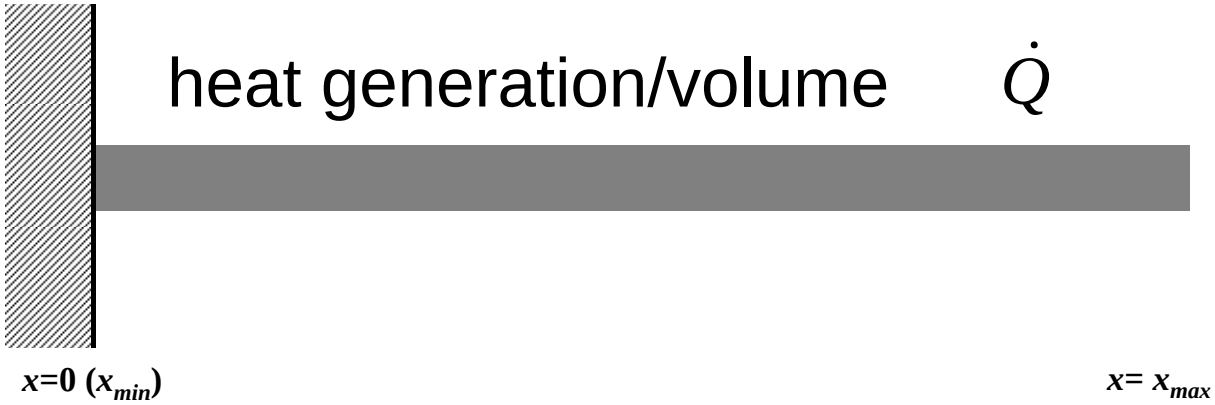
Report S2
C

Kengo Nakajima

Programming for Parallel Computing (616-2057)
Seminar on Advanced Computing (616-4009)

- Overview
- Distributed Local Data
- Program
- Results

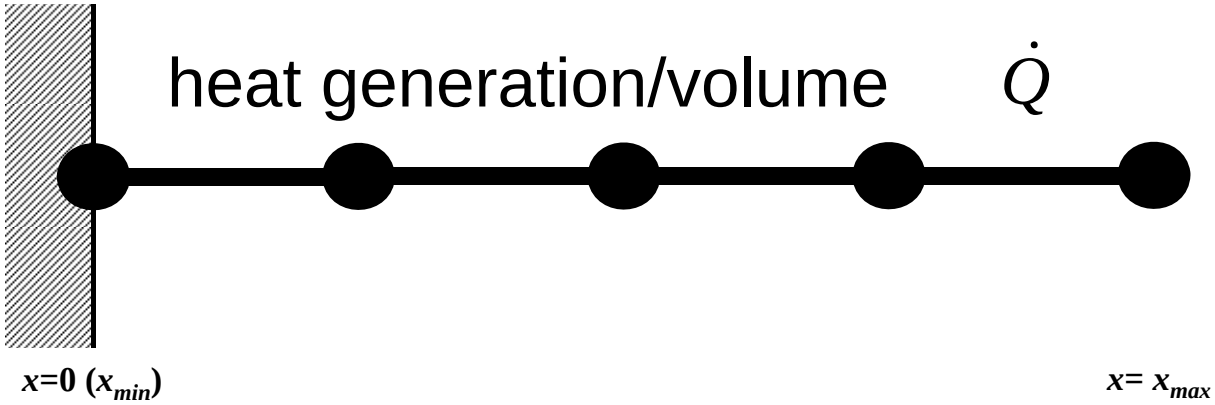
1D Steady State Heat Conduction



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

- 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} : $\frac{\partial T}{\partial x}=0$ (Insulated)

