Report S2
C

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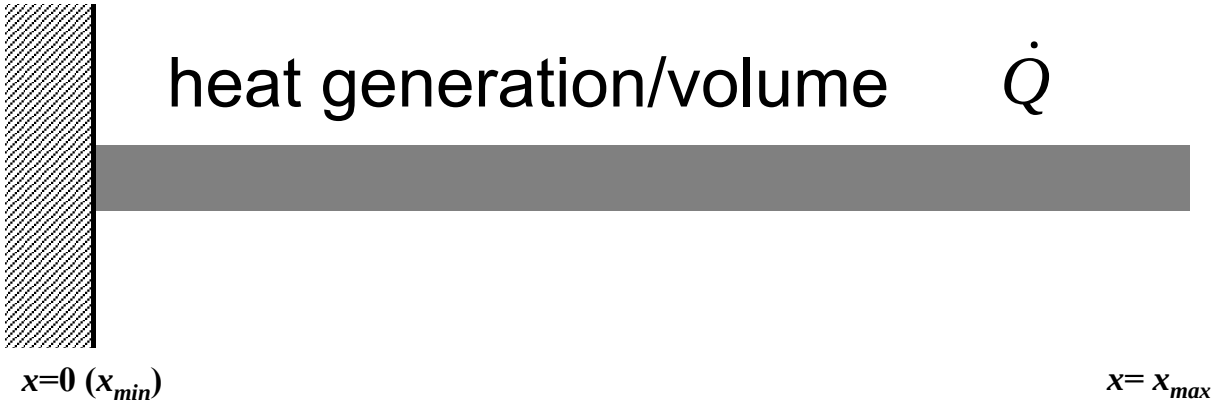
Technical & Scientific Computing II (4820-1028)
Seminar on Computer Science II (4810-1205)
Hybrid Distributed Parallel Computing (3747-111)

- Overview
- Distributed Local Data
- Program
- Results

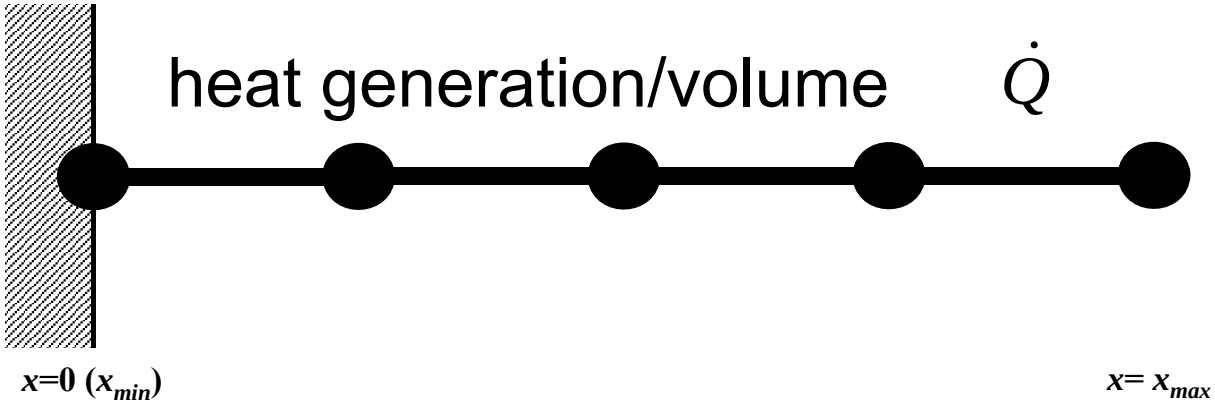
1D Steady State Heat Conduction



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

- Uniform: Sectional Area: A, Thermal Conductivity: λ
- Heat Generation Rate/Volume/Time [$QL^{-3}T^{-1}$] $\dot{Q}$
- Boundary Conditions
  - x=0 : T= 0 (Fixed Temperature)
  - x=x_{max} : $\dfrac{\partial T}{\partial x}=0$ (Insulated)

1D Steady State Heat Conduction



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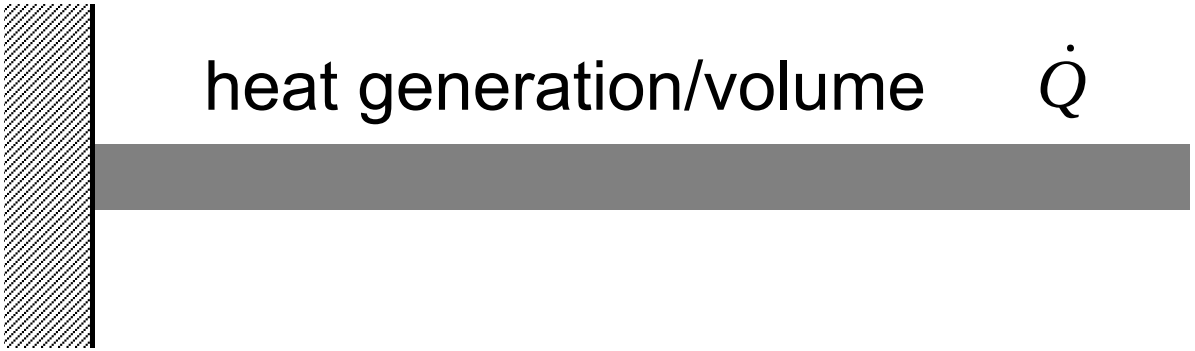
Analytical Solution



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

$$T=0\,@\,x=0$$

$$\frac{\partial T}{\partial x}=0\,@\,x=x_{\max}$$

$$\lambda T''=-\dot{Q}$$

$$\lambda T'=-\dot{Q}x+C_1\Rightarrow C_1=\dot{Q}x_{\max},\quad T'=0\,@\,x=x_{\max}$$

$$\lambda T=-\frac{1}{2}\dot{Q}x^2+C_1x+C_2\Rightarrow C_2=0,\quad T=0\,@\,x=0$$

$$\therefore\quad T=-\frac{1}{2\lambda}\dot{Q}x^2+\frac{\dot{Q}x_{\max}}{\lambda}x$$

Copy and Compile

Fortran

```
>$ cd <$O-TOP>
>$ cp /lustre/gt16/z30088/class_eps/F/s2r-f.tar .
>$ tar xvf s2r-f.tar
```

C

```
>$ cd <$O-TOP>
>$ cp /lustre/gt16/z30088/class_eps/C/s2r-c.tar .
>$ tar xvf s2r-c.tar
```

Confirm/Compile

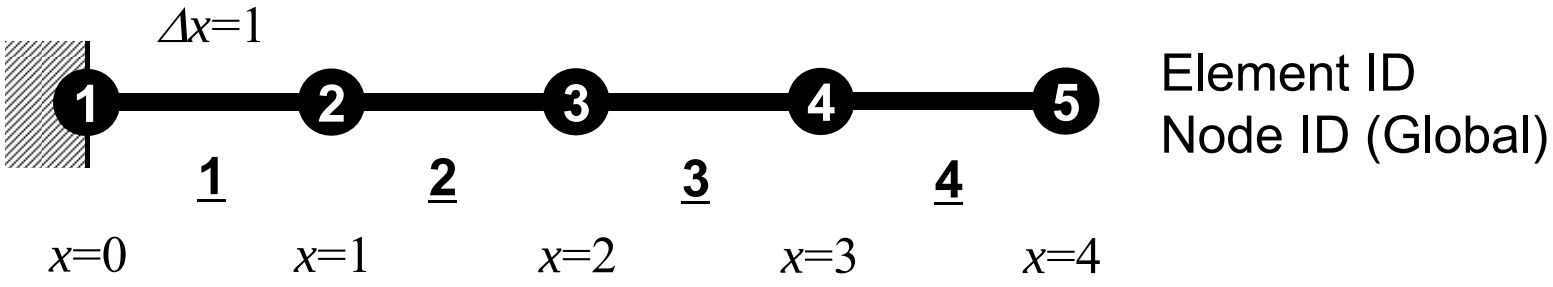
```
>$ cd mpi/S2-ref
>$ mpiifort -O3 -xCORE-AVX2 -align array32byte 1d.f
>$ mpicc -O3 -xCORE-AVX2 -align 1d.c
```

<$O-S2r> = <$O-TOP>/mpi/S2-ref

Control File: input.dat

Control Data `input.dat`

`4`	`NE` (Number of Elements)
`1.0 1.0 1.0 1.0`	Δx (Length of Each Elem.: `L`), `Q`, `A`, λ
`100`	Number of MAX. Iterations for CG Solver
`1.e-8`	Convergence Criteria for CG Solver

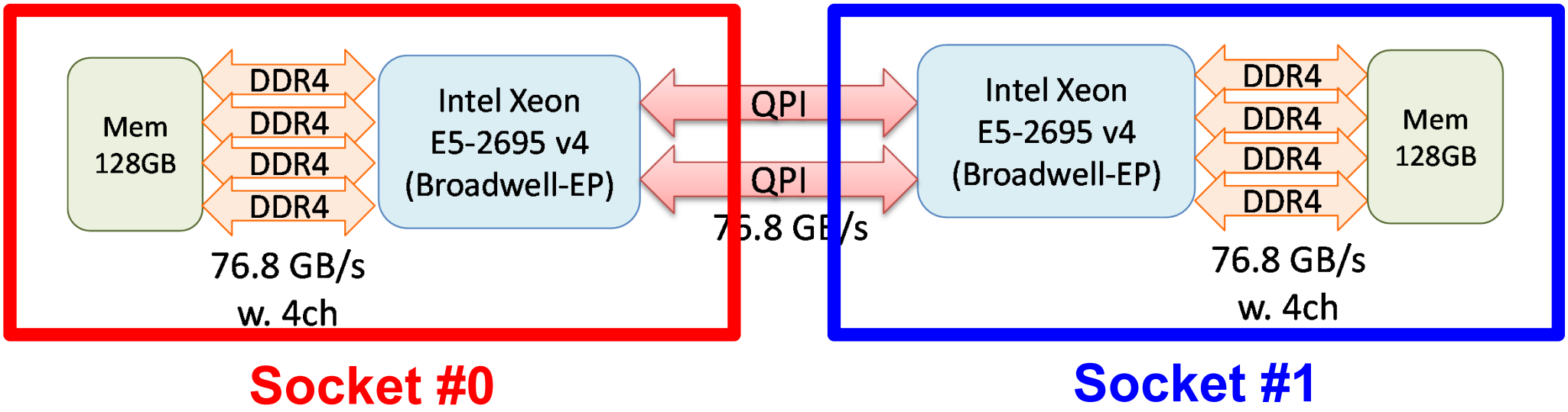


go.sh

```
#!/bin/sh
#PBS -q u-lecture                    Name of “QUEUE”
#PBS -N test                         Job Name
#PBS -l select=4:mpiprocs=32         node#, proc#/node
#PBS -Wgroup_list=gt16               Group Name (Wallet)
#PBS -l walltime=00:05:00            Computation Time
#PBS -e err                          Standard Error
#PBS -o test.lst                     Standard Outpt

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

export I_MPI_PIN_DOMAIN=socket       Execution on each socket
mpirun ./impimap.sh ./a.out          Exec’s
```

```
#PBS -l select=1:mpiprocs=4     1-node, 4-proc’s
#PBS –l select=1:mpiprocs=16    1-node, 16-proc’s
#PBS -l select=1:mpiprocs=36    1-node, 36-proc’s
#PBS –l select=2:mpiprocs=32    2-nodes, 32x2=64-proc’s
#PBS –l select=8:mpiprocs=36    8-nodes, 36x8=288-proc’s
```

export I_MPI_PIN_DOMAIN=socket



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

Procedures for Parallel FEM

- Reading control file, entire element number etc.
- Creating “distributed local data” in the program
- Assembling local and global matrices for linear solvers
- Solving linear equations by CG

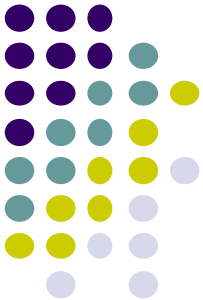
- Not so different from those of original code

- Overview
- **Distributed Local Data**
- Program
- Results

Finite Element Procedures

- 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

Distributed Local Data Structure for Parallel FEM

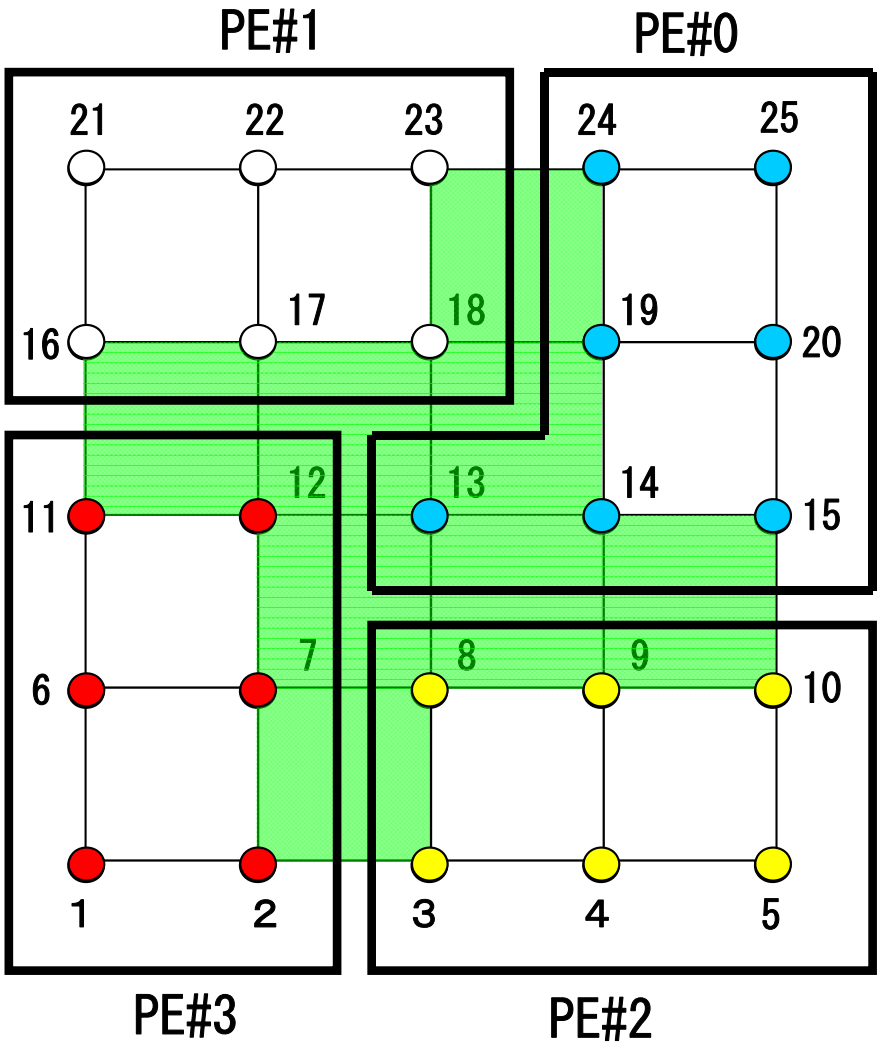


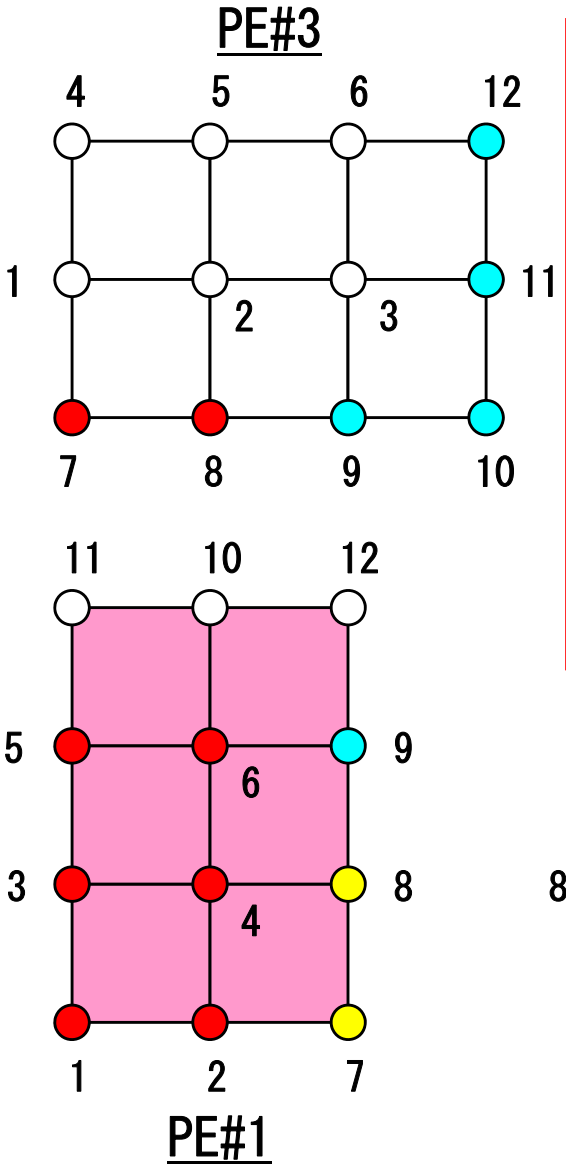
- Node-based partitioning
- Local data includes:
  - Nodes originally assigned to the domain/PE/partition
  - Elements which include above nodes
  - Nodes which are included above elements, and originally NOT-assigned to the domain/PE/partition
- 3 categories for nodes
  - Internal nodes Nodes originally assigned to the domain/PE/partition
  - External nodes Nodes originally NOT-assigned to the domain/PE/partition
  - Boundary nodes External nodes of other domains/PE's/partitions
- Communication tables

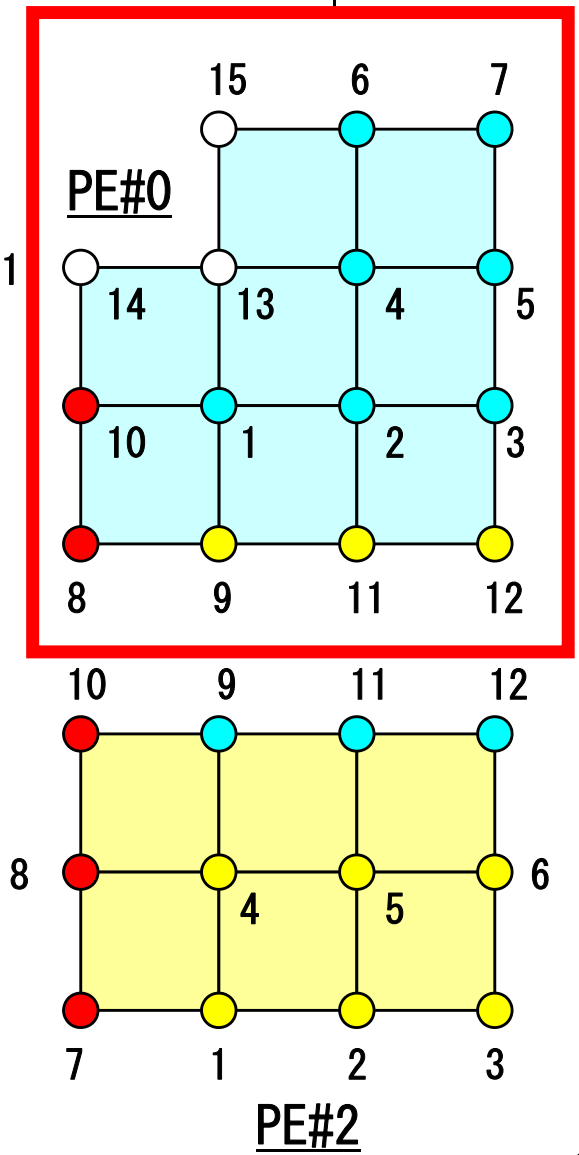
- Global info. is not needed except relationship between domains
  - Property of FEM: local element-by-element operations

Node-based Partitioning

internal nodes - elements - external nodes



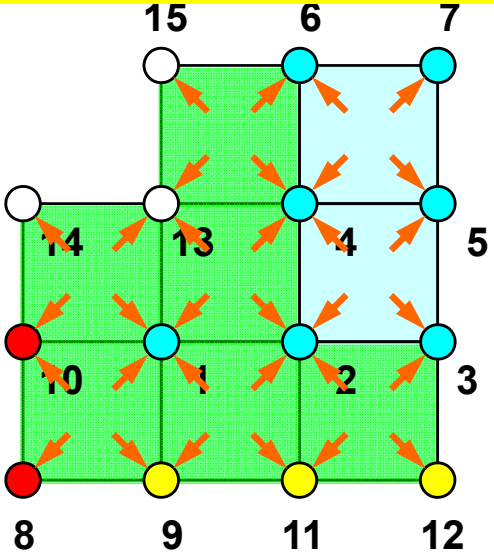


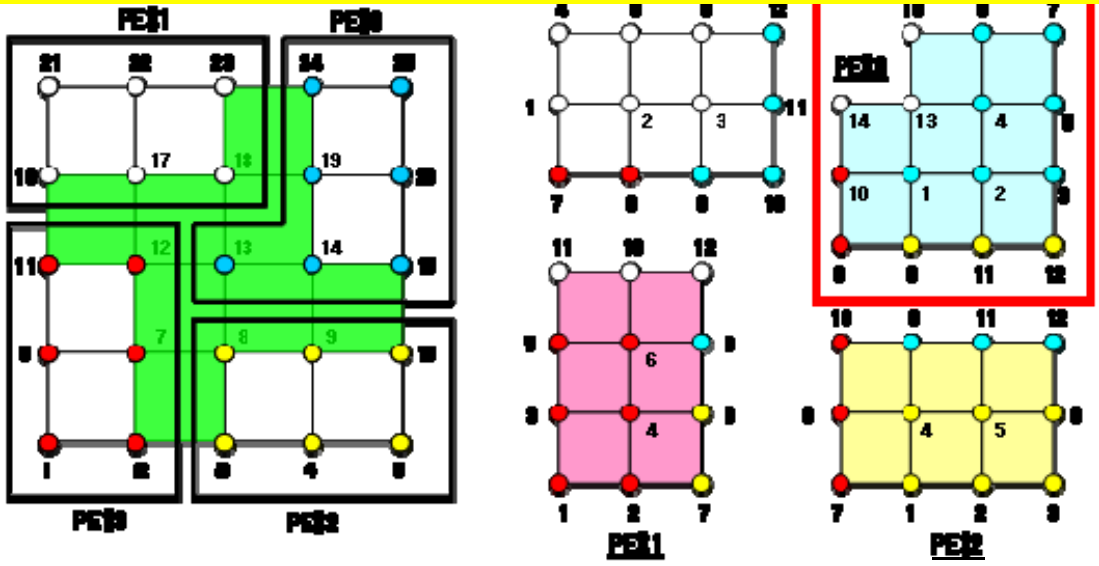


Node-based Partitioning

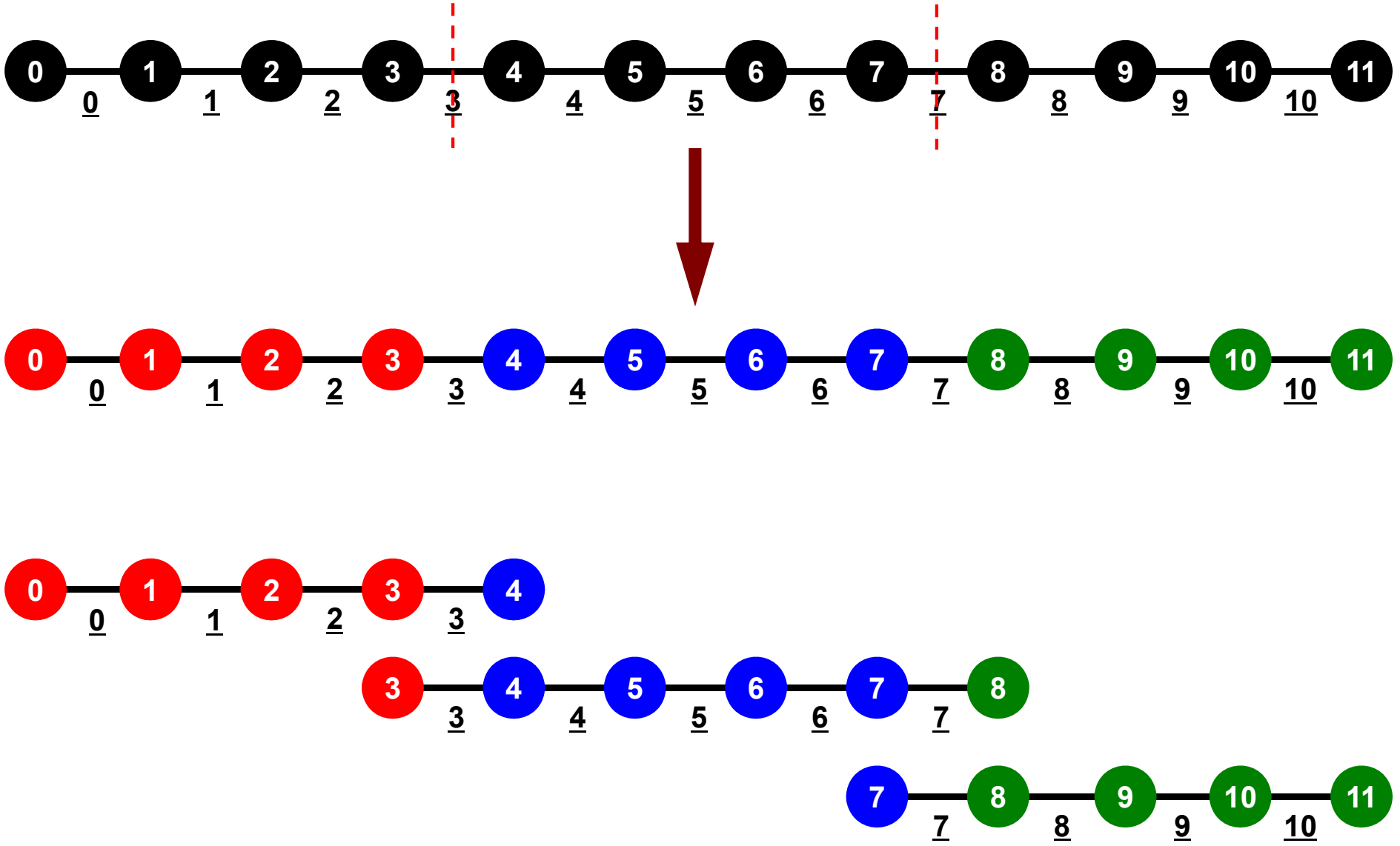
internal nodes - elements - external nodes

- Partitioned nodes themselves (Internal Nodes) 内点
- Elements which include Internal Nodes 内点を含む要素
- External Nodes included in the Elements 外点
  in overlapped region among partitions.
- Info of External Nodes are required for completely local element–based operations on each processor.

