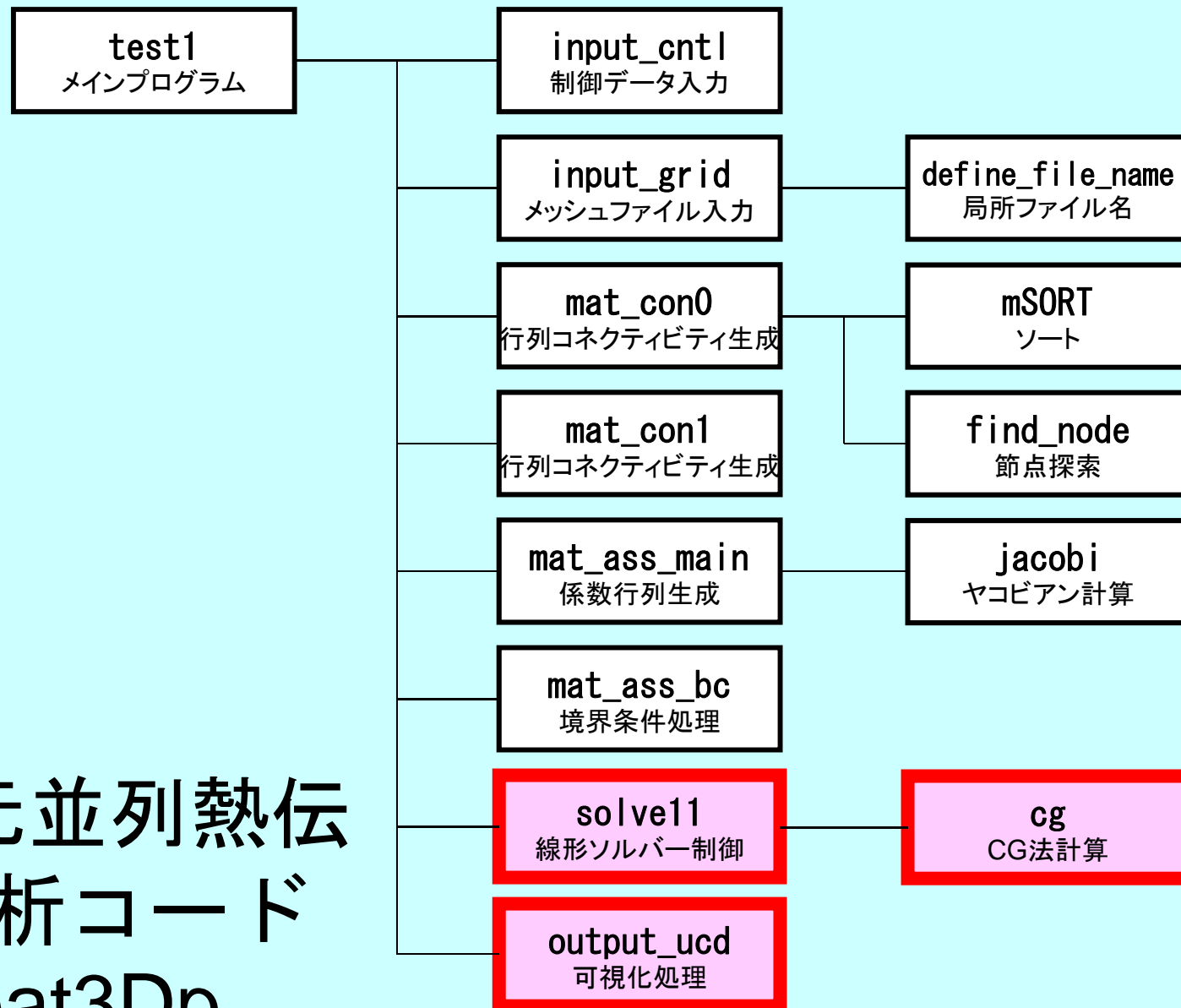


消去, ゼロクリア

ここでやっていることも1CPUの時と全く変わらない

並列有限要素法の処理：プログラム

- 初期化
 - 制御変数読み込み
 - 座標読み込み⇒要素生成 (N:節点数, NE:要素数)
 - 配列初期化 (全体マトリクス, 要素マトリクス)
 - 要素⇒全体マトリクスマッピング (Index, Item)
- マトリクス生成
 - 要素単位の処理 (do icel= 1, NE)
 - 要素マトリクス計算
 - 全体マトリクスへの重ね合わせ
 - 境界条件の処理
- 連立一次方程式
 - 共役勾配法 (CG)