1D Steady State Heat Conduction



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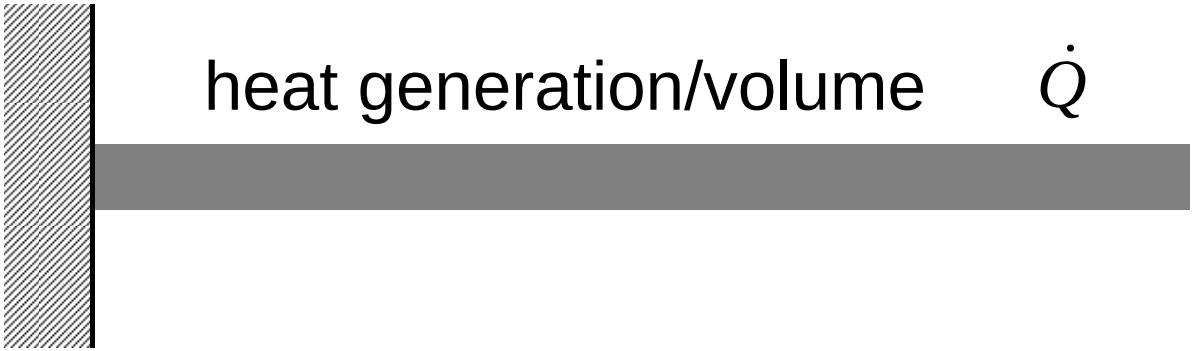
Analytical Solution



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

$$T=0 @ x=0$$

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

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

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

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

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

Copy and Compile

Fortran

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

C

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

Confirm/Compile

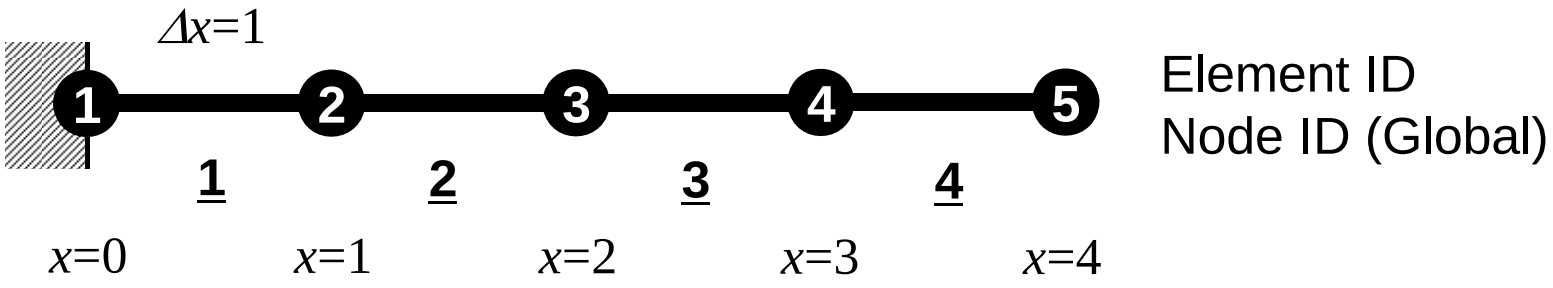
```
 >$ cd mpi/S2-ref
 >$ mpifrtpx –Kfast 1d.f
 >$ mpifccpx –Kfast 1d.c
```

<$O-S2r> = <$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
#PJM -L “node=4“                  Node # (.le.12)
#PJM -L “elapse=00:10:00“         Comp.Time (.le.15min)
#PJM -L “rscgrp=lecture“          “Queue” (or lecture1)
#PJM -g “gt71“                    “Wallet”
#PJM -
#PJM -o “test.lst“                Standard Output
#PJM --mpi “proc=64“              MPI Process # (.le.192)