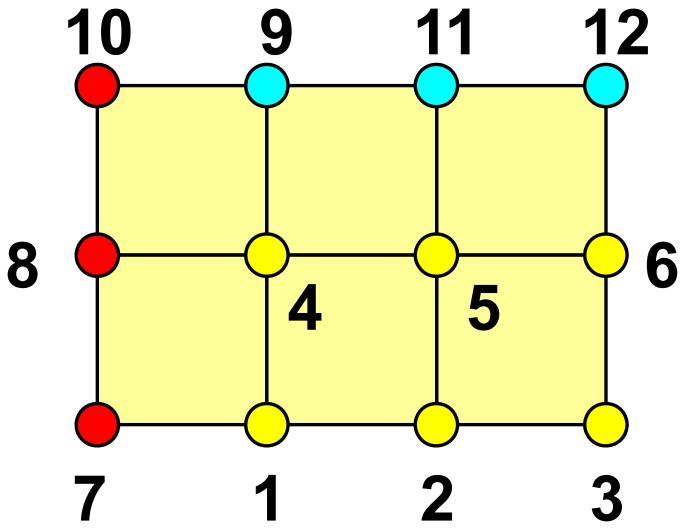




1D FEM: 12 nodes/11 elem's/3 domains



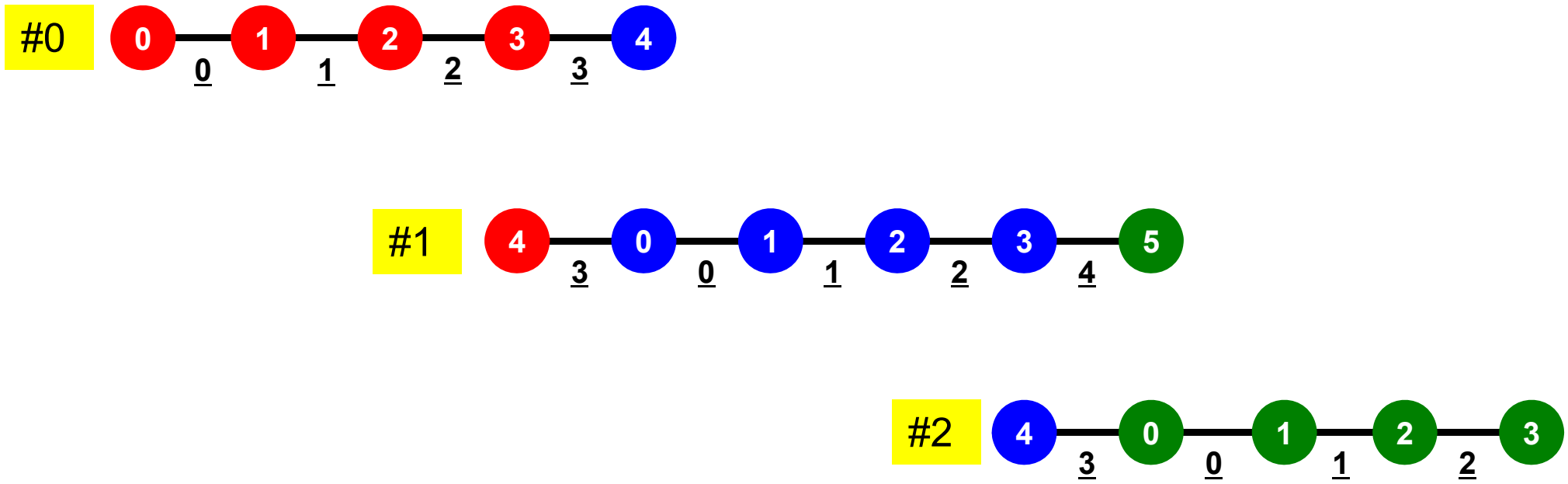
Description of Distributed Local Data



- Internal/External Points
  - Numbering: Starting from internal pts, then external pts after that
- Neighbors
  - Shares overlapped meshes
  - Number and ID of neighbors
- External Points
  - From where, how many, and which external points are received/imported ?
- Boundary Points
  - To where, how many and which boundary points are sent/exported ?

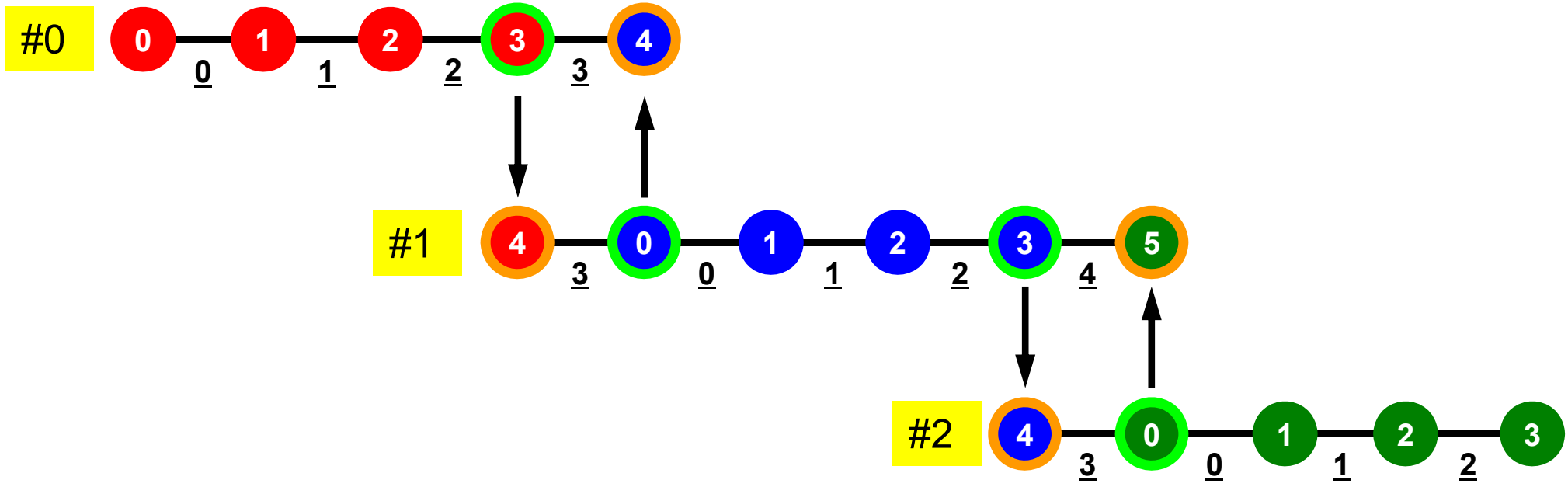
1D FEM: 12 nodes/11 elem's/3 domains

Local ID: Starting from 0 for node and elem at each domain

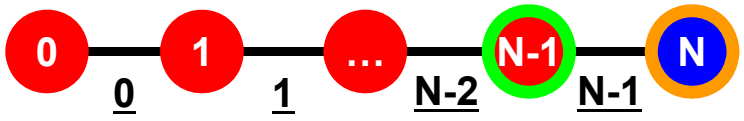


1D FEM: 12 nodes/11 elem's/3 domains

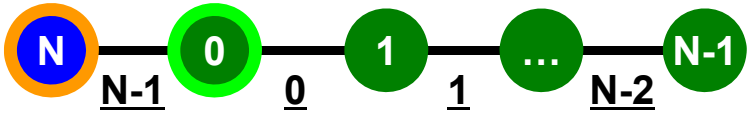
Internal/External Nodes



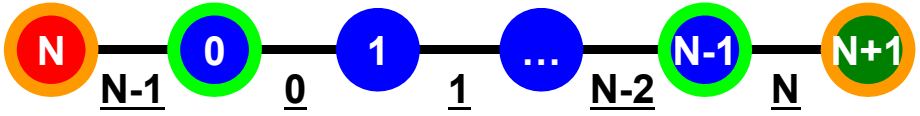
1D FEM: Numbering of Local ID



#0:
N+1 nodes
N elements



#PETot-1:
N+1 nodes
N elements

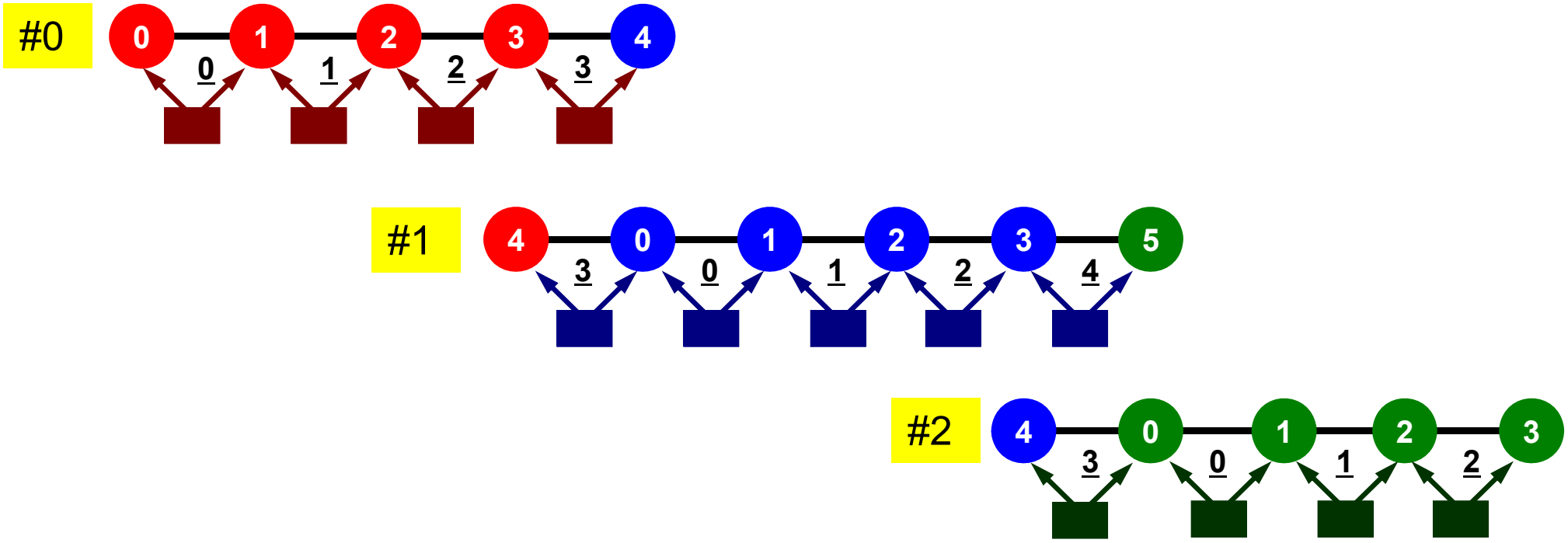


Others (General):
N+2 nodes
N+1 elements

1D FEM: 12 nodes/11 elem's/3 domains

Integration on each element, element matrix -> global matrix

Operations can be done by info. of internal/external nodes and elements which include these nodes



Preconditioned Conjugate Gradient Method (CG)

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

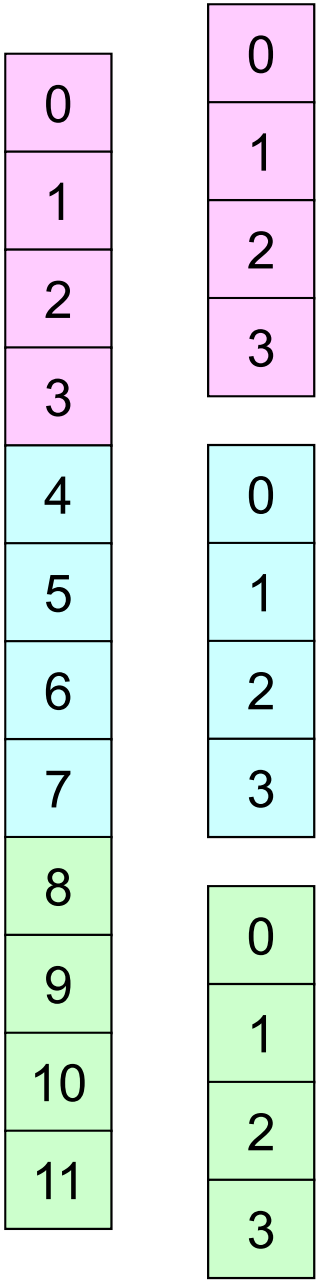
Preconditioning:
Diagonal Scaling
(or Point Jacobi)

Preconditioning, DAXPY

Local Operations by Only Internal Points: Parallel Processing is possible

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

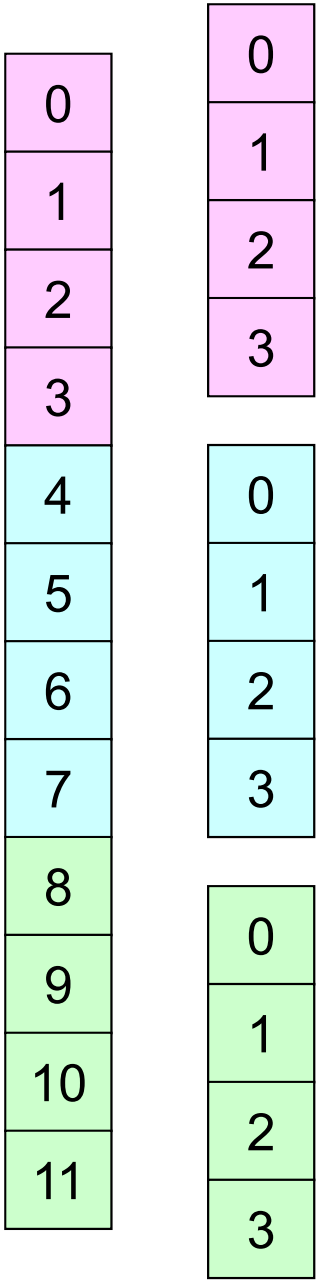
```
/*
//-- {x}= {x} + ALPHA*{p}
//   {r}= {r} - ALPHA*{q}
*/
  for(i=0;i<N;i++){
      U[i]    += Alpha * W[P][i];
      W[R][i] -= Alpha * W[Q][i];
  }
```



Dot Products

Global Summation needed: Communication ?

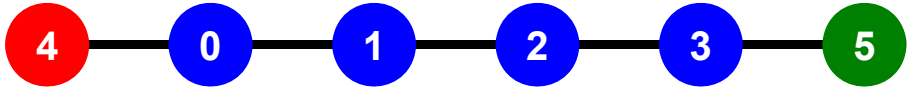
```
/*
//-- ALPHA= RHO / {p}{q}
*/
  C1 = 0.0;
  for(i=0;i<N;i++){
      C1 += W[P][i] * W[Q][i];
  }

  Alpha = Rho / C1;
```



Matrix-Vector Products

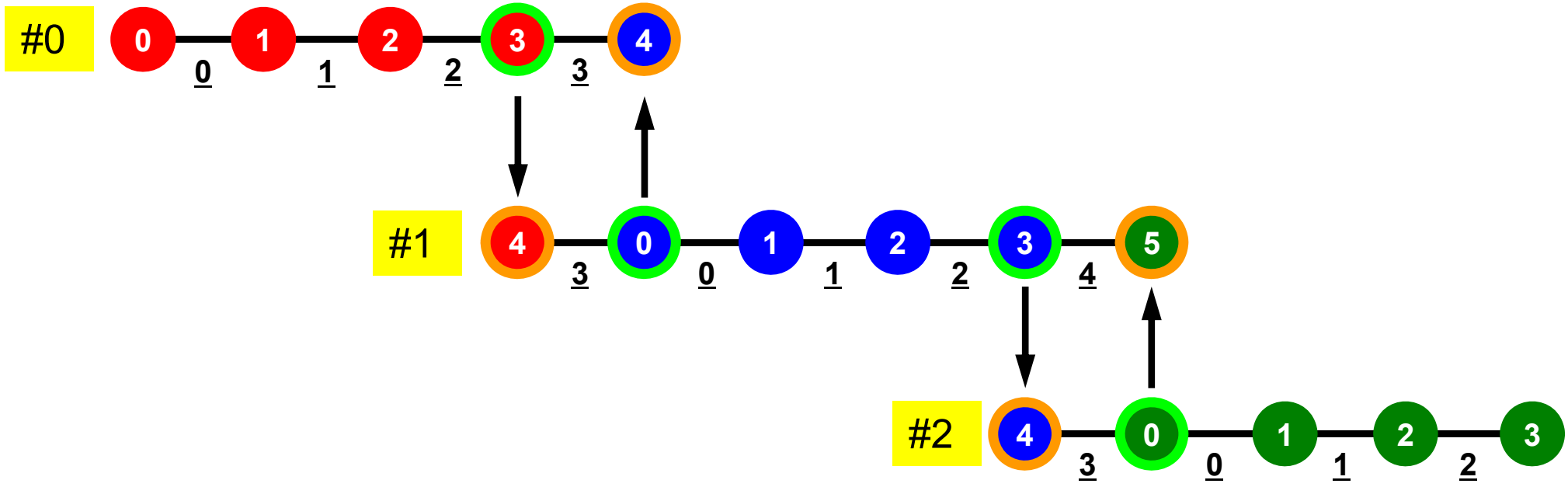
Values at External Points: P-to-P Communication

```
/*
//-- {q}= [A]{p}
*/
  for(i=0;i<N;i++){
      W[Q][i] = Diag[i] * W[P][i];
      for(j=Index[i];j<Index[i+1];j++){
          W[Q][i] += AMat[j]*W[P][Item[j]];
          }
      }
```