三次元並列熱伝 導解析コード heat3Dp

全体処理

```
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)
      RESID     = pfemRarray(1)
      !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

```

CG法の最大反復回数
CG法の収束判定値

前処理付き共役勾配法

Preconditioned Conjugate Gradient Method (CG)

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

前処理: 対角スケーリング

対角スケーリング, 点ヤコビ前処理

- 前処理行列として, もとの行列の対角成分のみを取り出した行列を前処理行列 $[M]$ とする。
 - 対角スケーリング, 点ヤコビ (point-Jacobi) 前処理

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

- $\text{solve } [M]z^{(i-1)} = r^{(i-1)}$ という場合に逆行列を簡単に求めることができる。

CG法 (2/6)

```

COMMtime= 0. d0
COMPtime= 0. d0

ERROR= 0

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

MAXIT = ITER
TOL = RESID

X = 0. d0
WS= 0. d0
WR= 0. d0

!C
!C +-----+
!C | {r0}= {b} - [A] {xini} |
!C +-----+
!C==

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

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

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

```

```

Compute  $r^{(0)} = b - [A]x^{(0)}$ 
for  $i = 1, 2, \dots$ 
  solve  $[M]z^{(i-1)} = r^{(i-1)}$ 
   $\rho_{i-1} = r^{(i-1)} \cdot z^{(i-1)}$ 
  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
   $q^{(i)} = [A]p^{(i)}$ 
   $\alpha_i = \rho_{i-1} / p^{(i)} \cdot q^{(i)}$ 
   $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$ 
   $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$ 
  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
  irstart= EXPORT_INDEX(neib-1)
  inum = EXPORT_INDEX(neib) - irstart
  do k= irstart+1, irstart+inum
    ii = EXPORT_ITEM(k)
    WS(k)= X(ii)
  enddo

  call MPI_Isend (WS(irstart+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法 (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法 (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)
          X1= WW(3*i-2,P)
          X2= WW(3*i-1,P)
          X3= WW(3*i,P)
          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  $i = 1, 2, \dots$ 
  solve  $[M]z^{(i-1)} = r^{(i-1)}$ 
   $\rho_{i-1} = r^{(i-1)} z^{(i-1)}$ 
  if  $i=1$ 
     $p^{(1)} = z^{(0)}$ 
  else
     $\beta_{i-1} = \rho_{i-1} / \rho_{i-2}$ 
     $p^{(i)} = z^{(i-1)} + \beta_{i-1} p^{(i-1)}$ 
  endif
   $q^{(i)} = [A]p^{(i)}$ 
   $\alpha_i = \rho_{i-1} / p^{(i)} q^{(i)}$ 
   $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$ 
   $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$ 
  check convergence  $|r|$ 
end

```

CG法 (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

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

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

      RHO1 = RHO

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

end

```

CG法 (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                                &          外点に最新のX (温度) 代入
&    ( NP, NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM, &
&    EXPORT_INDEX, EXPORT_ITEM, WS, WR, X , my_rank)

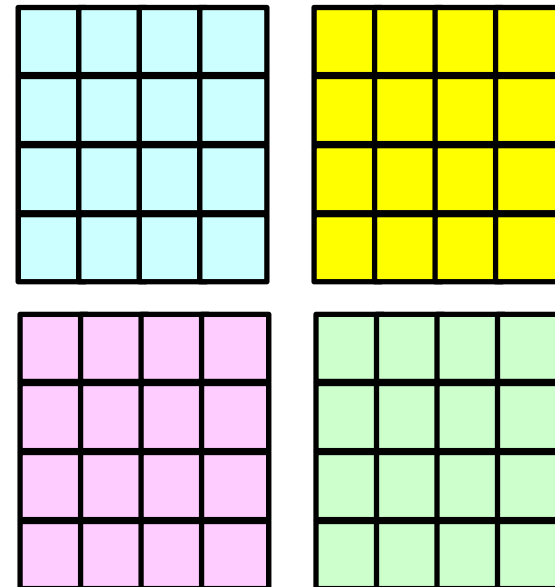
    deallocate (WW, WR, WS)

    end subroutine      CG
    end module          solver_CG