mpiexec ./a.out
```

N=8	N=16	N=32	N=64	N=192
“node=1“	“node=1“	“node=2“	“node=4“	“node=12“
“proc=8”	“proc=16”	“proc=32”	“proc=64”	“proc=192”

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

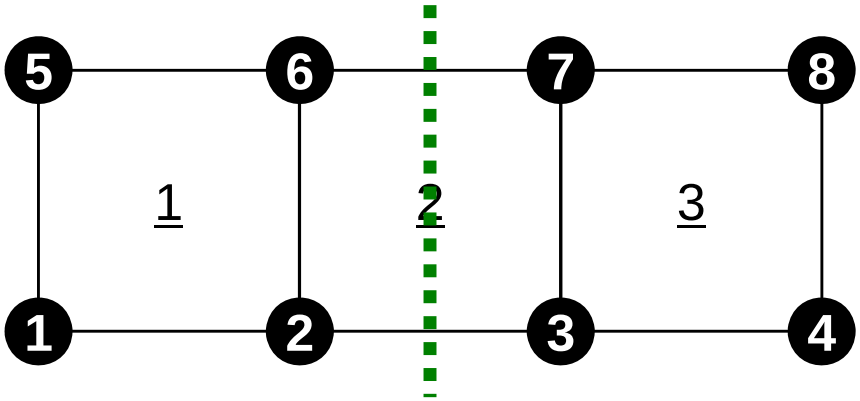
- Not so different from those of original code

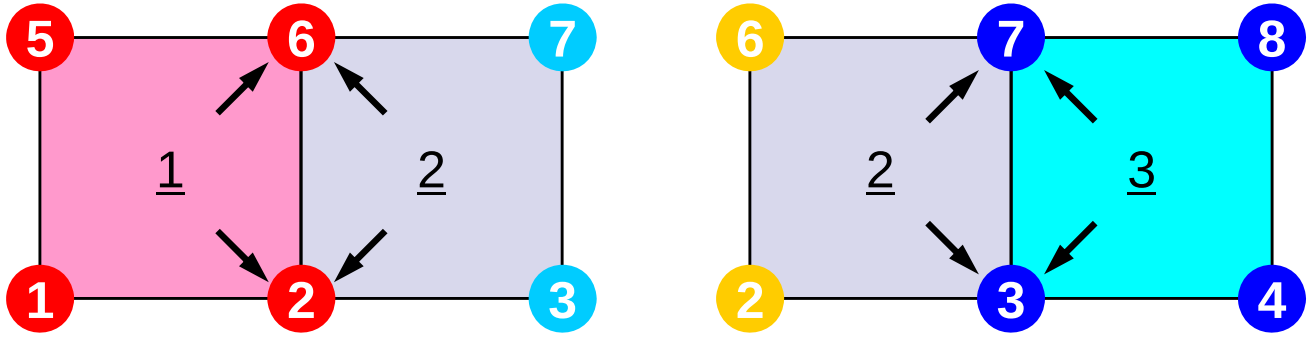
- Overview
- **Distributed Local Data**
- Program
- Results

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