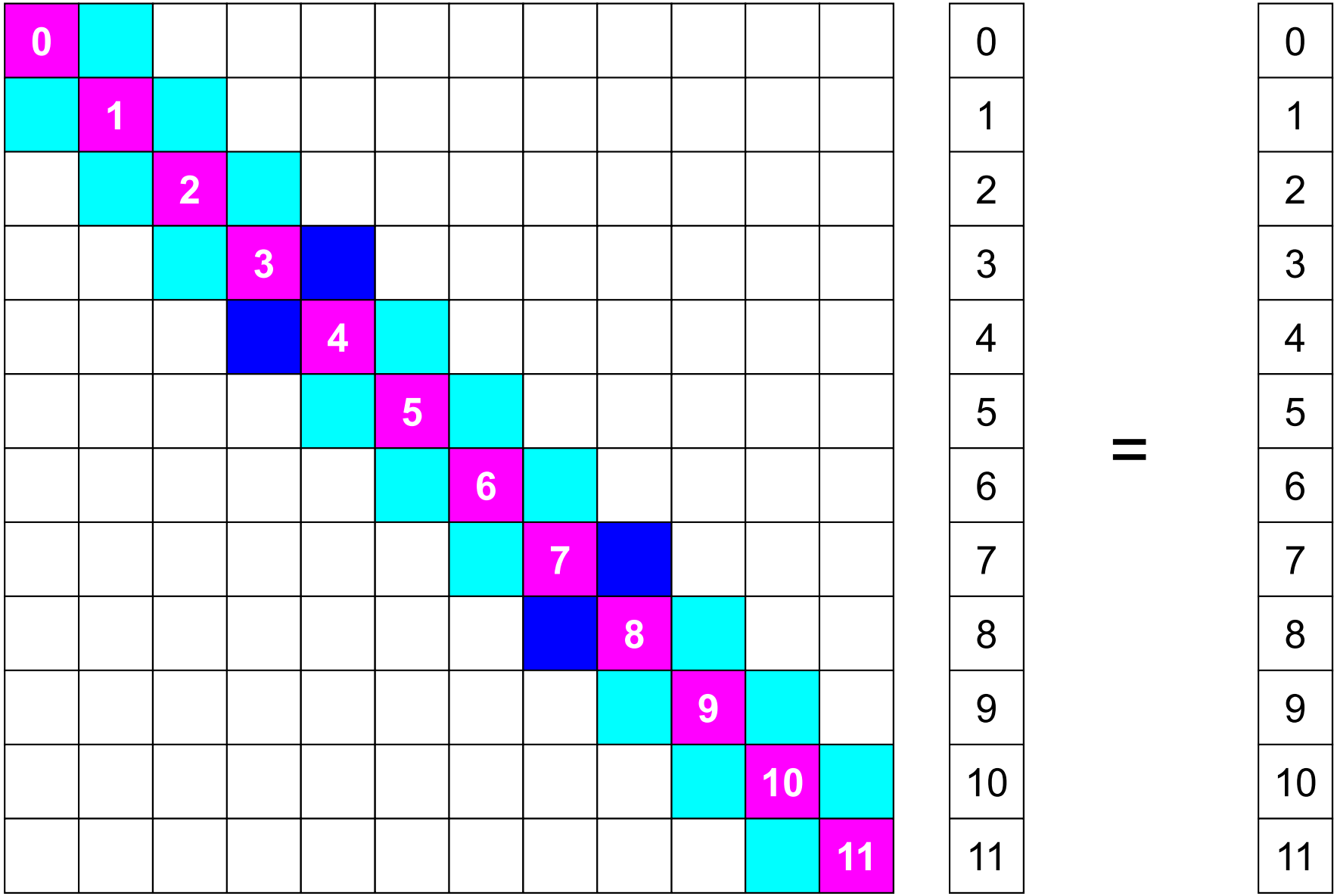


1D FEM: 12 nodes/11 elem's/3 domains

Internal/External Nodes



Mat-Vec Products: Local Op. Possible



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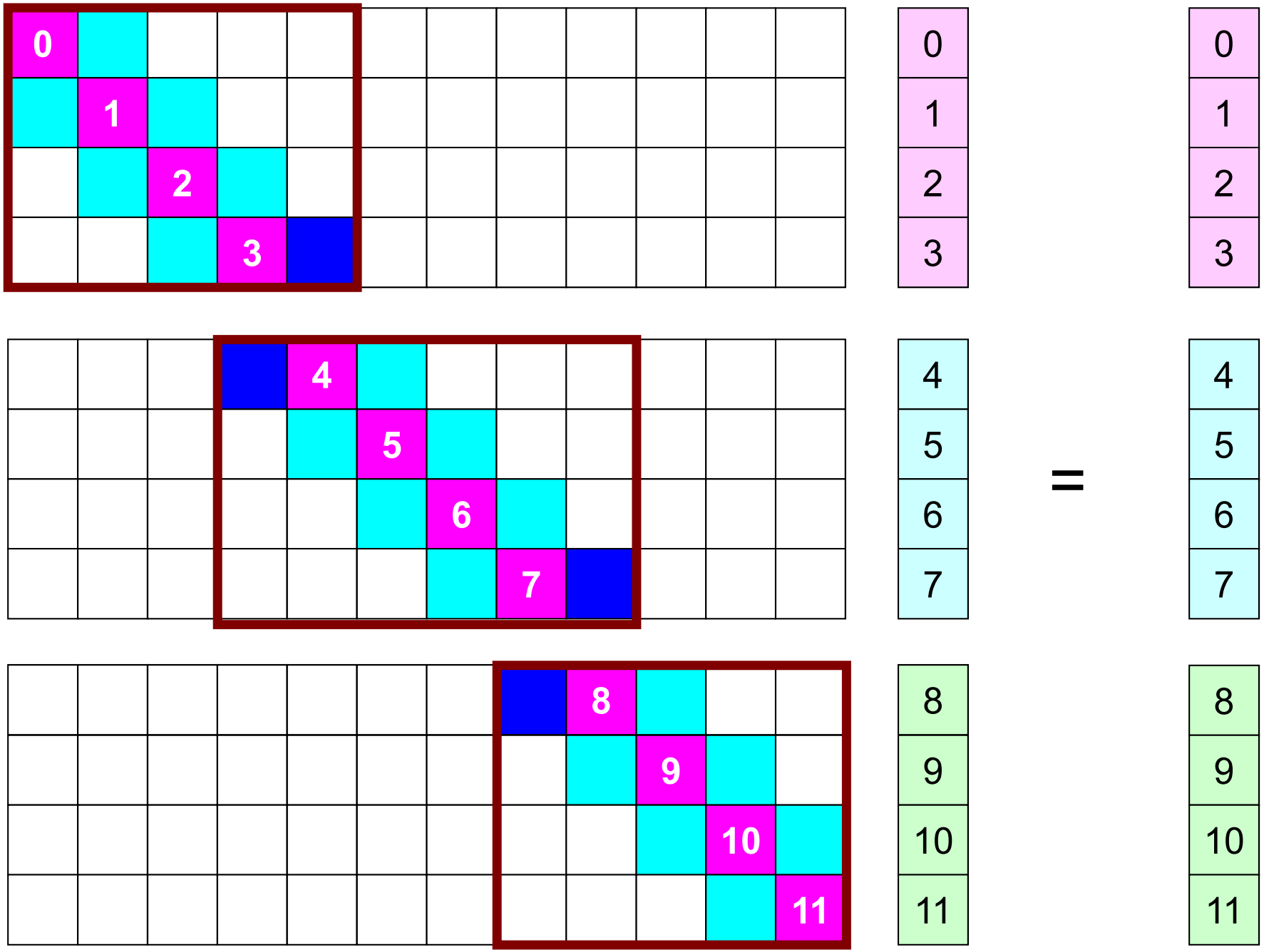
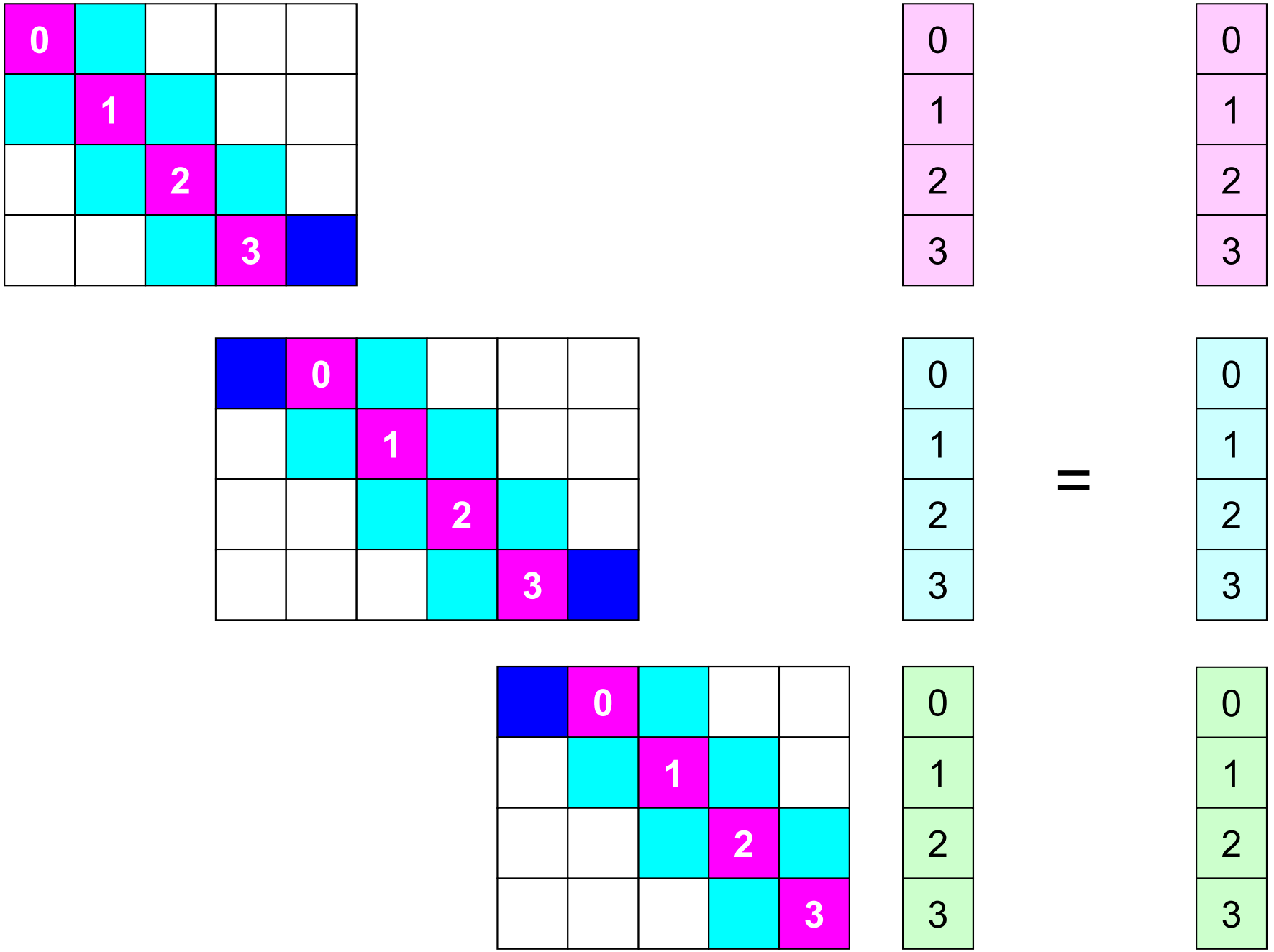
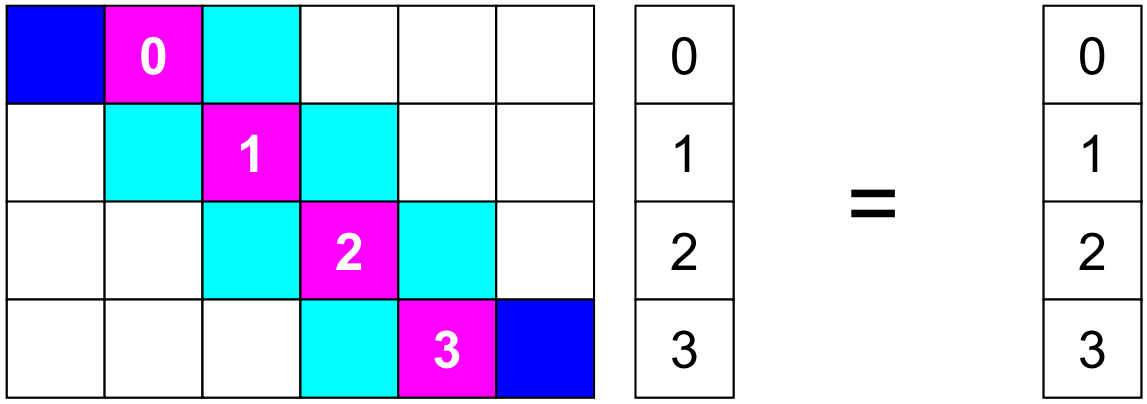
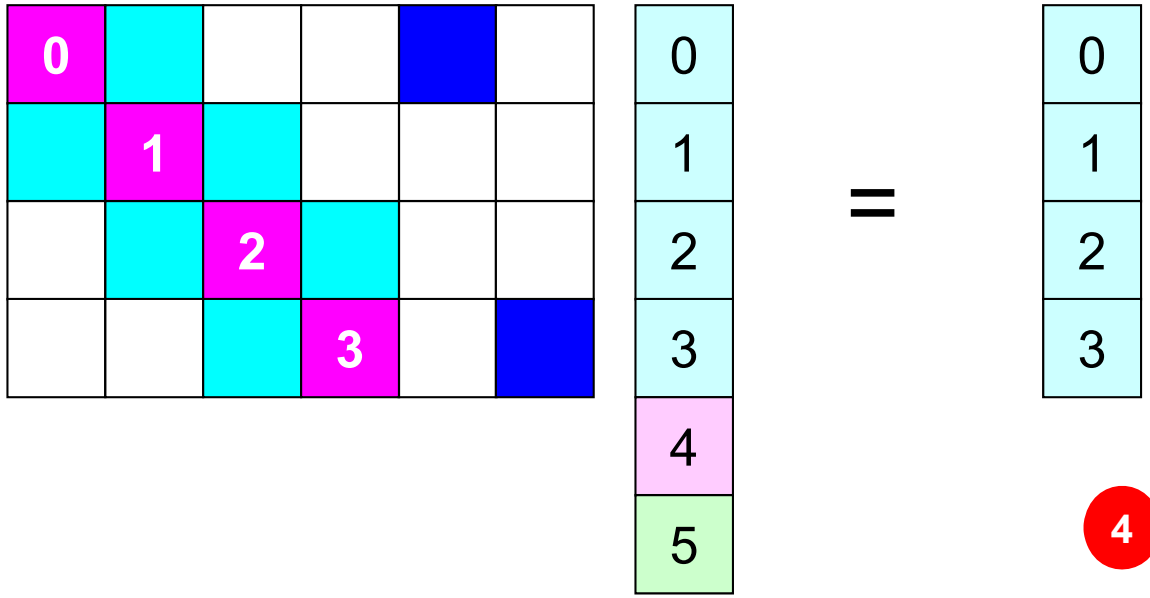


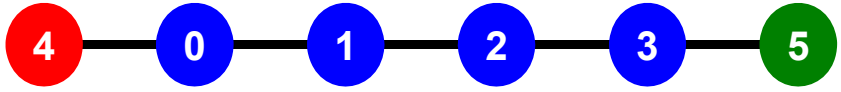
Mat-Vec Products: Local Op. Possible



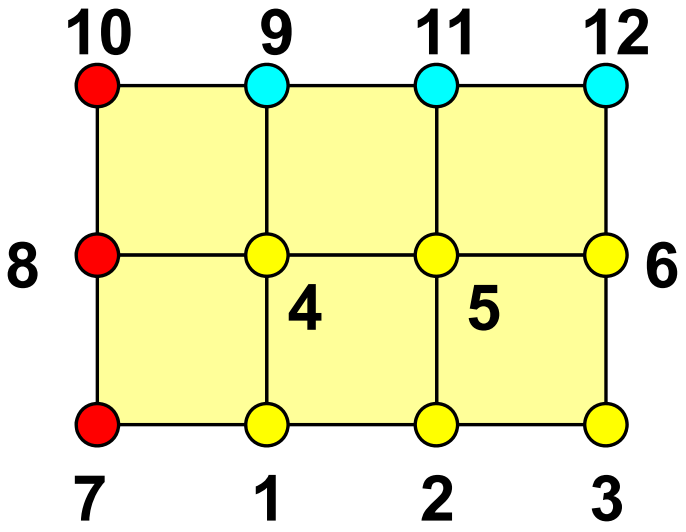
Mat-Vec Products: Local Op. #1







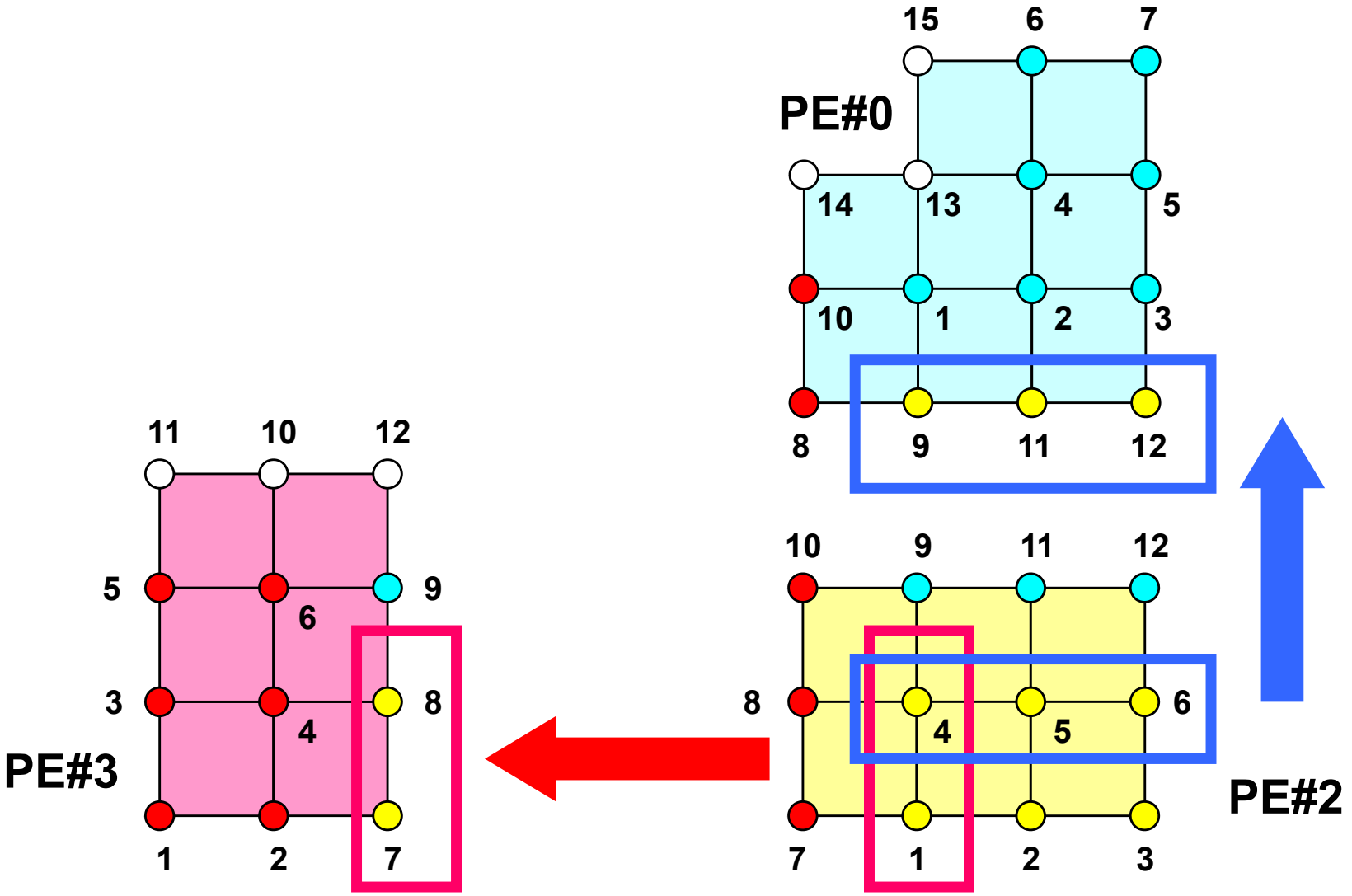
Description of Distributed Local Data



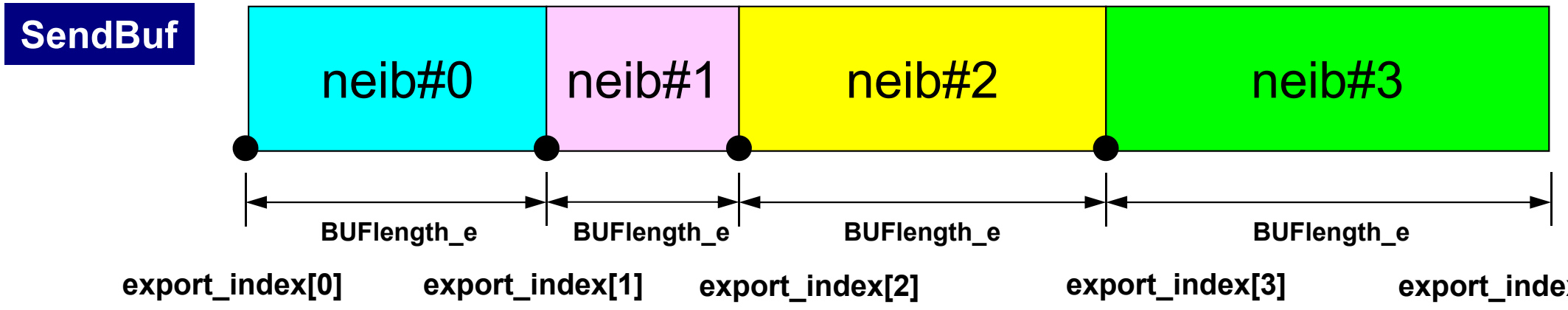
- Internal/External Points
  - Numbering: Starting from internal pts, then external pts after that
- Neighbors
  - Shares overlapped meshes
  - Number and ID of neighbors
- External Points
  - From where, how many, and which external points are received/imported ?
- Boundary Points
  - To where, how many and which boundary points are sent/exported ?

Boundary Nodes（境界点）：SEND

PE#2 : send information on “boundary nodes”



SEND: MPI_Isend/Irecv/Waitall



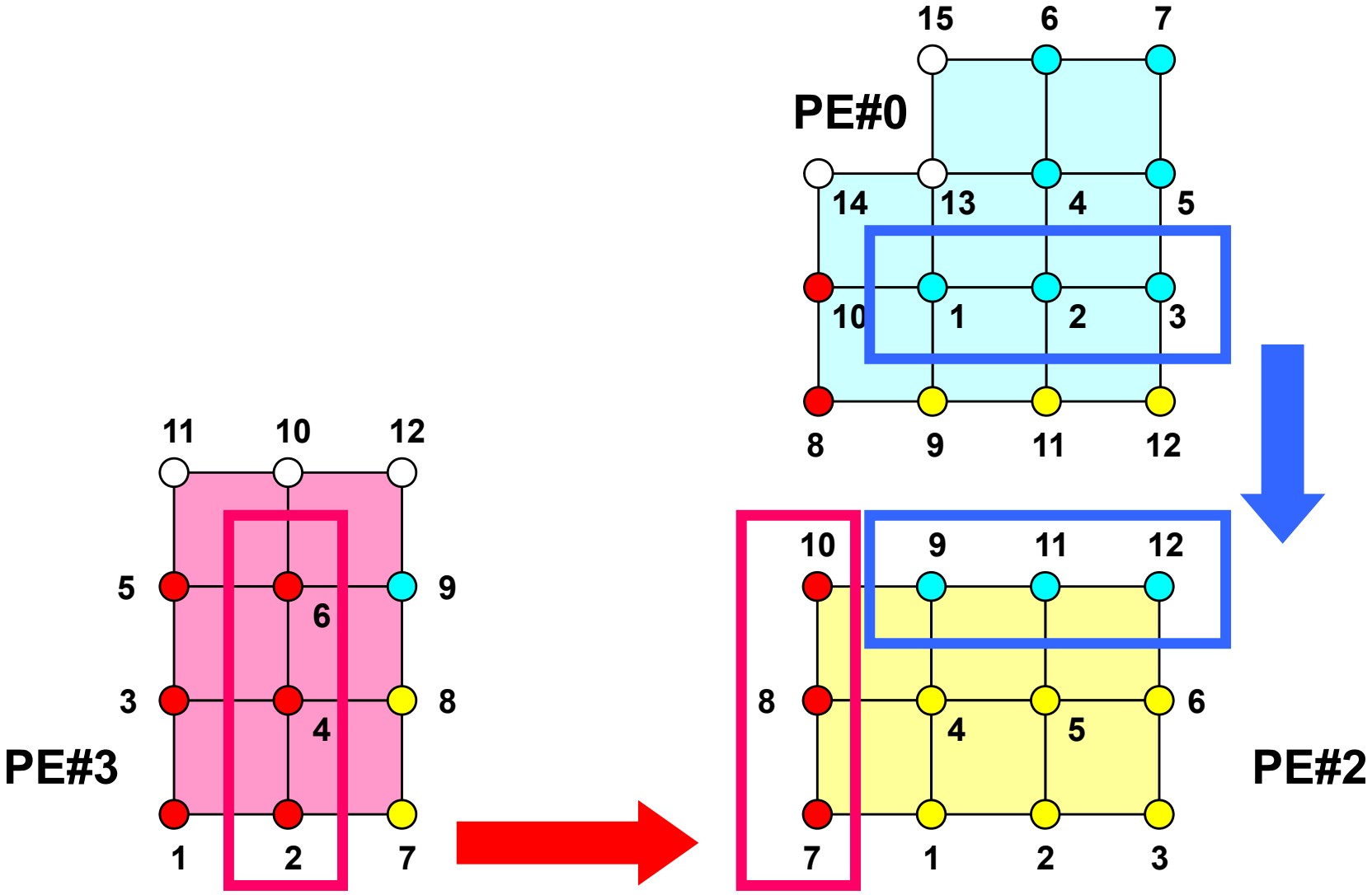
export_item (export_index[neib]:export_index[neib+1]-1) are sent to neib-th neighbor

```
for (neib=0; neib<NeibPETot;neib++){
   for (k=export_index[neib];k<export_index[neib+1];k++){
      kk= export_item[k];
      SendBuf[k]= VAL[kk];
   }
}

for (neib=0; neib<NeibPETot; neib++){
  tag= 0;
  iS_e= export_index[neib];
  iE_e= export_index[neib+1];
  BUFlength_e= iE_e - iS_e

  ierr= MPI_Isend
        (&SendBuf[iS_e], BUFlength_e, MPI_DOUBLE, NeibPE[neib], 0,
         MPI_COMM_WORLD, &ReqSend[neib])
}

MPI_Waitall(NeibPETot, ReqSend, StatSend);
```

Copied to sending buffers

External Nodes（外点）：RECEIVE

PE#2 : receive information for “external nodes”

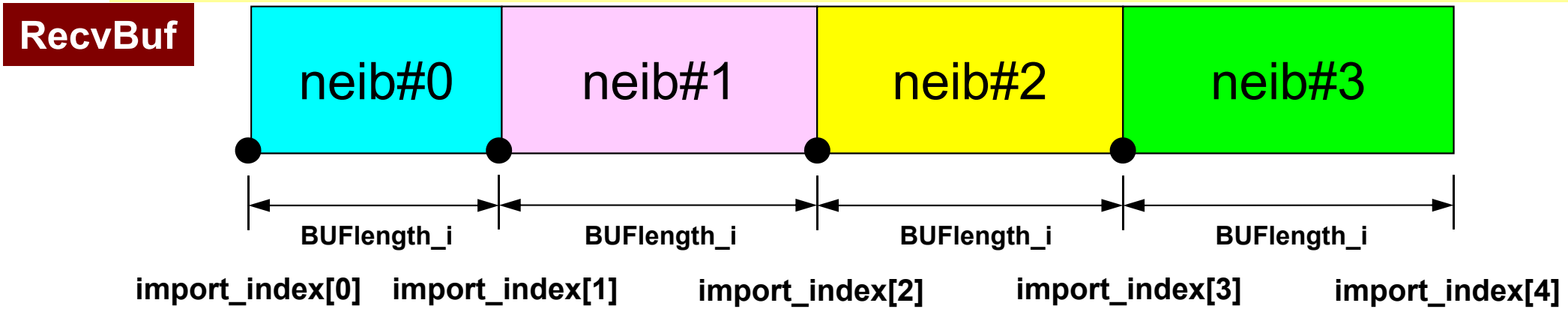


RECV: MPI_Isend/Irecv/Waitall

```
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];
    }
}
```