```


OUTPUT_UCD

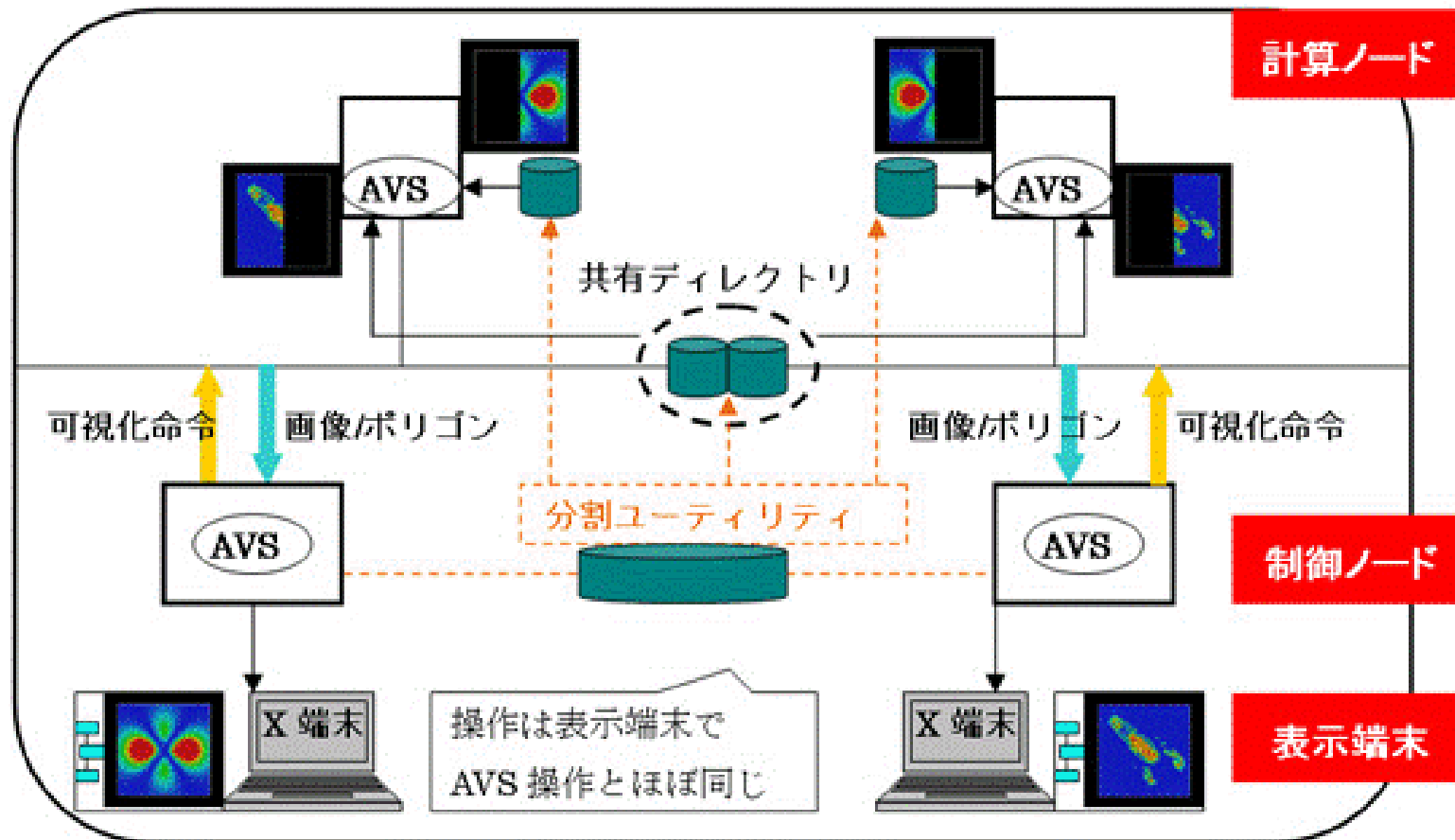
- 各領域からintELEM_listに所属する要素の情報を集める
 - intELEM_list: 各節点の属する領域番号のうち最も若い番号の領域に所属する・・・と見なす
- MPI_Allgathervを使って以下の情報を一箇所に集める
 - 節点: 節点座標, 温度
 - 要素: 要素コネクティビティ(要素を構成する節点)
- 節点の情報は一部重複
- 問題規模が大きくなると困難
 - あまり賢いやり方ではない
 - 並列可視化