Quadrilateral Elements





Node-based partitioning

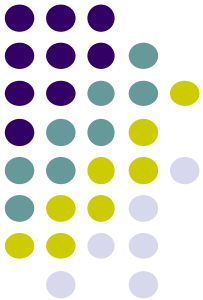
Independent variables are defined at nodes (vertices).

Information is not sufficient for assembling coefficient matrices.

Info. of nodes and elements in overlapped zones are required for assembling coef. matrices.

Computation of stress components needs same info.

Distributed Local Data Structure for Parallel FEM

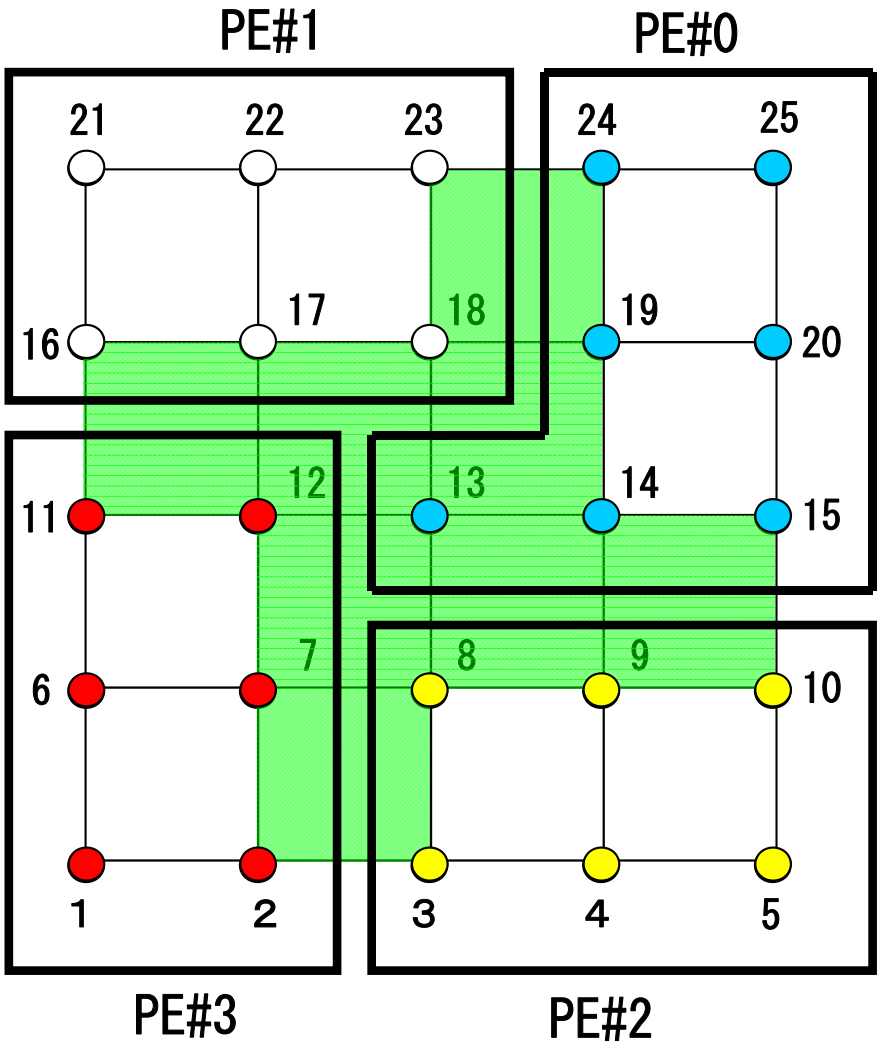