Copied from receiving buffer

import_item (import_index[neib]:import_index[neib+1]-1) are received from neib-th neighbor



- Overview
- Distributed Local Data
- **Program**
- Results

Program: 1d.c (1/11)
Variables

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <assert.h>
#include <mpi.h>

int main(int argc, char **argv){

  int NE, N, NP, NPLU, IterMax, NEg, Ng, errno;
  double dX, Resid, Eps, Area, QV, COND, QN;
  double X1, X2, DL, Ck;  double *PHI, *Rhs, *X, *Diag, *AMat;
  double *R, *Z, *Q, *P, *DD;
  int *Index, *Item, *Icelnod;
  double Kmat[2][2], Emat[2][2];

  int i, j, in1, in2, k, icel, k1, k2, jS;
  int iter, nr, neib;
  FILE *fp;
  double BNorm2, Rho, Rho1=0.0, C1, Alpha, Beta, DNorm2;
  int PETot, MyRank, kk, is, ir, len_s, len_r, tag;
  int NeibPETot, BufLength, NeibPE[2];

  int import_index[3], import_item[2];
  int export_index[3], export_item[2];
  double SendBuf[2], RecvBuf[2];

  double BNorm20, Rho0, C10, DNorm20;
  double StartTime, EndTime;
  int ierr = 1;

  MPI_Status  *StatSend,    *StatRecv;
  MPI_Request *RequestSend, *RequestRecv;
```

Program: 1d.c (2/11)
Control Data

```
/*
// +-------+
// | INIT. |
// +-------+
//=== */

/*
//-- CONTROL data
*/

    ierr = MPI_Init(&argc, &argv);                          Initialization
    ierr = MPI_Comm_size(MPI_COMM_WORLD, &PETot);           Entire Process #: PETot
    ierr = MPI_Comm_rank(MPI_COMM_WORLD, &MyRank);          Rank ID (0-PETot-1): MyRank

    if(MyRank == 0){
      fp = fopen("input.dat", "r");
      assert(fp != NULL);
      fscanf(fp, "%d", &NEg);
      fscanf(fp, "%lf %lf %lf %lf", &dX, &QV, &Area, &COND);
      fscanf(fp, "%d", &IterMax);
      fscanf(fp, "%lf", &Eps);
      fclose(fp);
    }

    ierr = MPI_Bcast(&NEg    , 1, MPI_INT, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&IterMax, 1, MPI_INT, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&dX     , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&QV     , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&Area   , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&COND   , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&Eps    , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

Program: 1d.c (2/11)

Control Data

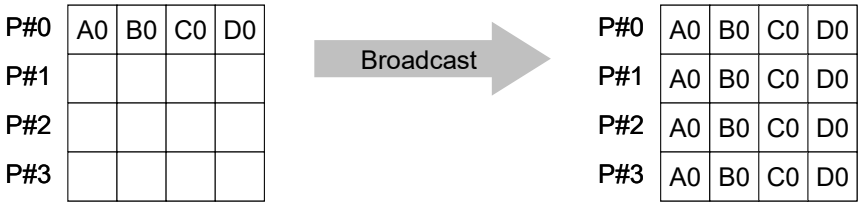
```
/*
// +-------+
// | INIT. |
// +-------+
//=== */

/*
//-- CONTROL data
*/

    ierr = MPI_Init(&argc, &argv);                          Initialization
    ierr = MPI_Comm_size(MPI_COMM_WORLD, &PETot);           Entire Process #: PETot
    ierr = MPI_Comm_rank(MPI_COMM_WORLD, &MyRank);          Rank ID (0-PETot-1): MyRank

    if(MyRank == 0){                                        Reading control file if MyRank=0
      fp = fopen("input.dat", "r");
      assert(fp != NULL);
      fscanf(fp, "%d", &NEg);                               Neg: Global Number of Elements
      fscanf(fp, "%lf %lf %lf %lf", &dX, &QV, &Area, &COND);
      fscanf(fp, "%d", &IterMax);
      fscanf(fp, "%lf", &Eps);
      fclose(fp);
    }

    ierr = MPI_Bcast(&NEg    , 1, MPI_INT, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&IterMax, 1, MPI_INT, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&dX     , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&QV     , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&Area   , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&COND   , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&Eps    , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

Program: 1d.c (2/11)

Control Data

```
/*
// +-------+
// | INIT. |
// +-------+
//=== */

/*
//-- CONTROL data
*/

 ierr = MPI_Init(&argc, &argv);                                  Initialization
    ierr = MPI_Comm_size(MPI_COMM_WORLD, &PETot);                Entire Process #: PETot
    ierr = MPI_Comm_rank(MPI_COMM_WORLD, &MyRank);               Rank ID (0-PETot-1): MyRank

    if(MyRank == 0){                                             Reading control file if MyRank=0
      fp = fopen("input.dat", "r");
      assert(fp != NULL);
      fscanf(fp, "%d", &NEg);                                    Neg: Global Number of Elements
      fscanf(fp, "%lf %lf %lf %lf", &dX, &QV, &Area, &COND);
      fscanf(fp, "%d", &IterMax);
      fscanf(fp, "%lf", &Eps);
      fclose(fp);
    }

    ierr = MPI_Bcast(&NEg    , 1, MPI_INT, 0, MPI_COMM_WORLD);  Parameters are sent to each process
    ierr = MPI_Bcast(&IterMax, 1, MPI_INT, 0, MPI_COMM_WORLD);  from Process #0.
    ierr = MPI_Bcast(&dX     , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&QV     , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&Area   , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&COND   , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
    ierr = MPI_Bcast(&Eps    , 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
```

MPI_Bcast



- Broadcasts a message from the process with rank "root" to all other processes of the communicator

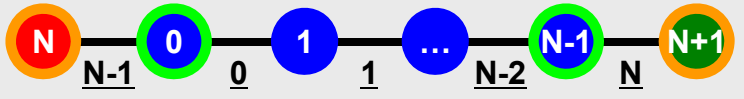
- **MPI_Bcast (buffer,count,datatype,root,comm)**
  - **buffer** choice I/O starting address of buffer
    type is defined by "**datatype**"
  - **count** int I number of elements in send/receive buffer
  - **datatype** MPI_Datatype I data type of elements of send/recive buffer
    FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.
    C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc.
  - **root** int I rank of root process
  - **comm** MPI_Comm I communicator

Program: 1d.c (3/11)
Distributed Local Mesh

```
/*
//-- LOCAL MESH size
*/
    Ng= NEg + 1;                Ng: Number of Nodes (Global)
    N = Ng / PETot;             N : Number of Nodes (Local)

    nr = Ng - N*PETot;          mod(Ng,PETot) .ne. 0
    if(MyRank < nr) N++;

    NE= N - 1 + 2;
    NP= N + 2;
    if(MyRank == 0) NE= N - 1 + 1;
    if(MyRank == 0) NP= N + 1;
    if(MyRank == PETot-1) NE= N - 1 + 1;
    if(MyRank == PETot-1) NP= N + 1;

    if(PETot==1){NE=N-1;}
    if(PETot==1){NP=N  ;}

/*
//-- Arrays
*/
    PHI    = calloc(NP, sizeof(double));
    Diag = calloc(NP, sizeof(double));
    AMat = calloc(2*NP-2, sizeof(double));
    Rhs  = calloc(NP, sizeof(double));
    Index= calloc(NP+1, sizeof(int));
    Item = calloc(2*NP-2, sizeof(int));
    Icelnod= calloc(2*NE, sizeof(int));
```

Program: 1d.c (3/11)
Distributed Local Mesh, Uniform Elements

```
/*
//-- LOCAL MESH size
*/
    Ng= NEg + 1;              Ng: Number of Nodes (Global)
    N = Ng / PETot;           N : Number of Nodes (Local)

    nr = Ng - N*PETot;        mod(Ng,PETot) .ne. 0
    if(MyRank < nr) N++;

    NE= N - 1 + 2;            Number of Elements (Local)
    NP= N + 2;                Total Number of Nodes (Local) (Internal + External Nodes)
    if(MyRank == 0) NE= N - 1 + 1;
    if(MyRank == 0) NP= N + 1;
    if(MyRank == PETot-1) NE= N - 1 + 1;
    if(MyRank == PETot-1) NP= N + 1;

    if(PETot==1){NE=N-1;}
    if(PETot==1){NP=N  ;}

/*
//-- Arrays
*/
    PHI  = calloc(NP, sizeof(double));
    Diag = calloc(NP, sizeof(double));
    AMat = calloc(2*NP-2, sizeof(double));
    Rhs  = calloc(NP, sizeof(double));
    Index= calloc(NP+1, sizeof(int));
    Item = calloc(2*NP-2, sizeof(int));
    Icelnod= calloc(2*NE, sizeof(int));
```



Others (General):
N+2 nodes
N+1 elements

Program: 1d.c (3/11)
Distributed Local Mesh, Uniform Elements

```
/*
//-- LOCAL MESH size
*/
    Ng= NEg + 1;                Ng: Number of Nodes (Global)
    N = Ng / PETot;             N : Number of Nodes (Local)

    nr = Ng - N*PETot;          mod(Ng,PETot) .ne. 0
    if(MyRank < nr) N++;

    NE= N - 1 + 2;
    NP= N + 2;
    if(MyRank == 0) NE= N - 1 + 1;
    if(MyRank == 0) NP= N + 1;
    if(MyRank == PETot-1) NE= N - 1 + 1;
    if(MyRank == PETot-1) NP= N + 1;

    if(PETot==1){NE=N-1;}
    if(PETot==1){NP=N  ;}

/*
//-- Arrays
*/
    PHI  = calloc(NP, sizeof(double));
    Diag = calloc(NP, sizeof(double));
    AMat = calloc(2*NP-2, sizeof(double));
    Rhs  = calloc(NP, sizeof(double));
    Index= calloc(NP+1, sizeof(int));
    Item = calloc(2*NP-2, sizeof(int));
    Icelnod= calloc(2*NE, sizeof(int));
```

#0:
N+1 nodes
N elements

Program: 1d.c (3/11)

Distributed Local Mesh, Uniform Elements

```
/*
//-- LOCAL MESH size
*/
    Ng= NEg + 1;                Ng: Number of Nodes (Global)
    N = Ng / PETot;             N : Number of Nodes (Local)

    nr = Ng - N*PETot;          mod(Ng,PETot) .ne. 0
    if(MyRank < nr) N++;
    NE= N - 1 + 2;
    NP= N + 2;
    if(MyRank == 0) NE= N - 1 + 1;
    if(MyRank == 0) NP= N + 1;
    if(MyRank == PETot-1) NE= N - 1 + 1;
    if(MyRank == PETot-1) NP= N + 1;

    if(PETot==1){NE=N-1;}
    if(PETot==1){NP=N  ;}

/*
//-- Arrays
*/
    PHI  = calloc(NP, sizeof(double));
    Diag = calloc(NP, sizeof(double));
    AMat = calloc(2*NP-2, sizeof(double));
    Rhs  = calloc(NP, sizeof(double));
    Index= calloc(NP+1, sizeof(int));
    Item = calloc(2*NP-2, sizeof(int));
    Icelnod= calloc(2*NE, sizeof(int));
```

#PETot-1:
N+1 nodes
N elements

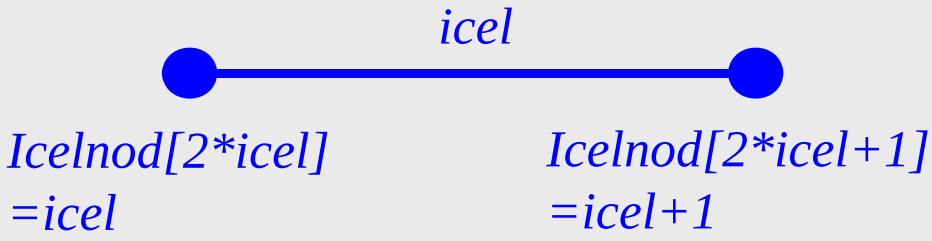
Program: 1d.c (3/11)
Distributed Local Mesh, Uniform Elements

```
/*
//-- LOCAL MESH size
*/
    Ng= NEg + 1;                Ng: Number of Nodes (Global)
    N = Ng / PETot;             N : Number of Nodes (Local)

    nr = Ng - N*PETot;          mod(Ng,PETot) .ne. 0
    if(MyRank < nr) N++;

    NE= N - 1 + 2;
    NP= N + 2;
    if(MyRank == 0) NE= N - 1 + 1;
    if(MyRank == 0) NP= N + 1;
    if(MyRank == PETot-1) NE= N - 1 + 1;
    if(MyRank == PETot-1) NP= N + 1;

    if(PETot==1){NE=N-1;}
    if(PETot==1){NP=N  ;}

/*
//-- Arrays
*/
    PHI  = calloc(NP, sizeof(double));          Size of arrays is  “NP”, not  “N”
    Diag = calloc(NP, sizeof(double));
    AMat = calloc(2*NP-2, sizeof(double));
    Rhs  = calloc(NP, sizeof(double));
    Index= calloc(NP+1, sizeof(int));
    Item = calloc(2*NP-2, sizeof(int));
    Icelnod= calloc(2*NE, sizeof(int));
```

Program: 1d.c (4/11)

Initialization of Arrays, Elements-Nodes

```
for(i=0;i<NP;i++)    U[i] = 0.0;
for(i=0;i<NP;i++) Diag[i] = 0.0;
for(i=0;i<NP;i++)  Rhs[i] = 0.0;
for(k=0;k<2*NP-2;k++)  AMat[k] = 0.0;

for(i=0;i<3;i++) import_index[i]= 0;
for(i=0;i<3;i++) export_index[i]= 0;
for(i=0;i<2;i++) import_item[i]= 0;
for(i=0;i<2;i++) export_item[i]= 0;

for(icel=0;icel<NE;icel++){
  Icelnod[2*icel  ]= icel;
  Icelnod[2*icel+1]= icel+1;
}

if(PETot>1){
  if(MyRank==0){
    icel= NE-1;
    Icelnod[2*icel  ]= N-1;
    Icelnod[2*icel+1]= N;
  }else if(MyRank==PETot-1){
    icel= NE-1;
    Icelnod[2*icel  ]= N;
    Icelnod[2*icel+1]= 0;
  }else{
    icel= NE-2;
    Icelnod[2*icel  ]= N;
    Icelnod[2*icel+1]= 0;
    icel= NE-1;
    Icelnod[2*icel  ]= N-1;
    Icelnod[2*icel+1]= N+1;
  }
}
```



Program: 1d.c (4/11)

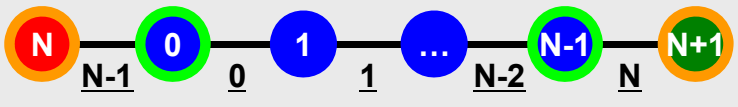
Initialization of Arrays, Elements-Nodes

```
for(i=0;i<NP;i++)    U[i] = 0.0;
for(i=0;i<NP;i++) Diag[i] = 0.0;
for(i=0;i<NP;i++)  Rhs[i] = 0.0;
for(k=0;k<2*NP-2;k++)  AMat[k] = 0.0;

for(i=0;i<3;i++) import_index[i]= 0;
for(i=0;i<3;i++) export_index[i]= 0;
for(i=0;i<2;i++) import_item[i]= 0;
for(i=0;i<2;i++) export_item[i]= 0;

for(icel=0;icel<NE;icel++){
  Icelnod[2*icel  ]= icel;
  Icelnod[2*icel+1]= icel+1;
}

if(PETot>1){
  if(MyRank==0){
    icel= NE-1;
    Icelnod[2*icel  ]= N-1;
    Icelnod[2*icel+1]= N;
  }else if(MyRank==PETot-1){
    icel= NE-1;
    Icelnod[2*icel  ]= N;
    Icelnod[2*icel+1]= 0;
  }else{
    icel= NE-2;
    Icelnod[2*icel  ]= N;
    Icelnod[2*icel+1]= 0;
    icel= NE-1;
    Icelnod[2*icel  ]= N-1;
    Icelnod[2*icel+1]= N+1;
  }
}
```

e.g. Element-0 includes node-0 and node-1

#0:
N+1 nodes
N elements

#PETot-1:
N+1 nodes
N elements



Others (General):
N+2 nodes
N+1 elements

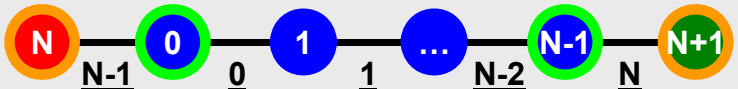
Program: 1d.c (5/11)

”Index”

```
    Kmat[0][0]= +1.0;
    Kmat[0][1]= -1.0;
    Kmat[1][0]= -1.0;
    Kmat[1][1]= +1.0;

/*
// +-------------+
// | CONNECTIVITY |
// +-------------+
*/
    for(i=0;i<N+1;i++)     Index[i] = 2;
    for(i=N+1;i<NP+1;i++)  Index[i] = 1;

    Index[0] = 0;
    if(MyRank == 0)        Index[1] = 1;
    if(MyRank == PETot-1)  Index[N] = 1;

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

    NPLU= Index[NP];
```

#0:
N+1 nodes
N elements

#PETot-1:
N+1 nodes
N elements



Others (General):
N+2 nodes
N+1 elements

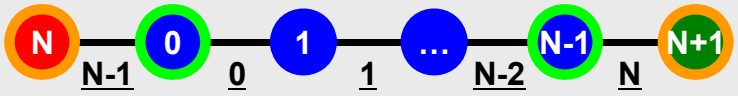
Program: 1d.c (6/11)

”Item”

```
for(i=0;i<N;i++){
  jS = Index[i];
  if((MyRank==0)&&(i==0)){
    Item[jS] = i+1;
  }else if((MyRank==PETot-1)&&(i==N-1)){
    Item[jS] = i-1;
  }else{
    Item[jS]   = i-1;
    Item[jS+1] = i+1;
    if(i==0)   { Item[jS]  = N;}
    if(i==N-1){ Item[jS+1]= N+1;}
    if((MyRank==0)&&(i==N-1)){Item[jS+1]= N;}
  }
}

i =N;
jS= Index[i];
  if (MyRank==0) {
    Item[jS]= N-1;
  }else {
    Item[jS]= 0;
  }

i =N+1;
jS= Index[i];
  if ((MyRank!=0)&&(MyRank!=PETot-1)) {
    Item[jS]= N-1;
  }
```

#0:
N+1 nodes
N elements

#PETot-1:
N+1 nodes
N elements



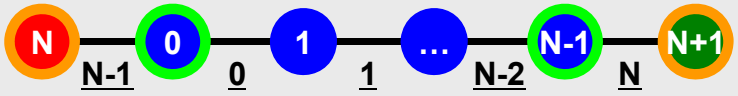
Others (General):
N+2 nodes
N+1 elements

Program: 1d.c (7/11)
Communication Tables

```
/*
//-- COMMUNICATION
*/
    NeibPETot = 2;
    if(MyRank == 0)        NeibPETot = 1;
    if(MyRank == PETot-1) NeibPETot = 1;
    if(PETot  == 1)        NeibPETot = 0;

    NeibPE[0] = MyRank - 1;
    NeibPE[1] = MyRank + 1;

    if(MyRank == 0)        NeibPE[0] = MyRank + 1;
    if(MyRank == PETot-1) NeibPE[0] = MyRank - 1;

    import_index[1]=1;
    import_index[2]=2;
    import_item[0]=  N;
    import_item[1]=  N+1;

    export_index[1]=1;
    export_index[2]=2;
    export_item[0]= 0;
    export_item[1]= N-1;

    if(MyRank == 0) import_item[0]=N;
    if(MyRank == 0) export_item[0]=N-1;

    BufLength = 1;

    StatSend = malloc(sizeof(MPI_Status) * NeibPETot);
    StatRecv = malloc(sizeof(MPI_Status) * NeibPETot);
    RequestSend = malloc(sizeof(MPI_Request) * NeibPETot);
    RequestRecv = malloc(sizeof(MPI_Request) * NeibPETot);
```

#0:
N+1 nodes
N elements

#PETot-1:
N+1 nodes
N elements



Others (General):
N+2 nodes
N+1 elements

MPI_Isend

- Begins a non-blocking send
  - Send the contents of sending buffer (starting from **`sendbuf`**, number of messages: **`count`**) to **`dest`** with **`tag`** .
  - Contents of sending buffer cannot be modified before calling corresponding **`MPI_Waitall`**.

- **`MPI_Isend (sendbuf,count,datatype,dest,tag,comm,request)`**

– **`sendbuf`**	choice	I	starting address of sending buffer
– **`count`**	int	I	number of elements in sending buffer
– **`datatype`**	MPI_Datatype	I	datatype of each sending buffer element
– **`dest`**	int	I	rank of destination
– **`tag`**	int	I	message tag This integer can be used by the application to distinguish messages. Communication occurs if `tag's` of `MPI_Isend` and `MPI_Irecv` are matched. Usually tag is set to be “0” (in this class),
– **`comm`**	MPI_Comm	I	communicator
– **`request`**	MPI_Request	O	communication request array used in `MPI_Waitall`

MPI_Irecv

- Begins a non-blocking receive
  - Receiving the contents of receiving buffer (starting from **`recvbuf`**, number of messages: **`count`**) from **`source`** with **`tag`** .
  - Contents of receiving buffer cannot be used before calling corresponding **`MPI_Waitall`**.

- **`MPI_Irecv (recvbuf,count,datatype,source,tag,comm,request)`**
  - **`recvbuf`** choice I starting address of receiving buffer
  - **`count`** int I number of elements in receiving buffer
  - **`datatype`** MPI_Datatype I datatype of each receiving buffer element
  - **`source`** int I rank of source
  - **`tag`** int I message tag
    This integer can be used by the application to distinguish messages. Communication occurs if `tag's` of `MPI_Isend` and `MPI_Irecv` are matched.
    Usually tag is set to be “0” (in this class),
  - **`comm`** MPI_Comm I communicator
  - **`request`** MPI_Request O communication request array used in `MPI_Waitall`

MPI_Waitall

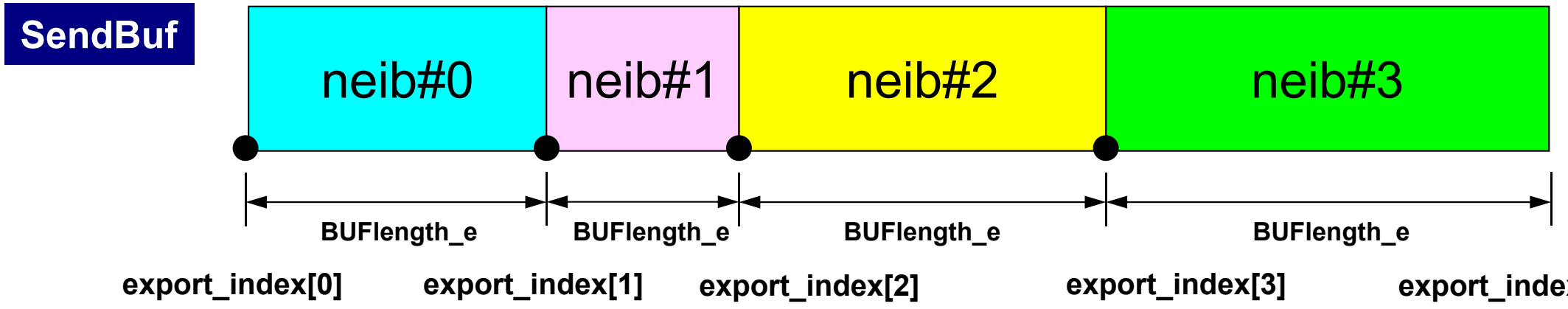
- **MPI_Waitall** blocks until all comm's, associated with **request** in the array, complete. It is used for synchronizing **MPI_Isend** and **MPI_Irecv** in this class.
- At sending phase, contents of sending buffer cannot be modified before calling corresponding **MPI_Waitall**. At receiving phase, contents of receiving buffer cannot be used before calling corresponding **MPI_Waitall**.
- **MPI_Isend** and **MPI_Irecv** can be synchronized simultaneously with a single **MPI_Waitall** if it is consitent.
  - Same **request** should be used in **MPI_Isend** and **MPI_Irecv**.
- Its operation is similar to that of **MPI_Barrier** but, **MPI_Waitall** can not be replaced by **MPI_Barrier.**
  - Possible troubles using **MPI_Barrier** instead of **MPI_Waitall**: Contents of **request** and **status** are not updated properly, very slow operations etc.

- **MPI_Waitall (count,request,status)**
  - **count** int I number of processes to be synchronized
  - **request** MPI_Request I/O comm. request used in MPI_Waitall (array size: count)
  - **status** MPI_Status O array of status objects
    MPI_STATUS_SIZE: defined in 'mpif.h', 'mpi.h'

Generalized Comm. Table: Send

- Neighbors
  - NeibPETot, NeibPE[neib]
- Message size for each neighbor
  - export_index[neib], neib= 0, NeibPETot-1
- ID of **boundary** points
  - export_item[k], k= 0, export_index[NeibPETot]-1
- Messages to each neighbor
  - SendBuf[k], k= 0, export_index[NeibPETot]-1

SEND: MPI_Isend/Irecv/Waitall

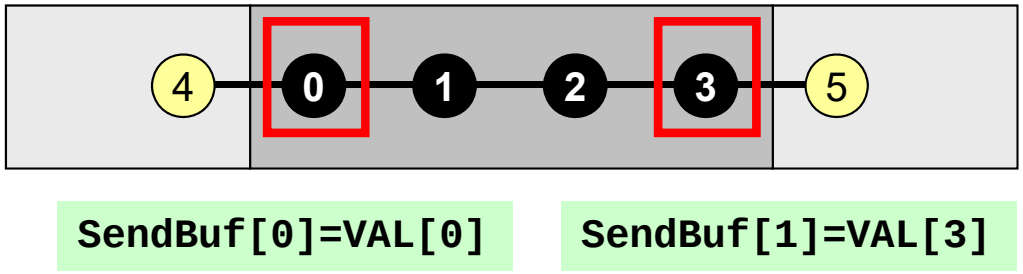


export_item (export_index[neib]:export_index[neib+1]-1) are sent to neib-th neighbor