AVS/Express PCE Parallel Cluster Edition

- <http://www.cybernet.co.jp/avs/products/pce/>
- AVS/Express PCEでは、クラスタ化された複数のLinuxマシンで、各計算ノードが持つ部分領域のみを可視化し、最終的な可視化結果のみ制御ノード上で表示するという構成になっている。
- 並列計算の結果、出力される大規模データを可視化する場合でも、高い精度を保ったまま、可視化処理を実現することが可能。
- **並列計算機上で対話処理可能**
 - 最新版ではWindowsより制御可能

AVS/Express PCE Parallel Cluster Edition

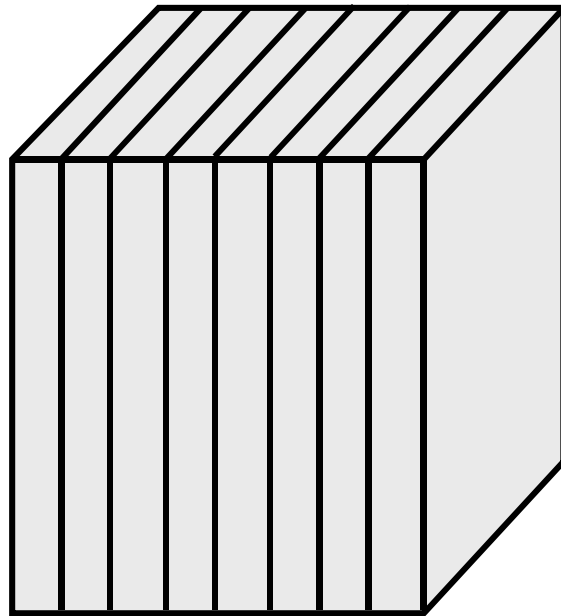


課題(1/2)

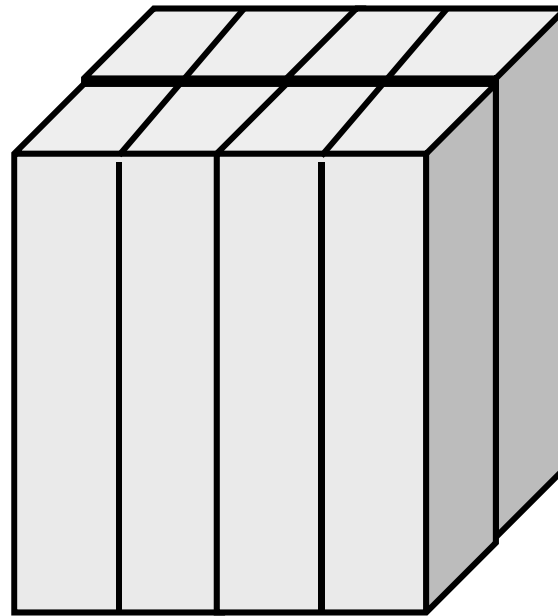
- 自分で問題設定を行い, 「sol」の挙動を分析してみよ
- 例
 - Strong Scaling
 - 問題サイズを固定, PE数を変化させて時間(全体, 各部分)を測定。
 - Weak Scaling
 - PEあたりの問題サイズを固定, 1反復あたりの計算時間を求める。
 - 考慮すべき項目
 - 問題サイズ
 - 領域分割手法(RCB, K-METIS, P-METIS, 1D~3D)の影響。
 - メッシュ生成, 領域分割におけるFX10の性能低い
 - 128^3 くらいが限界(領域分割に15分以上かかる)
- 「*.inp」の出力に時間がかかる場合がある。
 - OUTPUT_UCDの呼び出しのコメントアウト
 - src, part