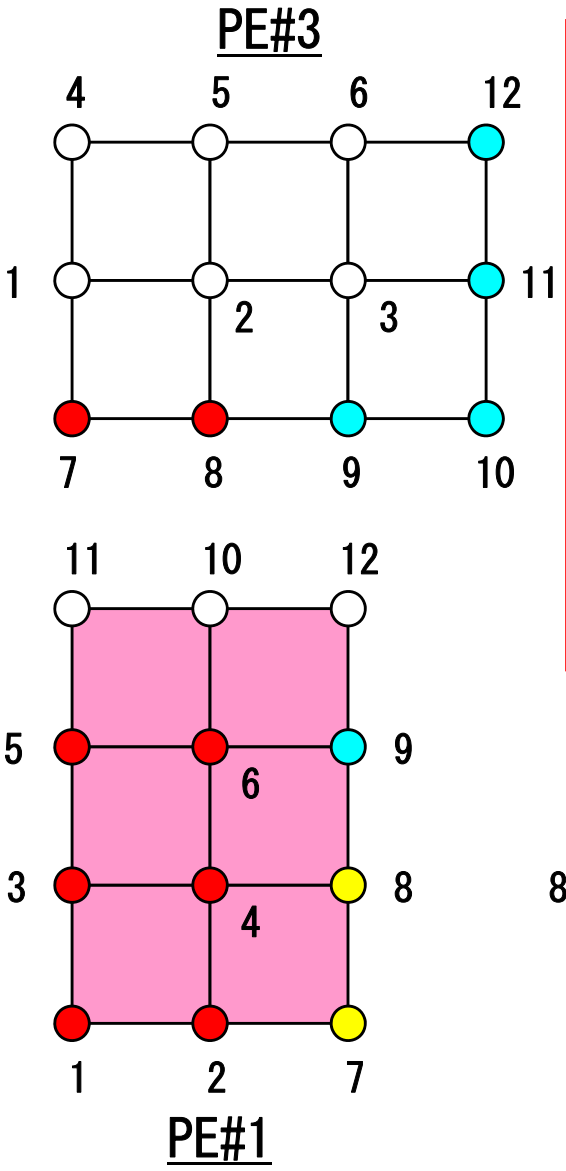
- Node-based partitioning
- Local data includes:
  - Nodes originally assigned to the domain/PE/partition
  - Elements which include above nodes
  - Nodes which are included above elements, and originally NOT-assigned to the domain/PE/partition
- 3 categories for nodes
  - Internal nodes Nodes originally 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

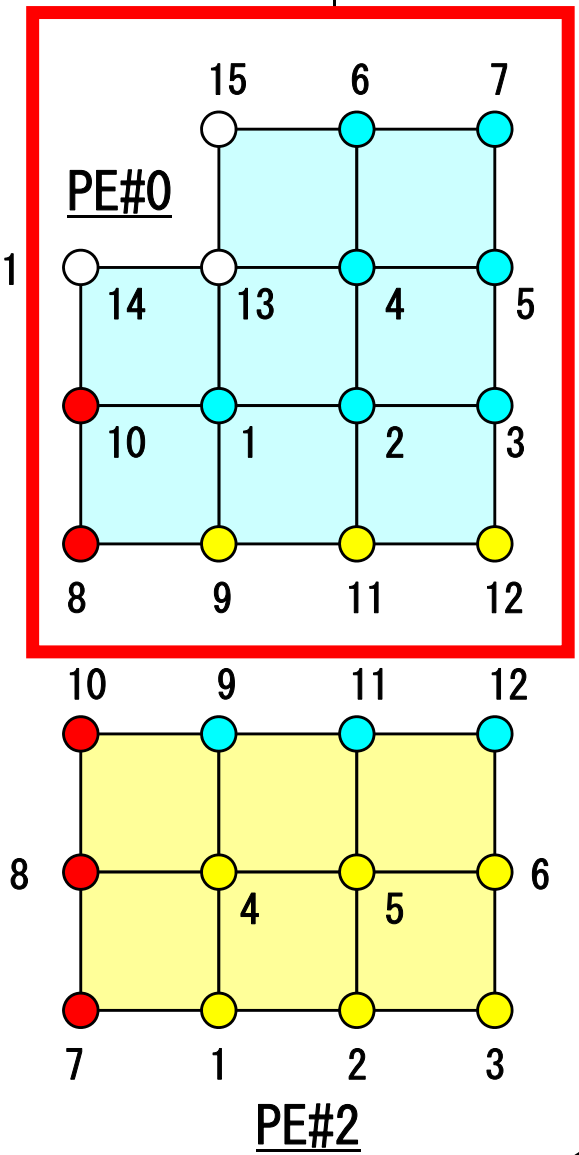