```
for (neib=0; neib<NeibPETot;neib++){
   for (k=export_index[neib];k<export_index[neib+1];k++){
      kk= export_item[k];
      SendBuf[k]= VAL[kk];
   }
}

for (neib=0; neib<NeibPETot; neib++){
  tag= 0;
  iS_e= export_index[neib];
  iE_e= export_index[neib+1];
  BUFlength_e= iE_e - iS_e

  ierr= MPI_Isend
        (&SendBuf[iS_e], BUFlength_e, MPI_DOUBLE, NeibPE[neib], 0,
         MPI_COMM_WORLD, &ReqSend[neib])
}

MPI_Waitall(NeibPETot, ReqSend, StatSend);
```

Copied to sending buffers

SEND/Export: 1D Problem



- Neighbors
  - NeibPETot, NeibPE[neib]
    - NeibPETot=2, NeibPE[0]= my_rank-1, NeibPE[1]= my_rank+1
- Message size for each neighbor
  - export_index[neib], neib= 0, NeibPETot-1
    - export_index[0]=0, export_index[1]= 1, export_index[2]= 2
- ID of **boundary** points
  - export_item[k], k= 0, export_index[NeibPETot]-1
    - export_item[0]= 0, export_item[1]= N-1
- Messages to each neighbor
  - SendBuf[k], k= 0, export_index[NeibPETot]-1
    - SendBuf[0]= VAL[0], SendBuf[1]= VAL[N-1]

Generalized Comm. Table: Receive

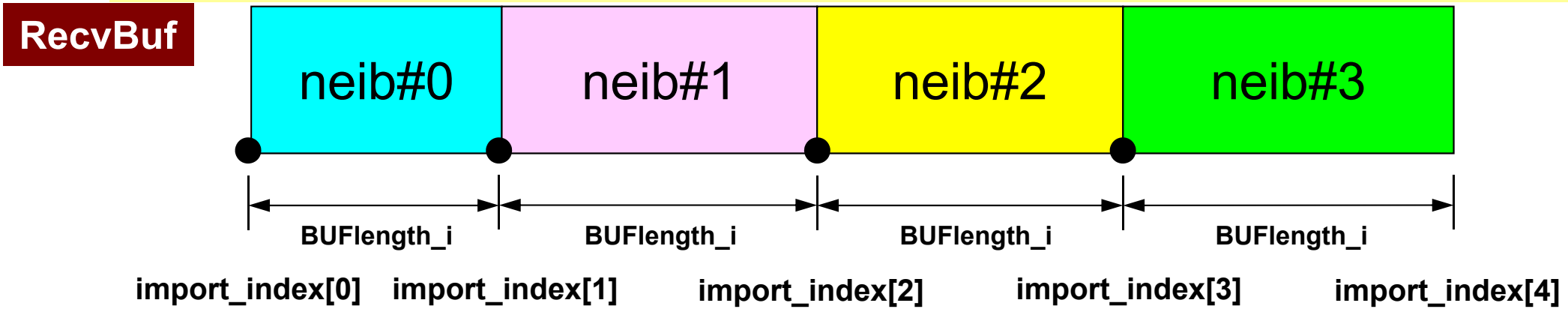
- Neighbors
  - NeibPETot , NeibPE[neib]
- Message size for each neighbor
  - import_index[neib], neib= 0, NeibPETot-1
- ID of **external** points
  - import_item[k], k= 0, import_index[NeibPETot]-1
- Messages from each neighbor
  - RecvBuf[k], k= 0, import_index[NeibPETot]-1

RECV: MPI_Isend/Irecv/Waitall

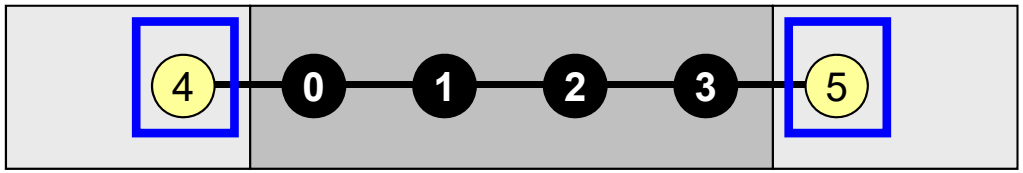
```
for (neib=0; neib<NeibPETot; neib++){
   tag= 0;
   iS_i= import_index[neib];
   iE_i= import_index[neib+1];
   BUFlength_i= iE_i - iS_i

   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];
    }
}
```

Copied from receiving buffer

import_item (import_index[neib]:import_index[neib+1]-1) are received from neib-th neighbor



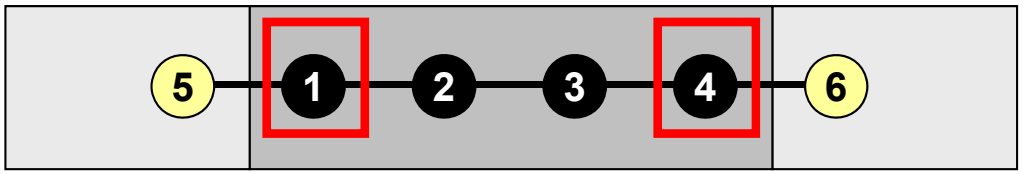
RECV/Import: 1D Problem



`VAL[4]=RecvBuf[0]` `VAL[5]=RecvBuf[1]`

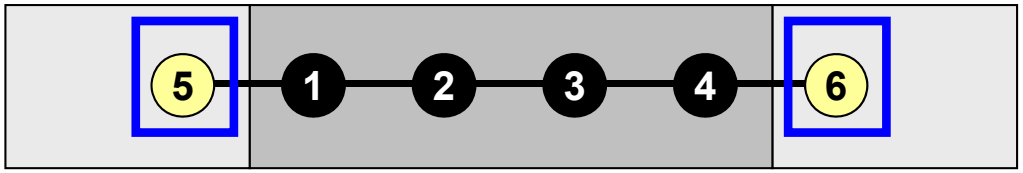
- Neighbors
  - NeibPETot, NeibPE[neib]
    - NeibPETot=2, NeibPE[0]= my_rank-1, NeibPE[1]= my_rank+1
- Message size for each neighbor
  - import_index[neib], neib= 0, NeibPETot-1
    - import_index[0]=0, import_index[1]= 1, import_index[2]= 2
- ID of **external** points
  - import_item[k], k= 0, import_index[NeibPETot]-1
    - import_item[0]= N, import_item[1]= N+1
- Messages from each neighbor
  - RECVbuf[k], k= 0, import_index[NeibPETot]-1
    - VAL[N]=RecvBuf[0], VAL[N+1]=RecvBuf[1]

Generalized Comm. Table: Fortran



SENDbuf(1)=BUF(1)

SENDbuf(2)=BUF(4)

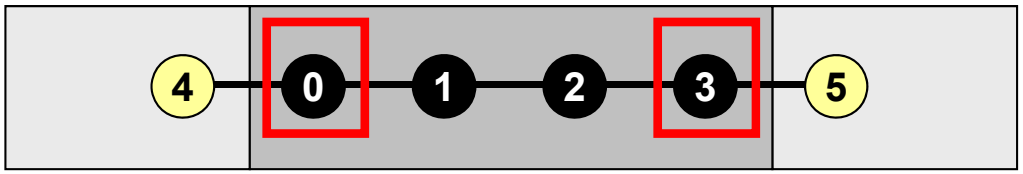


BUF(5)=RECVbuf(1)

BUF(6)=RECVbuf(2)

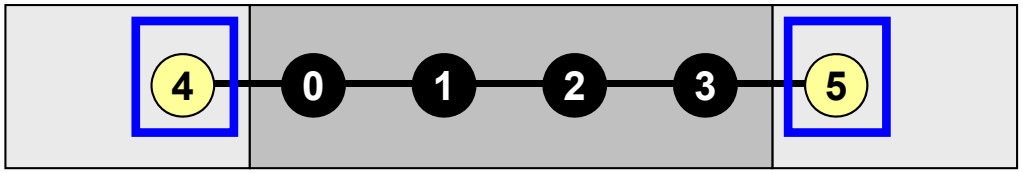
```
NEIBPETOT= 2
NEIBPE(1)= my_rank - 1
NEIBPE(2)= my_rank + 1

import_index(1)= 1
import_index(2)= 2
import_item (1)= N+1
import_item (2)= N+2

export_index(1)= 1
export_index(2)= 2
export_item (1)= 1
export_item (2)= N

if (my_rank.eq.0) then
  import_item (1)= N+1
  export_item (1)= N
  NEIBPE(1)= my_rank+1
endif
```

Generalized Comm. Table: C



SENDbuf[0]=BUF[0]

SENDbuf[1]=BUF[3]



BUF[4]=RECVbuf[0]

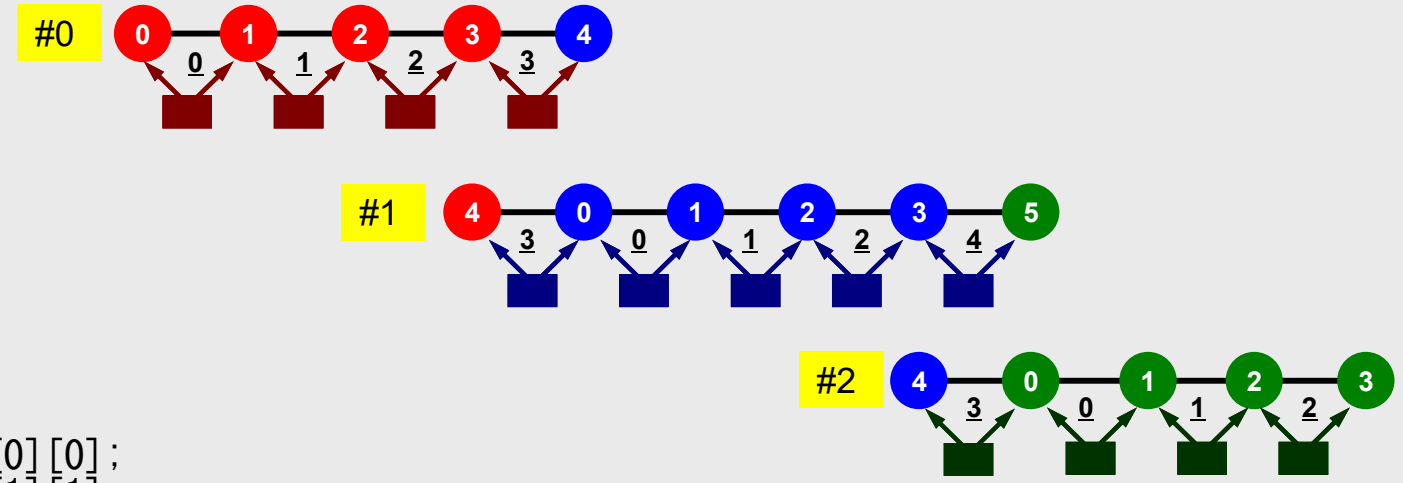
BUF[5]=RECVbuf[1]

```
NEIBPETOT= 2
NEIBPE[0]= my_rank - 1
NEIBPE[1]= my_rank + 1

import_index[1]= 0
import_index[2]= 1
import_item [0]= N
import_item [1]= N+1

export_index[1]= 0
export_index[2]= 1
export_item [0]= 0
export_item [1]= N-1

if (my_rank.eq.0) then
  import_item [0]= N
  export_item [0]= N-1
  NEIBPE[0]= my_rank+1
endif
```

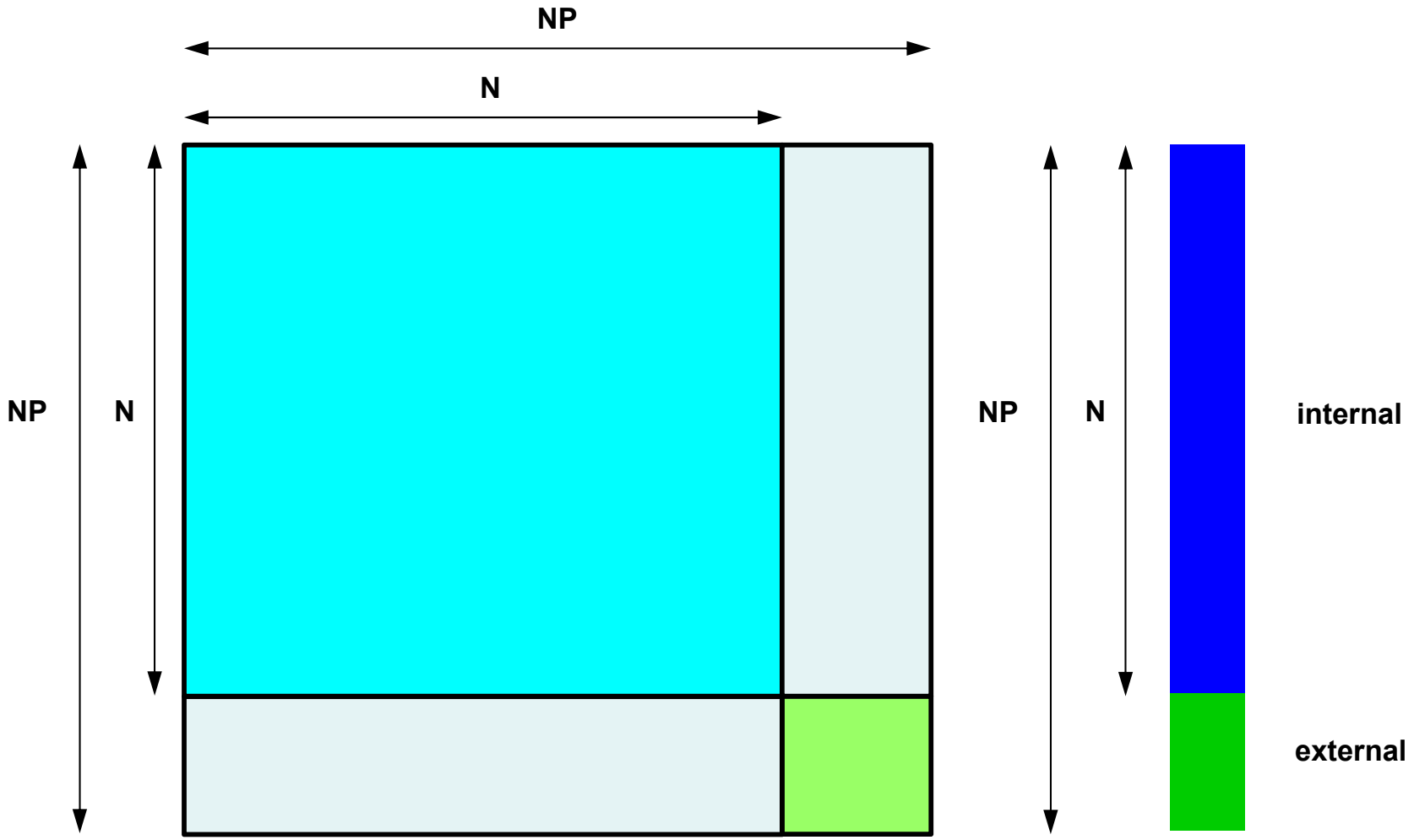
Program: 1d.c (8/11)

Matrix Assembling, NO changes from 1-CPU code

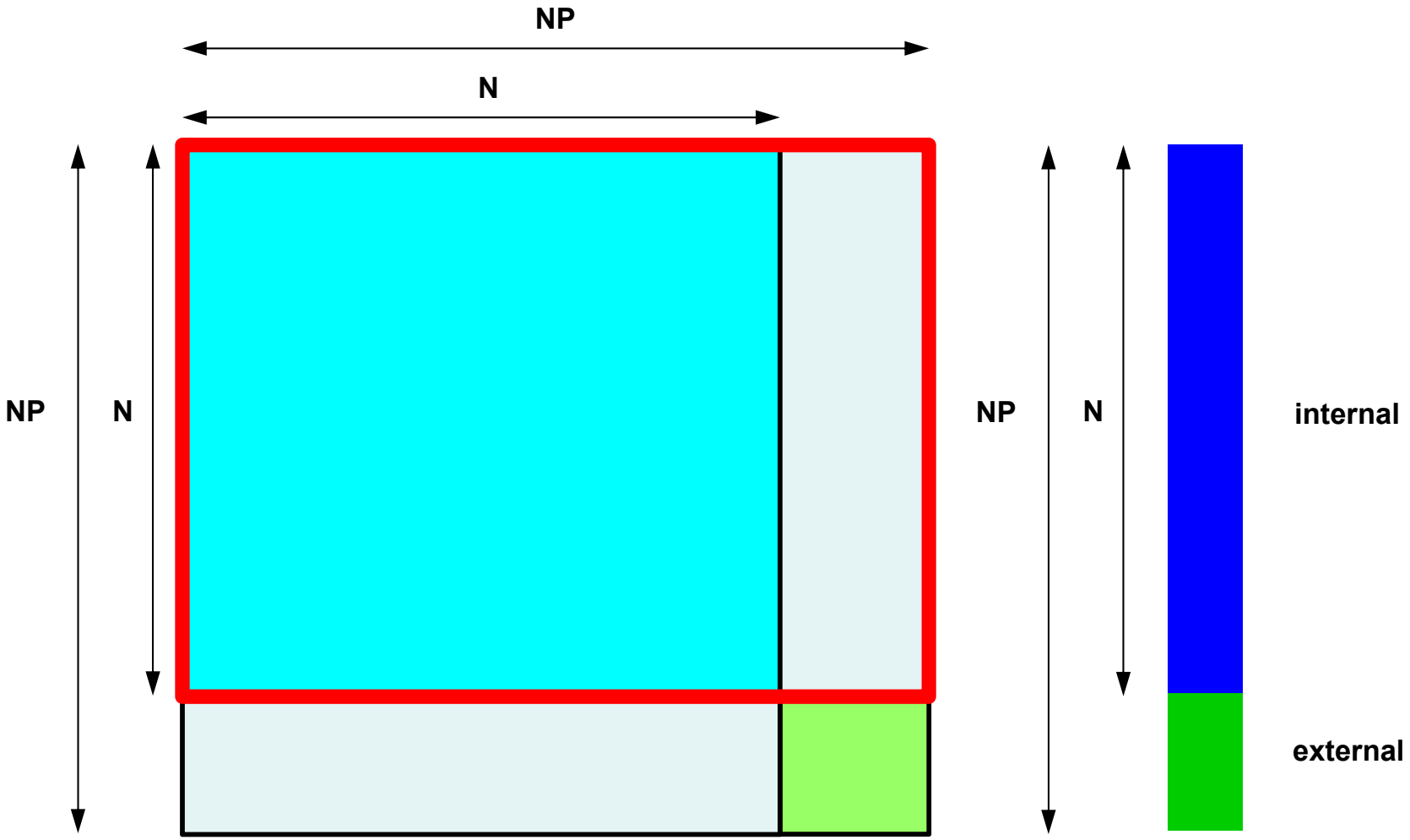
```
/*
// +-----------------+
// | MATRIX assemble |
// +-----------------+
*/
    for(icel=0;icel<NE;icel++){
      in1= Icelnod[2*icel];
      in2= Icelnod[2*icel+1];
      DL = dX;

      Ck= Area*COND/DL;
      Emat[0][0]= Ck*Kmat[0][0];
      Emat[0][1]= Ck*Kmat[0][1];
      Emat[1][0]= Ck*Kmat[1][0];
      Emat[1][1]= Ck*Kmat[1][1];

      Diag[in1]= Diag[in1] + Emat[0][0];
      Diag[in2]= Diag[in2] + Emat[1][1];

      if ((MyRank==0)&&(icel==0)){
        k1=Index[in1];
      }else {k1=Index[in1]+1;}

      k2=Index[in2];

      AMat[k1]= AMat[k1] + Emat[0][1];
      AMat[k2]= AMat[k2] + Emat[1][0];