1D~3D分割

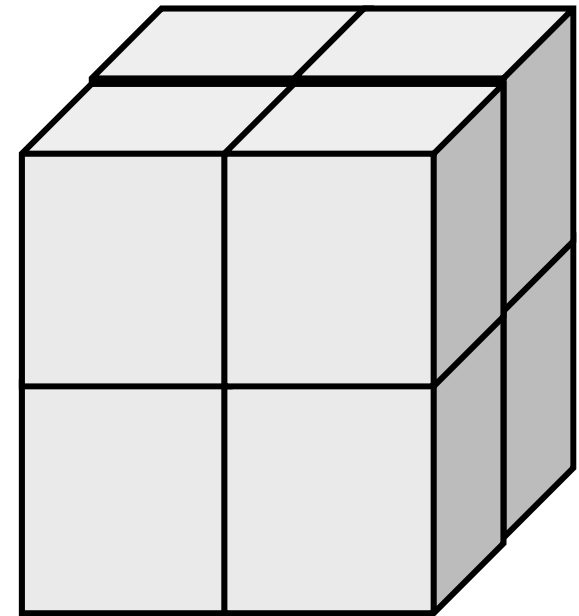
どの方法が良いか考えて見よ



1D型



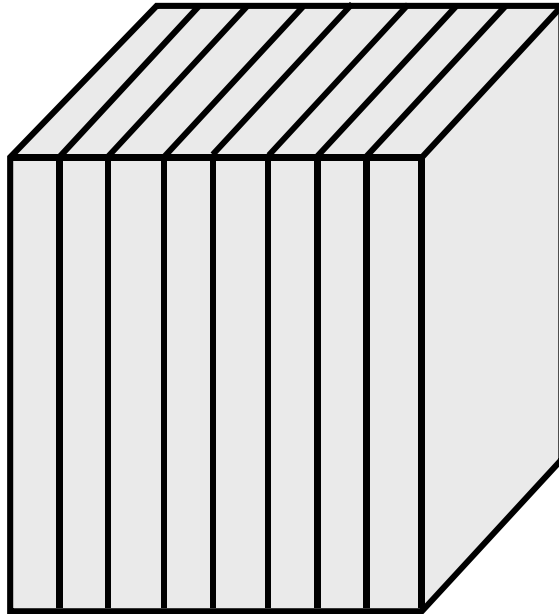
2D型



3D型

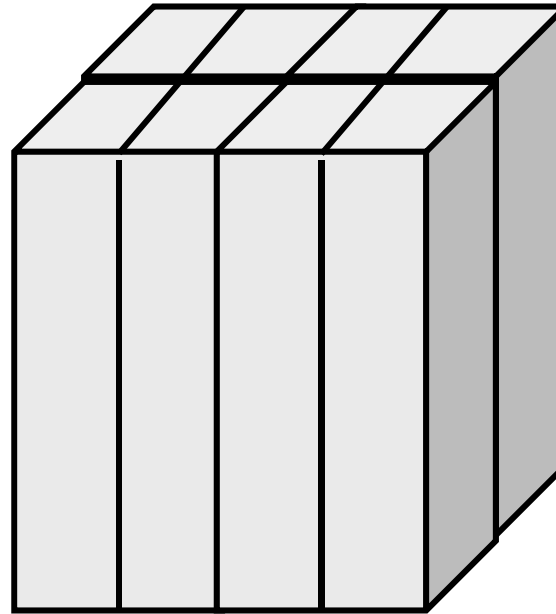
1D~3D分割

通信量の総和(各辺4N, 8領域とする)