      QN= 0.5*QV*Area*dX;
      Rhs[in1]= Rhs[in1] + QN;
      Rhs[in2]= Rhs[in2] + QN;
    }
```



Local Matrix



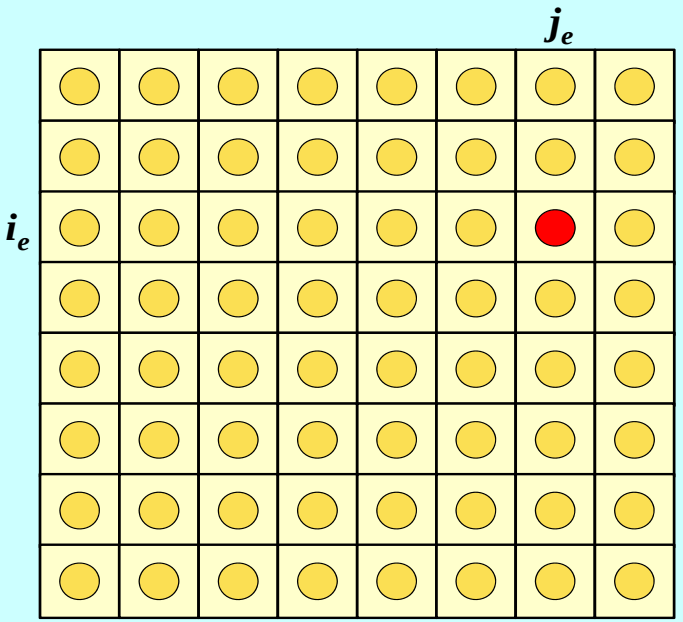
We really need these parts:



MAT_ASS_MAIN: Overview

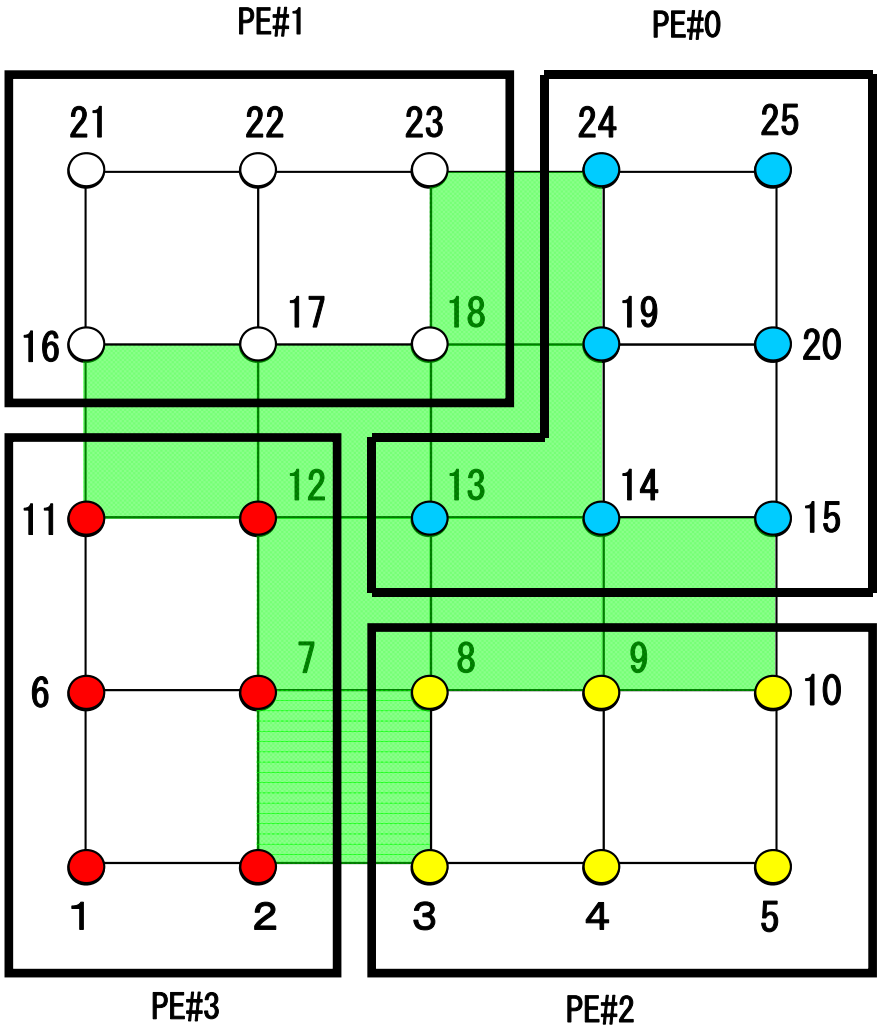
```
do kpn= 1, 2          Gaussian Quad. points in ζ-direction
  do jpn= 1, 2        Gaussian Quad. points in η-direction
    do ipn= 1, 2      Gaussian Quad. Pointe in ξ-direction
      Define Shape Function at Gaussian Quad. Points (8-points)
      Its derivative on natural/local coordinate is also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

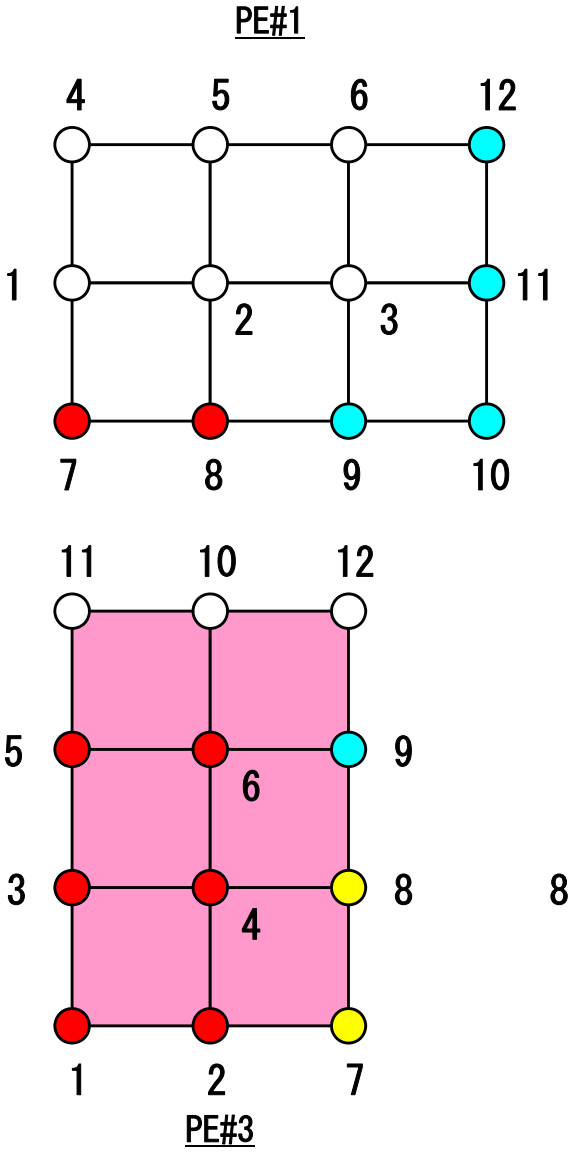
```
do icel= 1, ICELTOT    Loop for Element
  Jacobian and derivative on global coordinate of shape functions at
  Gaussian Quad. Points are defined according to coordinates of 8 nodes. (JACOBI)

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

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



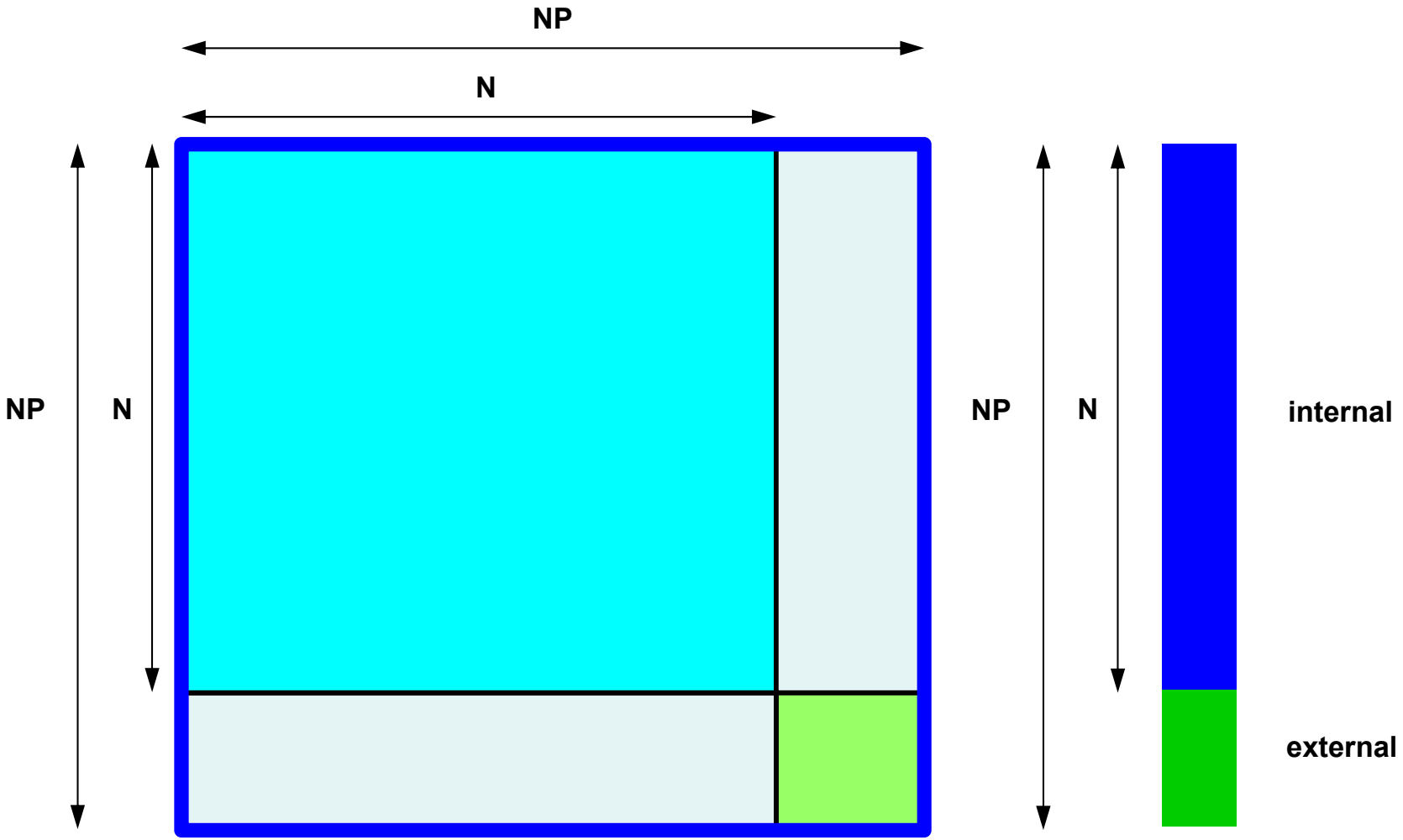
MAT_ASS_MAIN visits all elements

including overlapped elements with external nodes

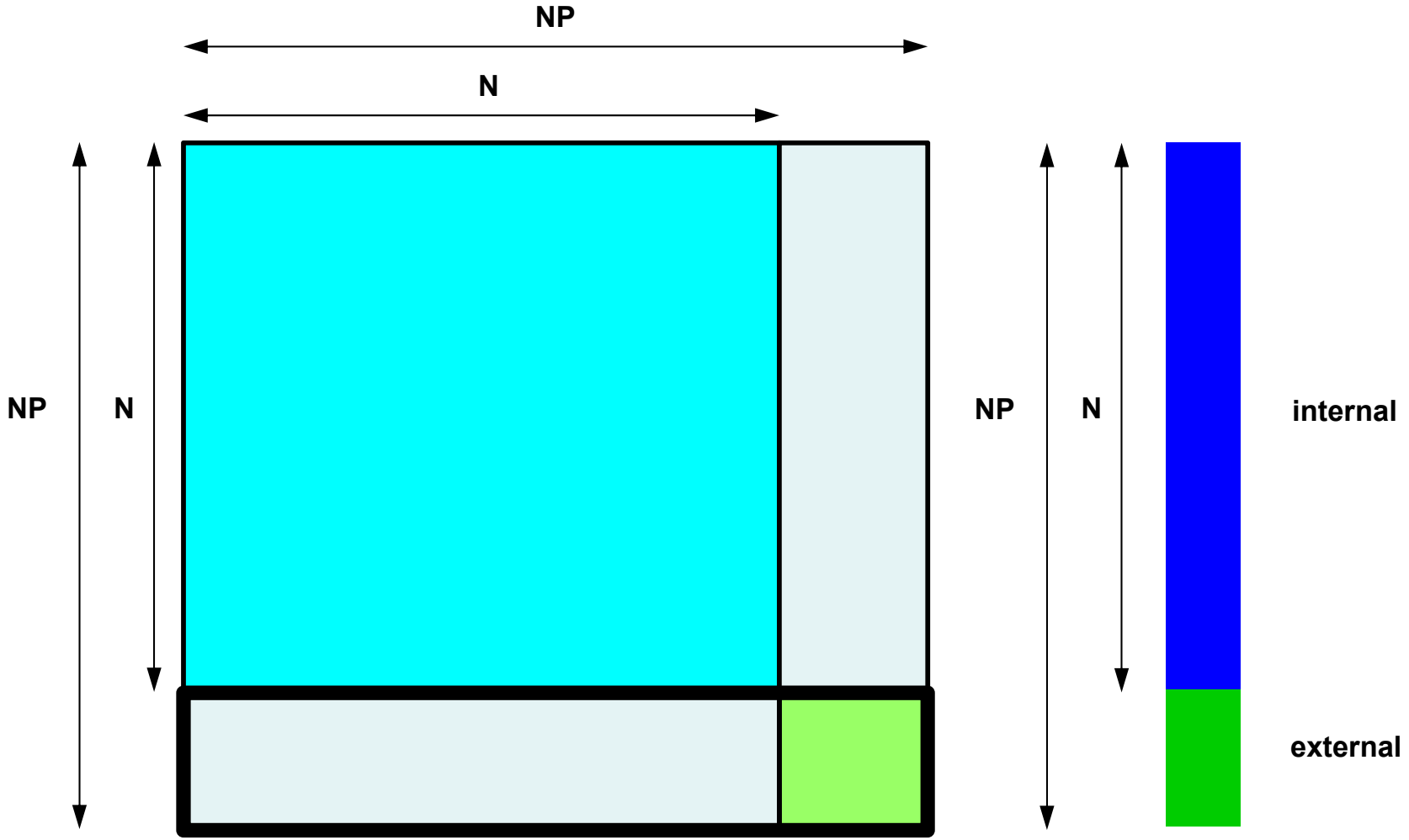




Therefore, we have this matrix



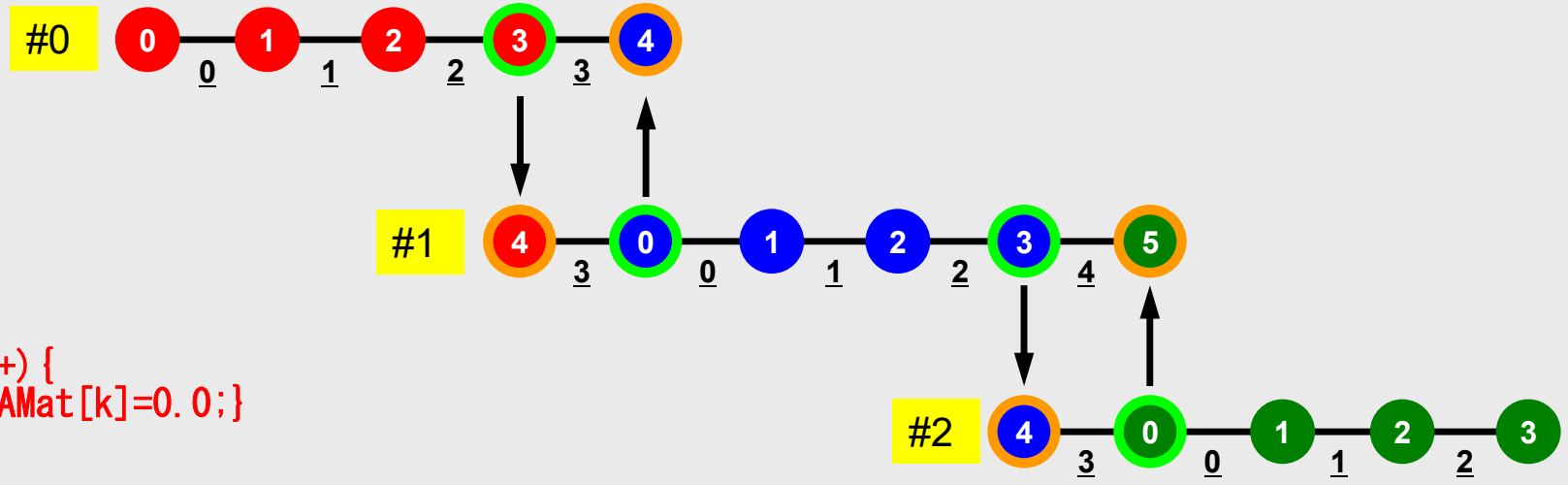
But components of this part are not complete, and not used in computation



Program: 1d.c (9/11)

Boundary Cond., ALMOST NO changes from 1-CPU code

```
/*
// +--------------------+
// | BOUNDARY conditions |
// +--------------------+
*/

/* X=Xmin */
    if (MyRank==0){
      i=0;
      jS= Index[i];
      AMat[jS]= 0.0;
      Diag[i ]= 1.0;
      Rhs [i ]= 0.0;

      for(k=0;k<NPLU;k++){
        if(Item[k]==0){AMat[k]=0.0;}
      }
    }
```



Program: 1d.c(10/11)
Conjugate Gradient Method

```
/*
// +---------------+
// | CG iterations |
// +---------------+
//=== */
    R = calloc(NP, sizeof(double));
    Z = calloc(NP, sizeof(double));
    P = calloc(NP, sizeof(double));
    Q = calloc(NP, sizeof(double));
    DD= calloc(NP, sizeof(double));

    for(i=0;i<N;i++){
      DD[i]= 1.0 / Diag[i];
    }

/*
//-- {r0}= {b} - [A]{xini} |
*/
    for(neib=0;neib<NeibPETot;neib++){
      for(k=export_index[neib];k<export_index[neib+1];k++){
        kk= export_item[k];
        SendBuf[k]= U[kk];
      }
    }
```

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

Conjugate Gradient Method (CG)

- Matrix-Vector Multiply
- Dot Product
- Preconditioning: in the same way as 1CPU code
- DAXPY: in the same way as 1CPU code

Preconditioning, DAXPY

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

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

Matrix-Vector Multiply (1/2)

Using Comm. Table, {p} is updated before computation

```
/*
//-- {q}= [A]{p}
*/
      for(neib=0;neib<NeibPETot;neib++){
         for(k=export_index[neib];k<export_index[neib+1];k++){
           kk= export_item[k];
           SendBuf[k]= P[kk];
         }
       }

         for(neib=0;neib<NeibPETot;neib++){
                 is   = export_index[neib];
                 len_s= export_index[neib+1] - export_index[neib];
                MPI_Isend(&SendBuf[is], len_s, MPI_DOUBLE, NeibPE[neib],
                                  0, MPI_COMM_WORLD, &RequestSend[neib]);
         }

         for(neib=0;neib<NeibPETot;neib++){
                 ir   = import_index[neib];
                 len_r= import_index[neib+1] - import_index[neib];
                MPI_Irecv(&RecvBuf[ir], len_r, MPI_DOUBLE, NeibPE[neib],
                                  0, MPI_COMM_WORLD, &RequestRecv[neib]);
         }

         MPI_Waitall(NeibPETot, RequestRecv, StatRecv);

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

Matrix-Vector Multiply (2/2)

{q}= [A]{p}

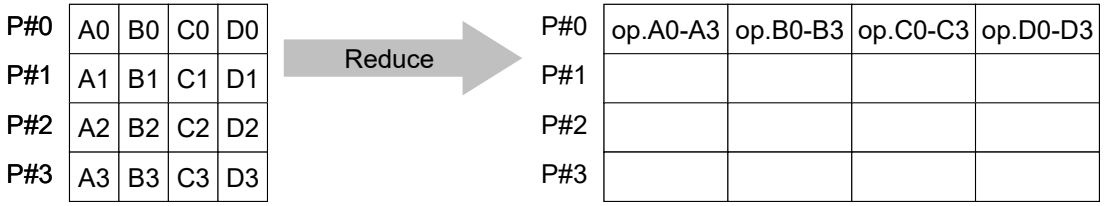
```
MPI_Waitall(NeibPETot, RequestSend, StatSend);

for(i=0;i<N;i++){
  Q[i] = Diag[i] * P[i];
  for(j=Index[i];j<Index[i+1];j++){
    Q[i] += AMat[j]*P[Item[j]];
  }
}
```

Dot Product

Global Summation by MPI_Allreduce

```
/*
//-- RHO= {r}{z}
*/
      Rho0= 0.0;
      for(i=0;i<N;i++){
        Rho0 += R[i] * Z[i];
      }

      ierr = MPI_Allreduce(&Rho0, &Rho, 1, MPI_DOUBLE,
                           MPI_SUM, MPI_COMM_WORLD);
```

MPI_Reduce



- Reduces values on all processes to a single value
  - Summation, Product, Max, Min etc.

- **MPI_Reduce (sendbuf,recvbuf,count,datatype,op,root,comm)**
  - **sendbuf** choice I starting address of send buffer
  - **recvbuf** choice O starting address receive buffer
    type is defined by "**datatype**"
  - **count** int I number of elements in send/receive buffer
  - **datatype** MPI_Datatype I data type of elements of send/recive buffer
    FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.
    C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc

  - **op** MPI_Op I reduce operation
    MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD, MPI_LAND, MPI_BAND etc
    Users can define operations by **MPI_OP_CREATE**

  - **root** int I rank of root process
  - **comm** MPI_Comm I communicator

Send/Receive Buffer (Sending/Receiving)

- Arrays of “send (sending) buffer” and “receive (receiving) buffer” often appear in MPI.

- Addresses of “send (sending) buffer” and “receive (receiving) buffer” must be different.

Example of MPI_Reduce (1/2)

```
call MPI_REDUCE
(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

```
real(kind=8):: X0, X1

call MPI_REDUCE
(X0, X1, 1, MPI_DOUBLE_PRECISION, MPI_MAX, 0, <comm>, ierr)
```

```
real(kind=8):: X0(4), XMAX(4)

call MPI_REDUCE
(X0, XMAX, 4, MPI_DOUBLE_PRECISION, MPI_MAX, 0, <comm>, ierr)
```

Global Max values of X0[i] go to XMAX[i] on #0 process（i=0~3）

Example of MPI_Reduce (2/2)

```
call MPI_REDUCE
(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

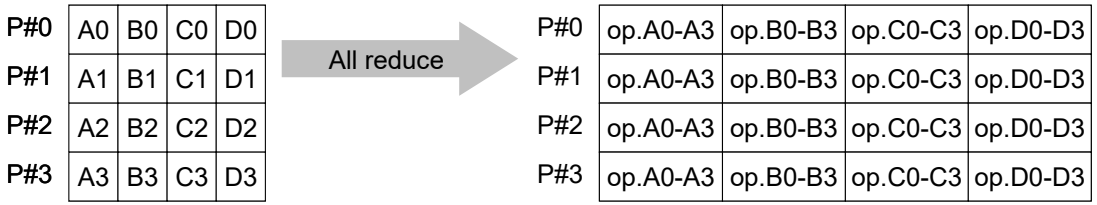
```
real(kind=8):: X0, XSUM

call MPI_REDUCE
(X0, XSUM, 1, MPI_DOUBLE_PRECISION, MPI_SUM, 0, <comm>, ierr)
```

Global summation of X0 goes to XSUM on #0 process.

```
real(kind=8):: X0(4)

call MPI_REDUCE
(X0(1), X0(3), 2, MPI_DOUBLE_PRECISION, MPI_SUM, 0, <comm>, ierr)
```

- Global summation of X0[0] goes to X0[2] on #0 process.
- Global summation of X0[1] goes to X0[3] on #0 process.

MPI_Allreduce



- MPI_Reduce + MPI_Bcast
- Summation (of dot products) and MAX/MIN values are likely to utilized in each process

- **`call MPI_Allreduce (sendbuf,recvbuf,count,datatype,op, comm)`**
  - **`sendbuf`** choice I starting address of send buffer
  - **`recvbuf`** choice O starting address receive buffer
    type is defined by "**`datatype`**"
  - **`count`** int I number of elements in send/receive buffer
  - **`datatype`** MPI_Datatype I data type of elements of send/recive buffer
  - **`op`** MPI_Op I reduce operation
  - **`comm`** MPI_Comm I communicator

CG method (1/5)

```
/*
//-- {r0}= {b} - [A]{xini} |
*/
    for(neib=0;neib<NeibPETot;neib++){
      for(k=export_index[neib];k<export_index[neib+1];k++){
        kk= export_item[k];
        SendBuf[k]= PHI[kk];
      }
    }

    for(neib=0;neib<NeibPETot;neib++){
      is   = export_index[neib];
      len_s= export_index[neib+1] - export_index[neib];
      MPI_Isend(&SendBuf[is], len_s, MPI_DOUBLE, NeibPE[neib],
                0, MPI_COMM_WORLD, &RequestSend[neib]);
    }

    for(neib=0;neib<NeibPETot;neib++){
      ir   = import_index[neib];
      len_r= import_index[neib+1] - import_index[neib];
      MPI_Irecv(&RecvBuf[ir], len_r, MPI_DOUBLE, NeibPE[neib],
                0, MPI_COMM_WORLD, &RequestRecv[neib]);
    }

    MPI_Waitall(NeibPETot, RequestRecv, StatRecv);

    for(neib=0;neib<NeibPETot;neib++){
      for(k=import_index[neib];k<import_index[neib+1];k++){
        kk= import_item[k];
        PHI[kk]=RecvBuf[k];
      }
    }
    MPI_Waitall(NeibPETot, RequestSend, StatSend);
```

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 method (2/5)

```
    for(i=0;i<N;i++){
      R[i] = Diag[i]*PHI[i];
      for(j=Index[i];j<Index[i+1];j++){
        R[i] += AMat[j]*PHI[Item[j]];
      }
    }

    BNorm20 = 0.0;
    for(i=0;i<N;i++){
      BNorm20 += Rhs[i] * Rhs[i];
      R[i] = Rhs[i] - R[i];
    }
    ierr = MPI_Allreduce(&BNorm20, &BNorm2, 1, MPI_DOUBLE,
                         MPI_SUM, MPI_COMM_WORLD);

  for(iter=1;iter<=IterMax;iter++){

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

/*
//-- RHO= {r}{z}
*/
    Rho0= 0.0;
    for(i=0;i<N;i++){
      Rho0 += R[i] * Z[i];
    }
    ierr = MPI_Allreduce(&Rho0, &Rho, 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

CG method (3/5)

```
/*
//-- {p} = {z} if      ITER=1
//   BETA= RHO / RHO1  otherwise
*/
    if(iter == 1){
      for(i=0;i<N;i++){
        P[i] = Z[i];
      }
    }else{
      Beta = Rho / Rho1;
      for(i=0;i<N;i++){
        P[i] = Z[i] + Beta*P[i];
      }
    }

/*
//-- {q}= [A]{p}
*/
    for(neib=0;neib<NeibPETot;neib++){
      for(k=export_index[neib];k<export_index[neib+1];k++){
        kk= export_item[k];
        SendBuf[k]= P[kk];
      }
    }

    for(neib=0;neib<NeibPETot;neib++){
      is   = export_index[neib];
      len_s= export_index[neib+1] - export_index[neib];
      MPI_Isend(&SendBuf[is], len_s, MPI_DOUBLE, NeibPE[neib],
                0, MPI_COMM_WORLD, &RequestSend[neib]);
    }
```

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 method (4/5)

```
    for(neib=0;neib<NeibPETot;neib++){
      ir   = import_index[neib];
      len_r= import_index[neib+1] - import_index[neib];
      MPI_Irecv(&RecvBuf[ir], len_r, MPI_DOUBLE, NeibPE[neib],
                0, MPI_COMM_WORLD, &RequestRecv[neib]);
    }

    MPI_Waitall(NeibPETot, RequestRecv, StatRecv);

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

    MPI_Waitall(NeibPETot, RequestSend, StatSend);

    for(i=0;i<N;i++){
      Q[i] = Diag[i] * P[i];
      for(j=Index[i];j<Index[i+1];j++){
        Q[i] += AMat[j]*P[Item[j]];
      }
    }
/*
//-- ALPHA= RHO / {p}{q}
*/
    C10 = 0.0;
    for(i=0;i<N;i++){
      C10 += P[i] * Q[i];
    }
    ierr = 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 method (5/5)

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

    DNorm20 = 0.0;
    for(i=0;i<N;i++){
      DNorm20 += R[i] * R[i];
    }

    ierr = MPI_Allreduce(&DNorm20, &DNorm2, 1, MPI_DOUBLE,
                         MPI_SUM, MPI_COMM_WORLD);

    Resid = sqrt(DNorm2/BNorm2);
    if (MyRank==0)
      printf("%8d%s%16.6e¥n", iter, " iters, RESID=", Resid);

    if(Resid <= Eps){
      ierr = 0;
      break;
    }

    Rho1 = Rho;

    }
```

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

Program: 1d.c (11/11)
Output by Each Process

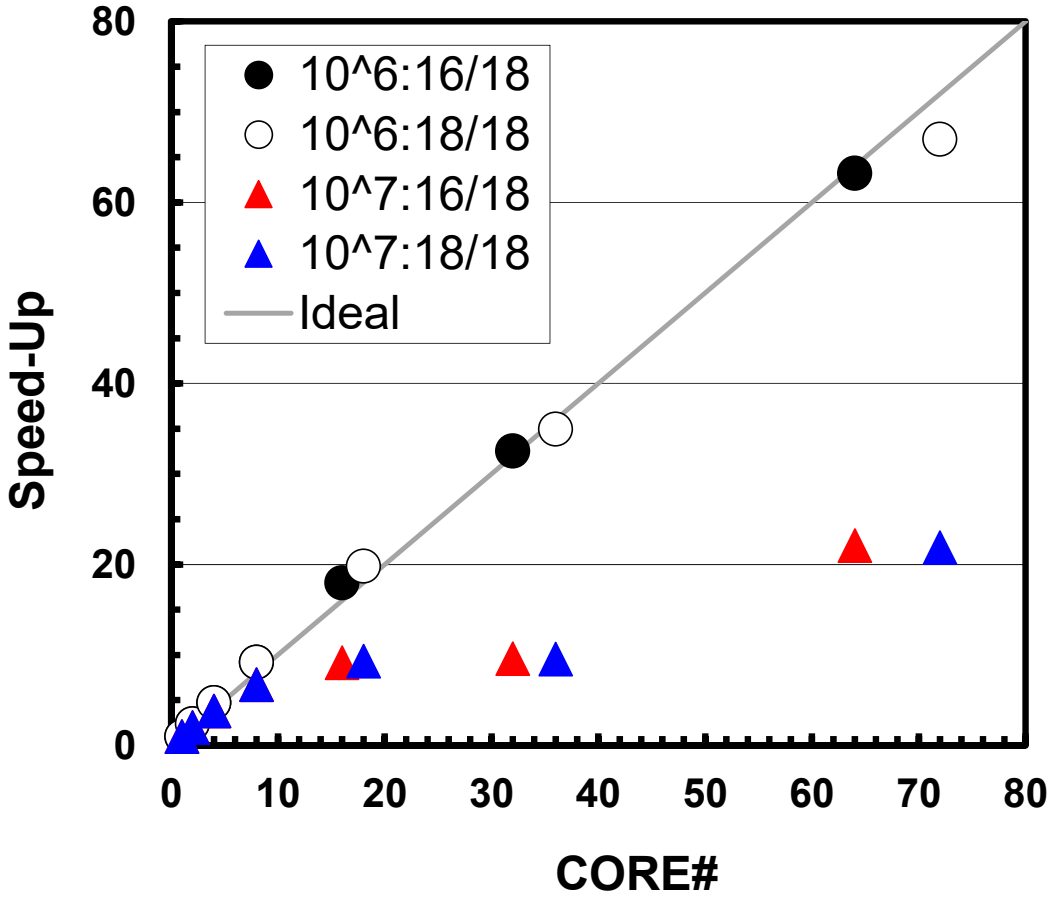
```
/*
//-- OUTPUT
*/
    printf("¥n%s¥n", "### TEMPERATURE");
    for(i=0;i<N;i++){
      printf("%3d%8d%16.6E¥n", MyRank, i+1, PHI[i]);
    }

    ierr = MPI_Finalize();
    return ierr;
}
```

- Overview
- Distributed Local Data
- Program
- **Results**

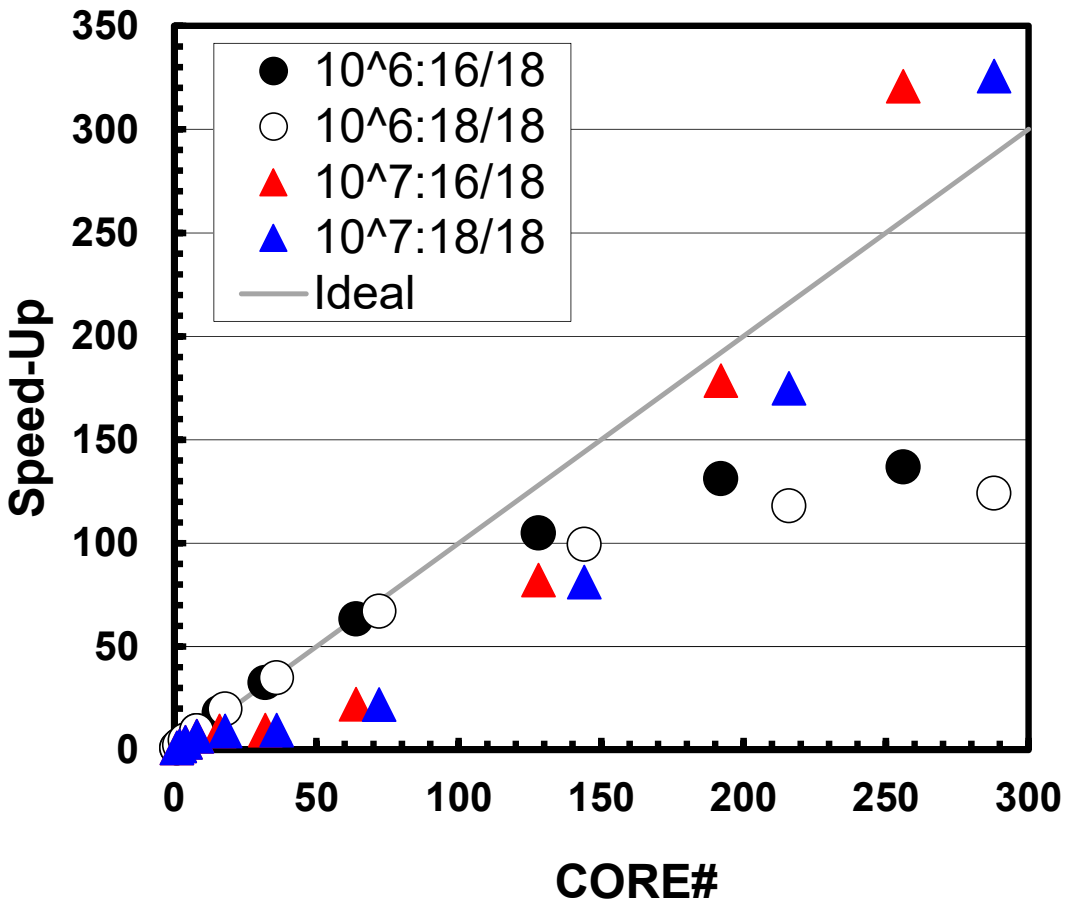
Results: Time for CG Solver

Time for 1,000 iterations, Strong Scaling
16/18: 16 of 18 cores on socket, 18/18: 18 of 18 cores
16/18 is rather better, if number of nodes is large

up to 2 nodes



up to 8 nodes



Performance is lower than ideal one

- Time for MPI communication
  - Time for sending data
  - Communication bandwidth between nodes
  - Time is proportional to size of sending/receiving buffers
- Time for starting MPI
  - latency
  - does not depend on size of buffers
    - depends on number of calling, increases according to process #
  - $O(10^0)$-$O(10^1)$ μsec.
- Synchronization of MPI
  - Increases according to number of processes

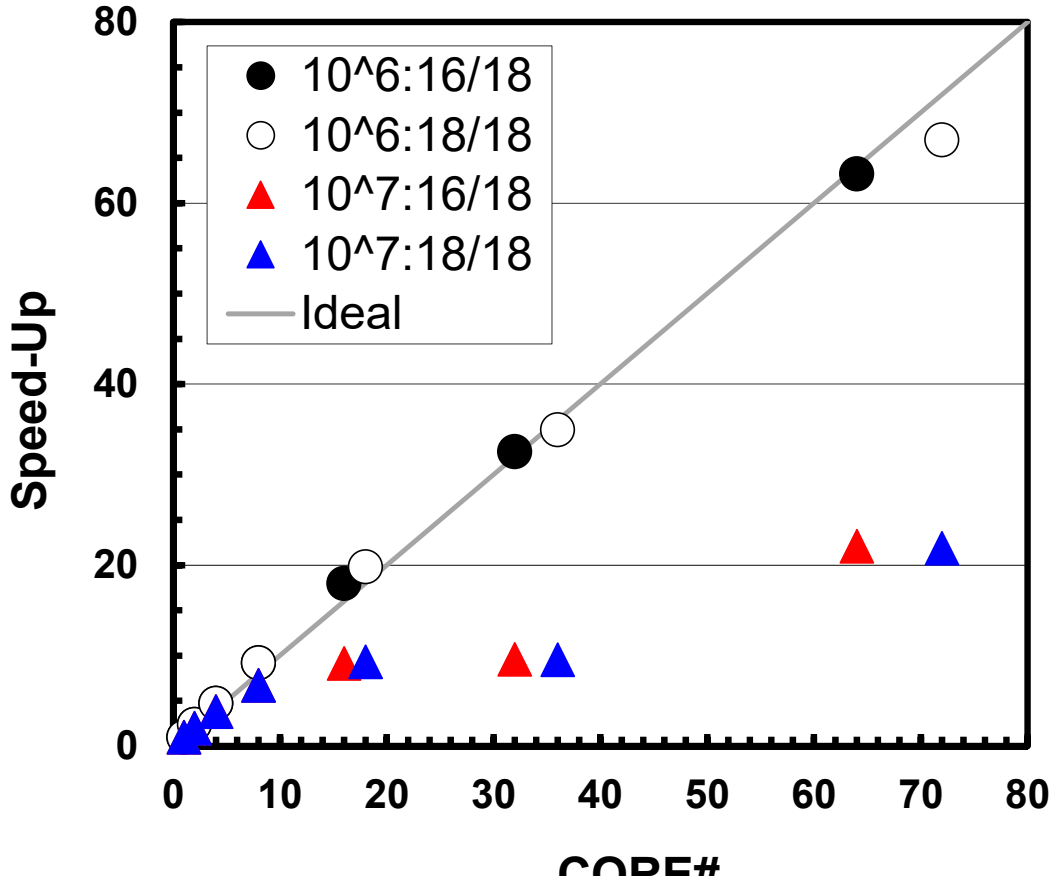
Performance is lower than ideal one (cont.)

- If computation time is relatively small (N is small in S1-3), these effects are not negligible.
  - If the size of messages is small, effect of “latency” is significant.

Results: Time for CG Solver

Time for 1,000 iterations, Strong Scaling
16/18: 16 of 18 cores on socket, 18/18: 18 of 18 cores
16/18 is rather better, if number of nodes is large

up to 2 nodes



- in a single node (< 36 cores), performance of small cases ($N=10^6$) are rather better.
- Effect of memory contention/saturation (not communication)
- Memory throughput on each node is constant for 8+ cores
- If problem size is small, cache can be well-utilized. Therefore, effect of memory bandwidth is small.

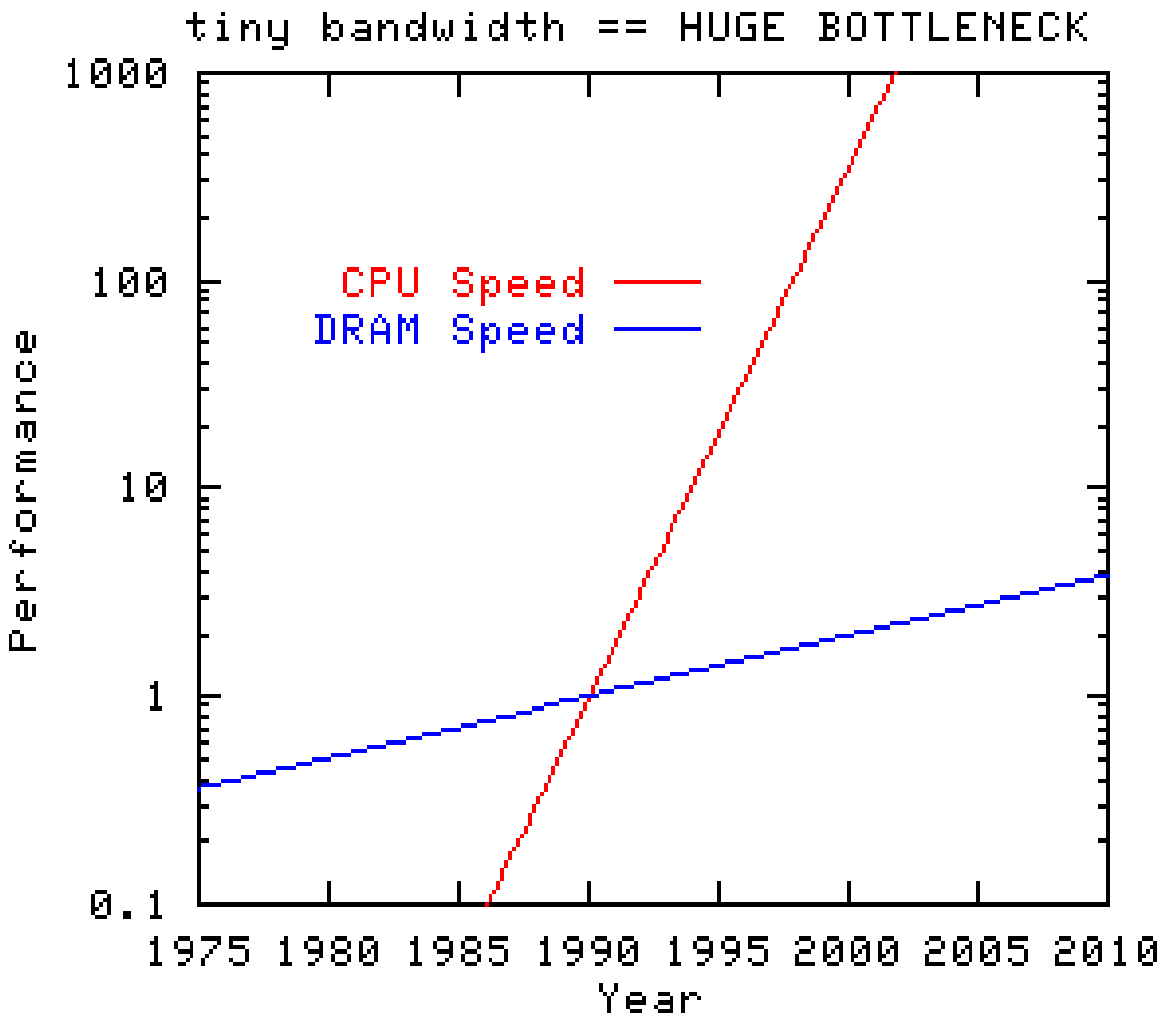
STREAM benchmark

http://www.cs.virginia.edu/stream/

- Benchmarks for Memory Bandwidth
  - Copy: c(i)= a(i)
  - Scale: c(i)= s*b(i)
  - Add: c(i)= a(i) + b(i)
  - Triad: c(i)= a(i) + s*b(i)

```
-------------------------------------------------
 Double precision appears to have 16 digits of accuracy
 Assuming 8 bytes per DOUBLE PRECISION word
-------------------------------------------------
 Number of processors =           16
 Array size =    2000000
 Offset     =          0
 The total memory requirement is     732.4 MB (
45.8MB/task)
 You are running each test  10 times
 --
 The *best* time for each test is used
 *EXCLUDING* the first and last iterations
 -----------------------------------------------------
 -----------------------------------------------------
Function     Rate (MB/s)  Avg time   Min time  Max time
Copy:      18334.1898      0.0280      0.0279      0.0280
Scale:     18035.1690      0.0284      0.0284      0.0285
Add:       18649.4455      0.0412      0.0412      0.0413
Triad:     19603.8455      0.0394      0.0392      0.0398
```

Gap between performance of CPU and Memory



http://www.cs.virginia.edu/stream/

How to run: MPI Version

```
>$ cd <$O-S2r>
>$ mpiifort -O3 -xCORE-AVX2 -align array32byte stream.f –o stream

>$ qsub stream.sh
```

stream.sh

```
#!/bin/sh

#PBS -q u-lecture
#PBS -N stream
#PBS -l select=1:mpiprocs=2   MPI Process # (1-36)
#PBS -Wgroup_list=gt16
#PBS -l walltime=00:05:00
#PBS -e err
#PBS -o stream.lst