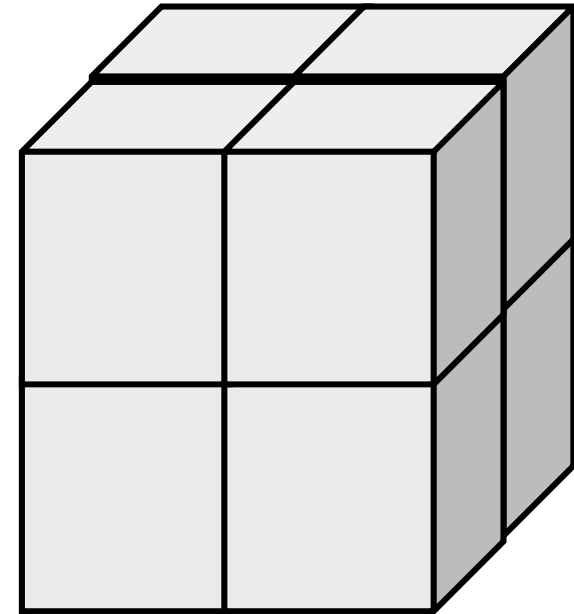
1D型

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



2D型

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

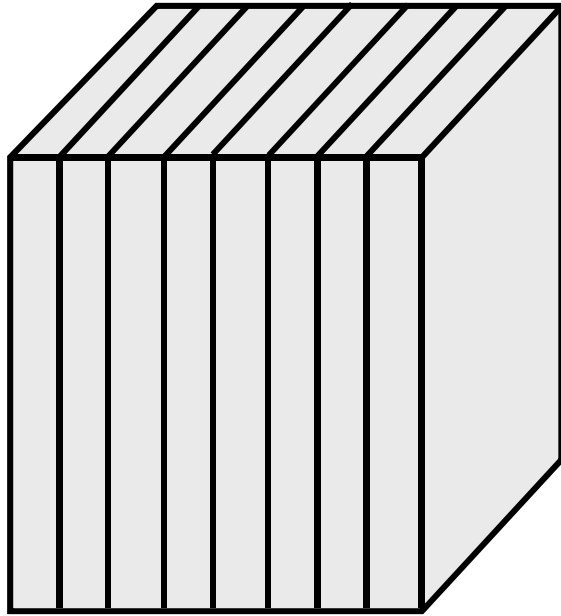


3D型

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

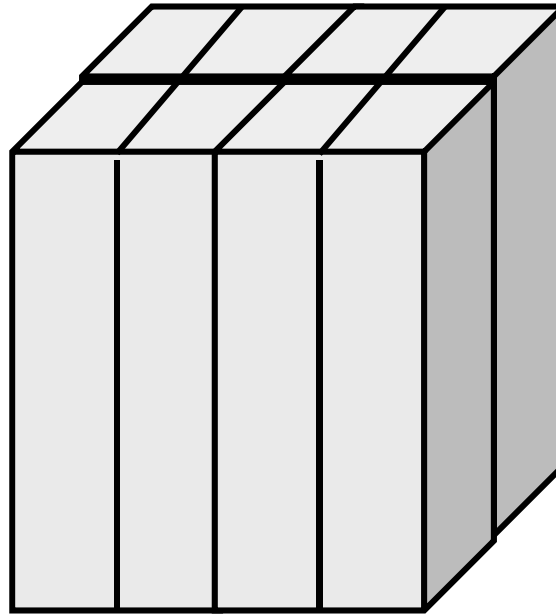
1D~3D分割

mesh.inp



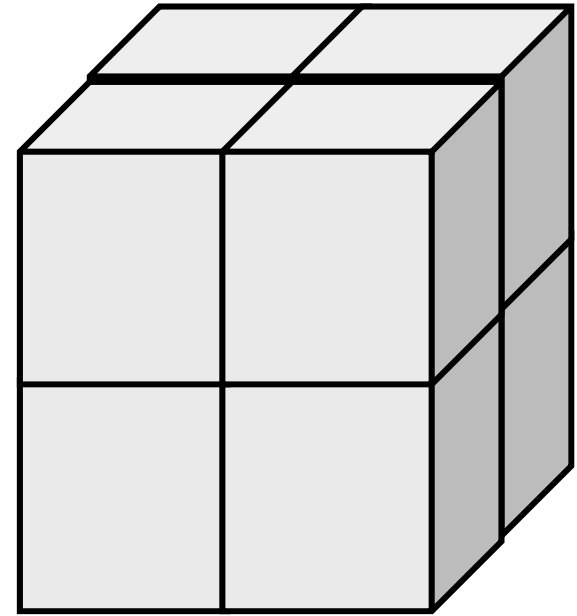
1D型

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



2D型

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



3D型

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

課題 (2/2)

- 領域間通信 (solver_SR) の性能改善ができないかどうか考えてみよ。
 - Recv. Bufferへのコピーを効率的に実施できないか?

```
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	

計算例(通信最適化済)@東大

Strong Scaling

- $192 \times 192 \times 128$ 節点 (4,718,592節点, 4,633,087要素)
- 16~192コア
- Solver計算時間

core #	sec. (speed-up)
16 (4x2x2)	16.6 (16.0)
32 (4x4x2)	8.69 (30.5)
64 (4x4x4)	4.55 (59.6)
96 (6x4x4)	3.54 (74.7)
128 (8x4x4)	2.69 (98.4)
192 (8x6x4)	1.84 (144.)