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

export I_MPI_PIN_DOMAIN=socket
mpirun ./impimap.sh ./stream
```

Results of Triad on a Single Node of Reedbush-U Peak is 153.6 GB/sec.

Thread #	GB/sec	Speed-up
1	16.0	1.00E+00
2	32.0	2.00E+00
4	61.7	3.85E+00
8	108.4	6.77E+00
16	128.7	8.04E+00
18	129.6	8.09E+00
32	130.0	8.12E+00
36	129.4	8.09E+00

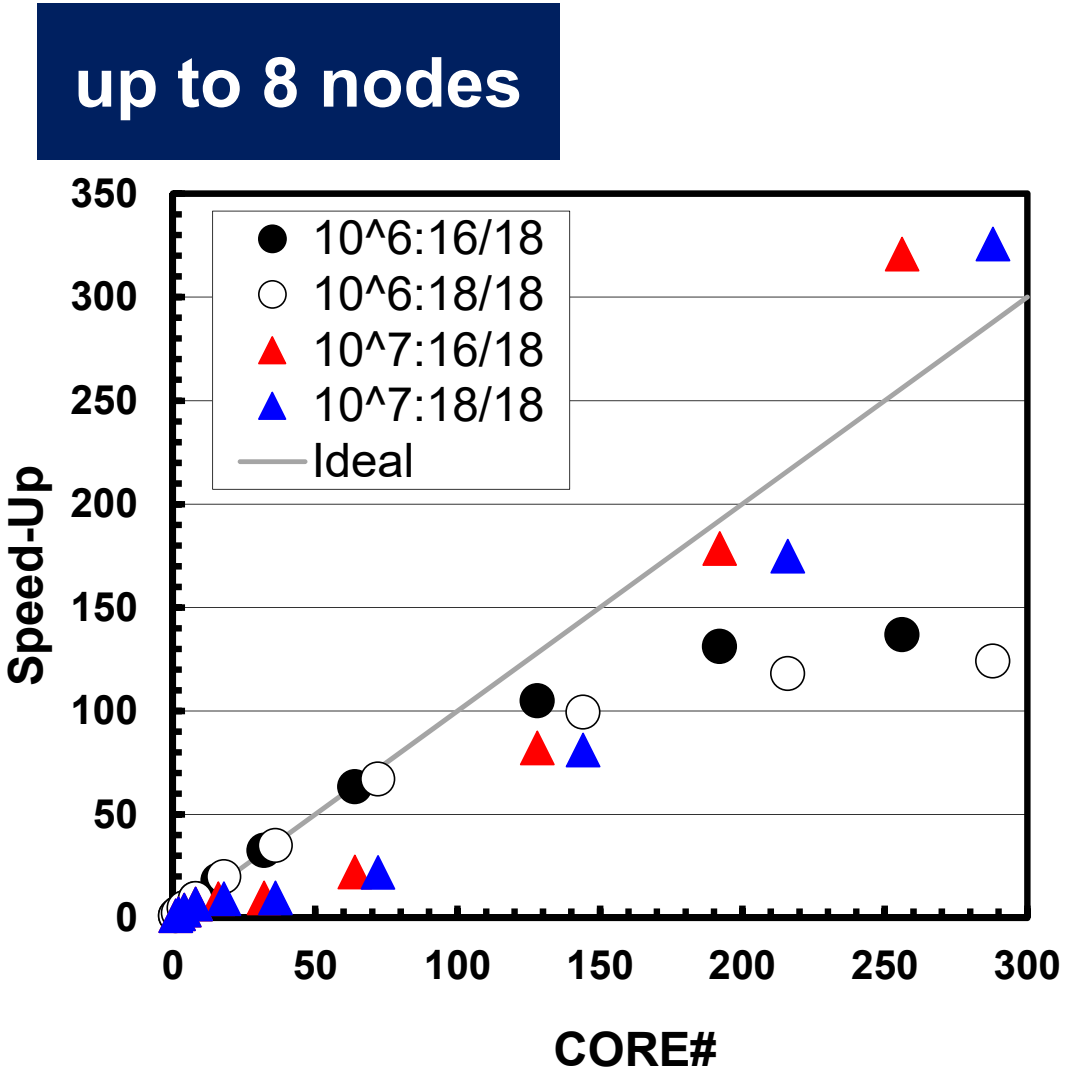
Exercises

- Running the code
- Try various number of processes (1-36)
- OpenMP-version and Single PE version are available
  - Fortran, C
  - Web-site of STREAM
  - http://www.cs.virginia.edu/stream/

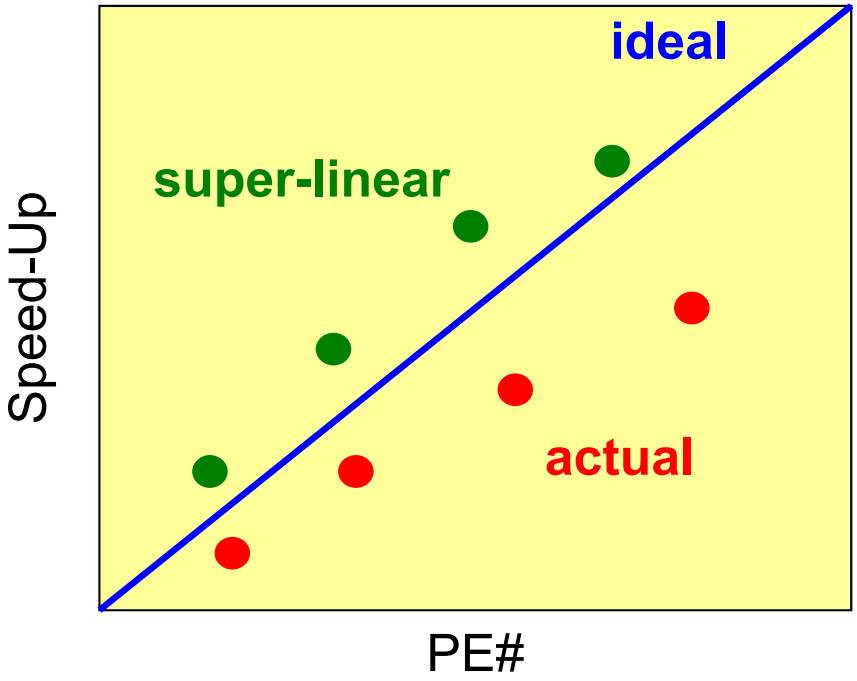
Results: Time for CG Solver

Time for 1,000 iterations, Strong Scaling
16/18: 16 of 18 cores on socket, 18/18: 18 of 18 cores
16/18 is rather better, if number of nodes is large

- Performance of N=10^6 case decreases, as node# increases.
- Performance of N=10^7 becomes close to ideal one gradually, and superlinear situation occurs at 256 cores (8 nodes).
- 16/18 is rather better if number of node is large.
  - Memory is more well-utilized

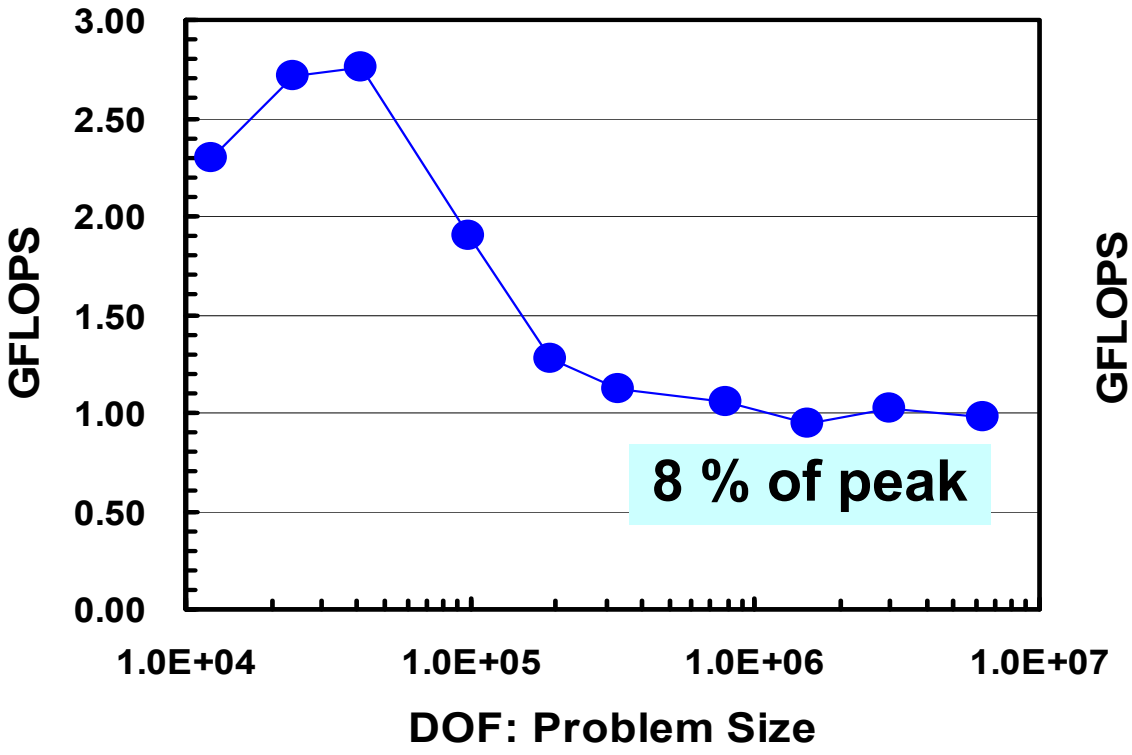


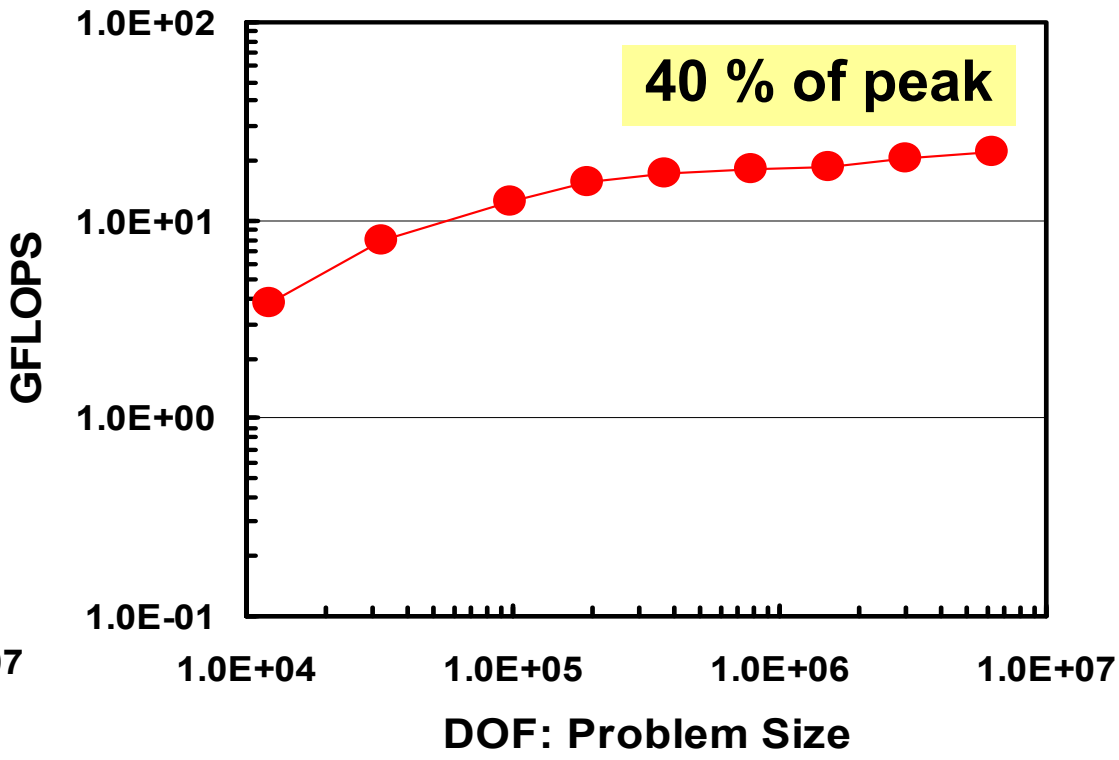
Super-Linear in Strong Scaling



- In strong scaling case where entire problem size is fixed, performance is generally lower than the ideal one due to communication overhead.
- But sometime, actual performance may be better than the ideal one. This is called “super-linear”
  - only for scalar processors
  - does not happen in vector processors

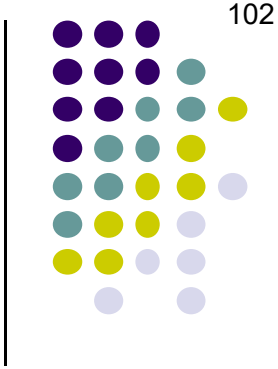
Typical Behaviors



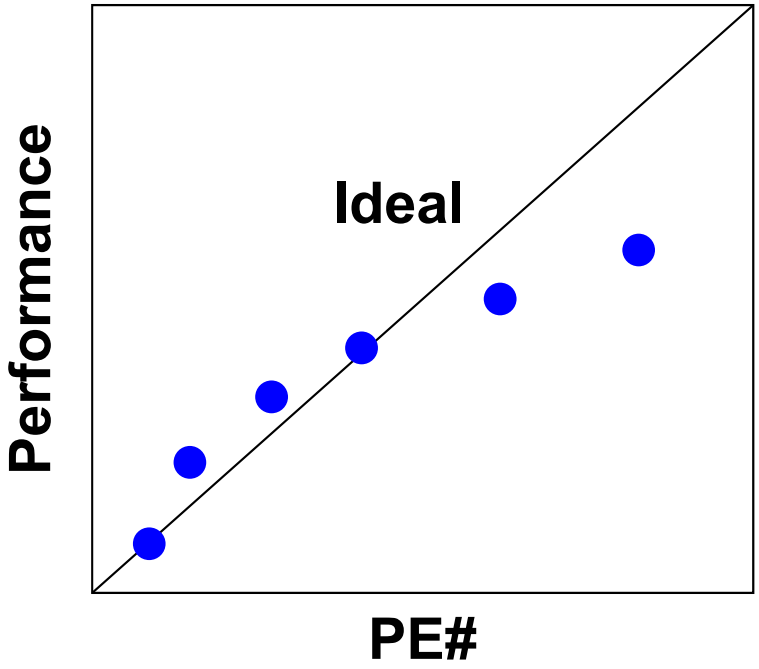


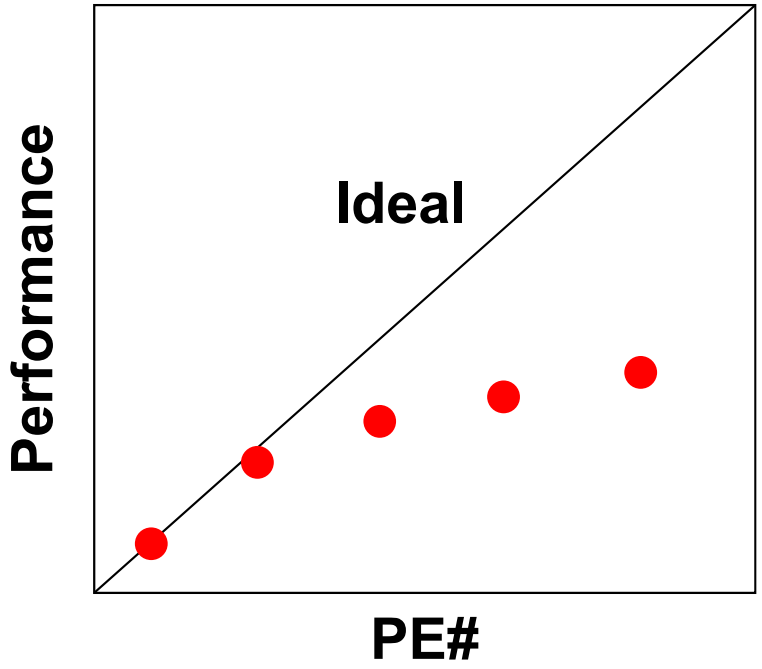
IBM-SP3:
Higher performance for small problems, effect of cache

Earth Simulator:
Higher performance for large-scale problems with longer loops



Strong Scaling



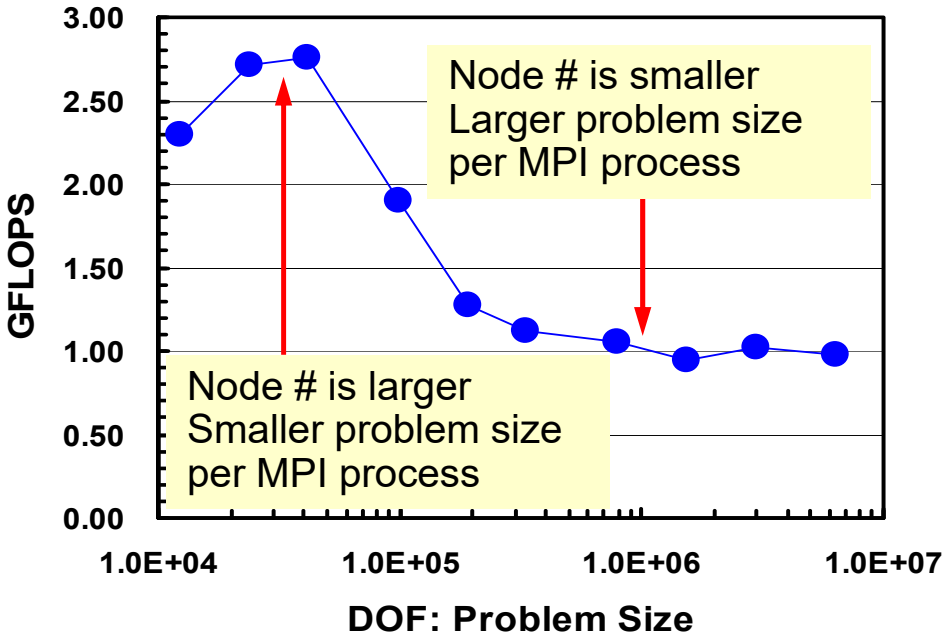


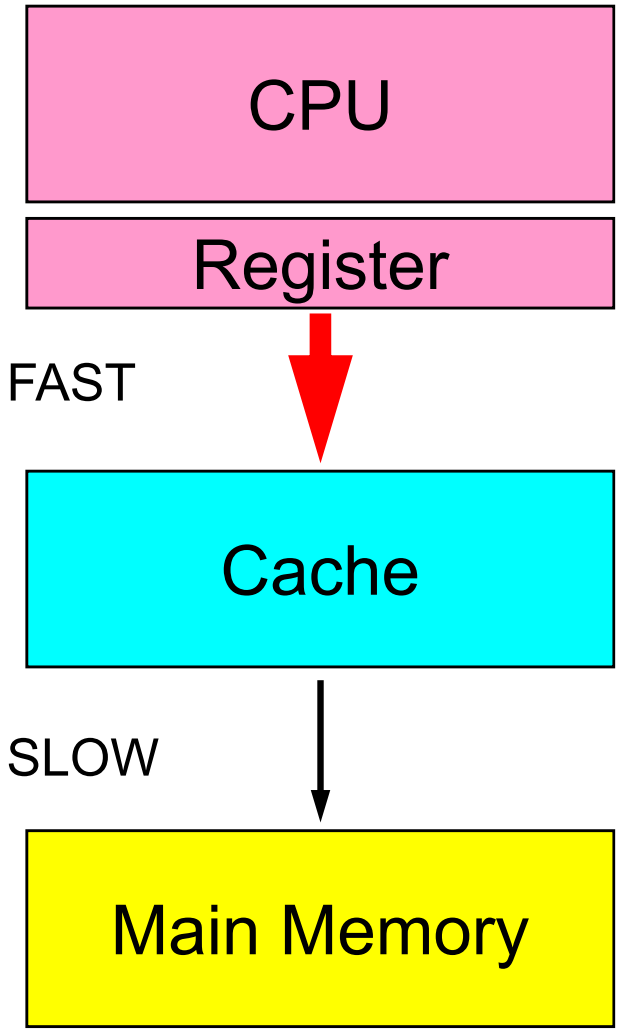
IBM-SP3:
"Super-linear" happens if number of PE is not so large. Performance is getting worse due to communication overhead if PE number is larger.

Earth Simulator:
Performance is getting worse due to communication overhead and smaller loop length if PE number is larger.

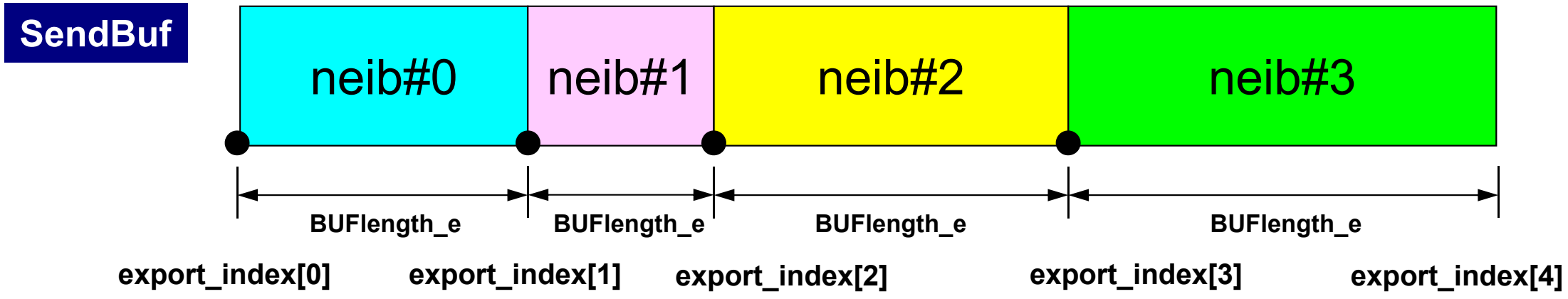
Why does “Super-Linear” happen ?

- Effect of Cache
- In scalar processors, performance for smaller problem is generally better.
  - Cache is well-utilized.





Memory Copy is expensive (1/2)



export_item (export_index[neib]:export_index[neib+1]-1) are sent to neib-th neighbor

```
for (neib=0; neib<NeibPETot;neib++){
   for (k=export_index[neib];k<export_index[neib+1];k++){
      kk= export_item[k];
      SendBuf[k]= VAL[kk];
   }
}

for (neib=0; neib<NeibPETot; neib++){
  tag= 0;
  iS_e= export_index[neib];
  iE_e= export_index[neib+1];
  BUFlength_e= iE_e - iS_e

  ierr= MPI_Isend
        (&SendBuf[iS_e], BUFlength_e, MPI_DOUBLE, NeibPE[neib], 0,
         MPI_COMM_WORLD, &ReqSend[neib])
}

MPI_Waitall(NeibPETot, ReqSend, StatSend);
```

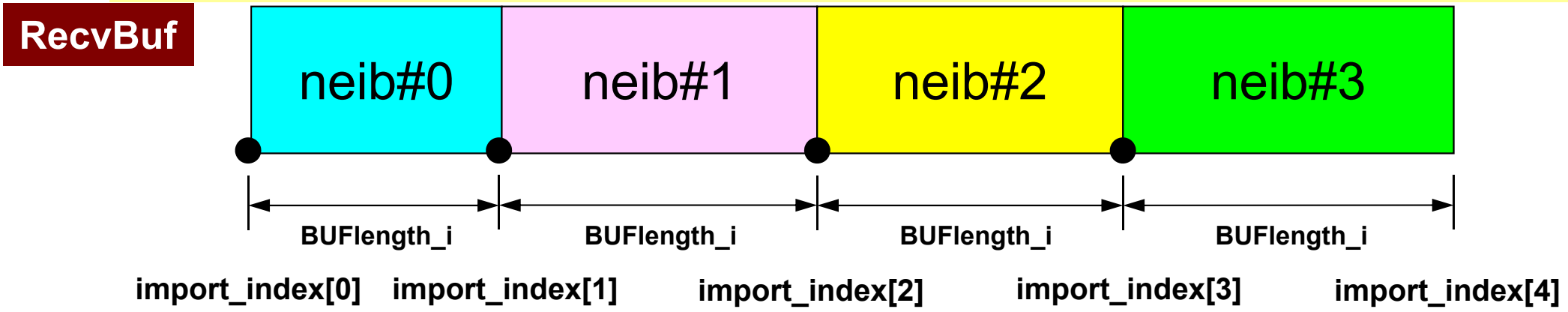
Copied to sending buffers

Memory Copy is expensive (2/2)

```
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];
    }
}
```

Copied from receiving buffer

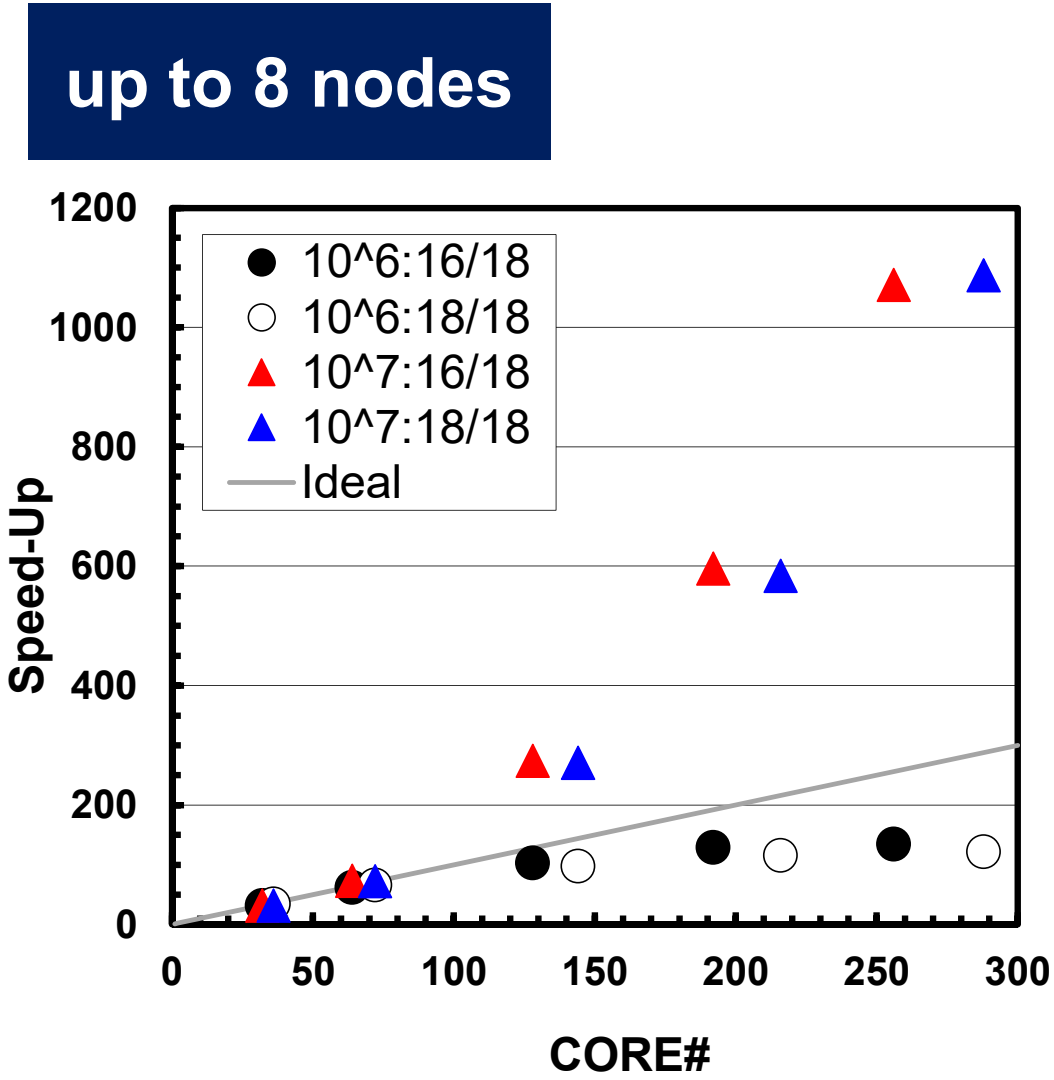
import_item (import_index[neib]:import_index[neib+1]-1) are received from neib-th neighbor



Results: Time for CG Solver

Time for 1,000 iterations, Strong Scaling
16/18: 16 of 18 cores on socket, 18/18: 18 of 18 cores
16/18 is rather better, if number of nodes is large

- It is reasonable to evaluate strong scalability for multiple nodes based on the performance by a node with 32/36 cores
- In this figure, performance of the case with 32 cores is set to 32 (results of 16/18 and 18/18 are directly compared).
- L2 cache: 256kB/core
- L3: 45MB/socket (shared)



Summary: Parallel FEM

- Proper design of data structure of distributed local meshes.

- Open Technical Issues
  - Parallel Mesh Generation, Parallel Visualization
  - Parallel Preconditioner for Ill-Conditioned Problems
  - Large-Scale I/O

Distributed Local Data Structure for Parallel Computation

- Distributed local data structure for domain-to-doain communications has been introduced, which is appropriate for such applications with sparse coefficient matrices (e.g. FDM, FEM, FVM etc.).
  - SPMD
  - Local Numbering: Internal pts to External pts
  - Generalized communication table

- Everything is easy, if proper data structure is defined:
  - Values at boundary pts are copied into sending buffers
  - Send/Recv
  - Values at external pts are updated through receiving buffers