- Global info. is not needed except relationship between domains
  - Property of FEM: local element-by-element operations

Node-based Partitioning

internal nodes - elements - external nodes



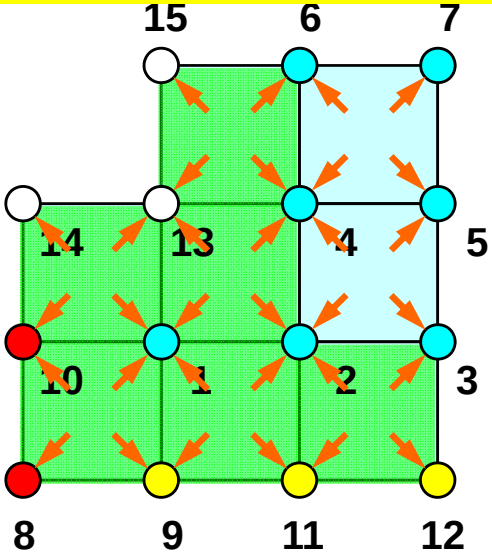


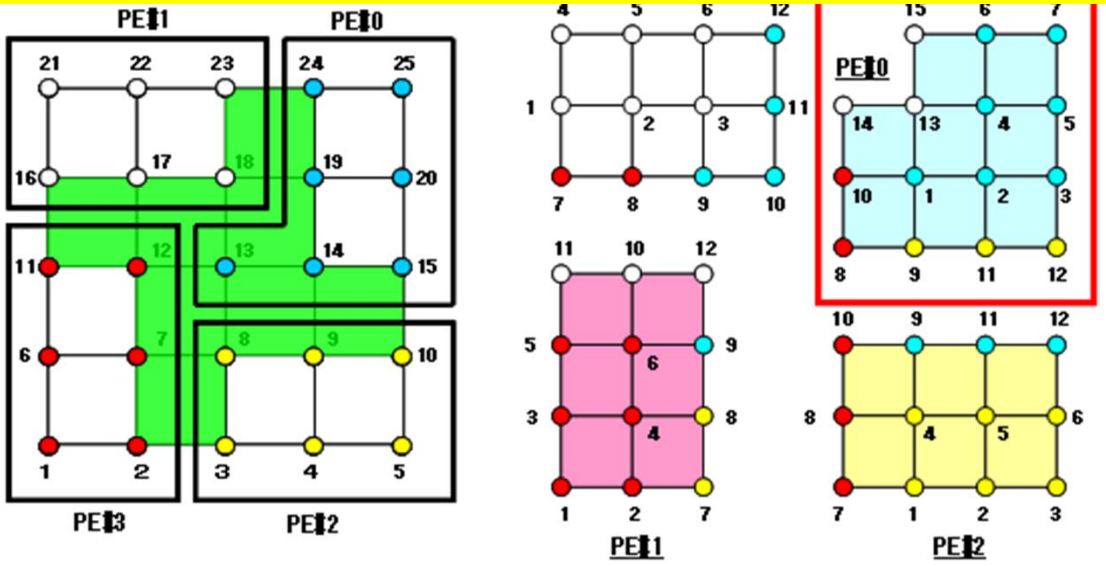


Node-based Partitioning

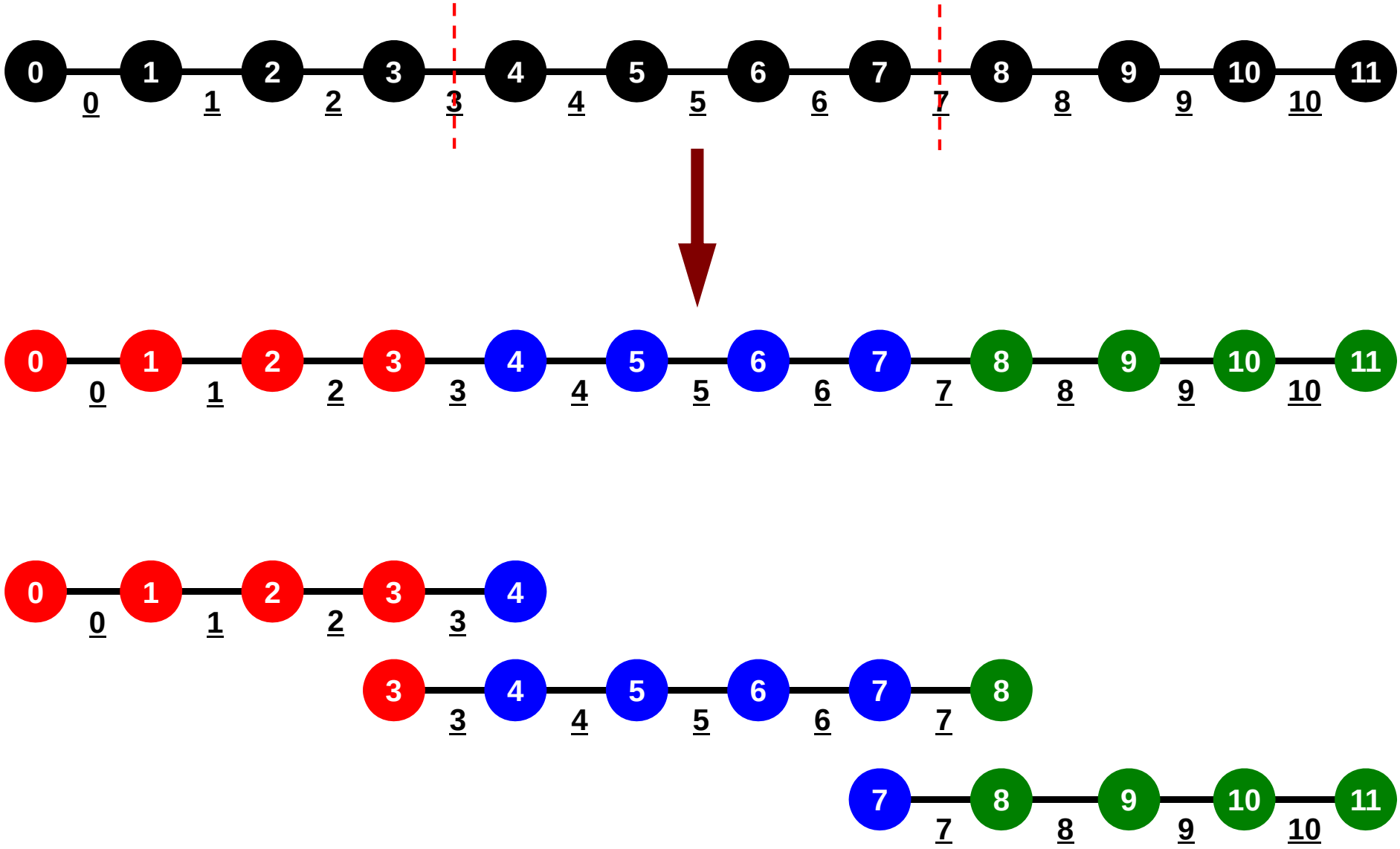
internal nodes - elements - external nodes

- 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.



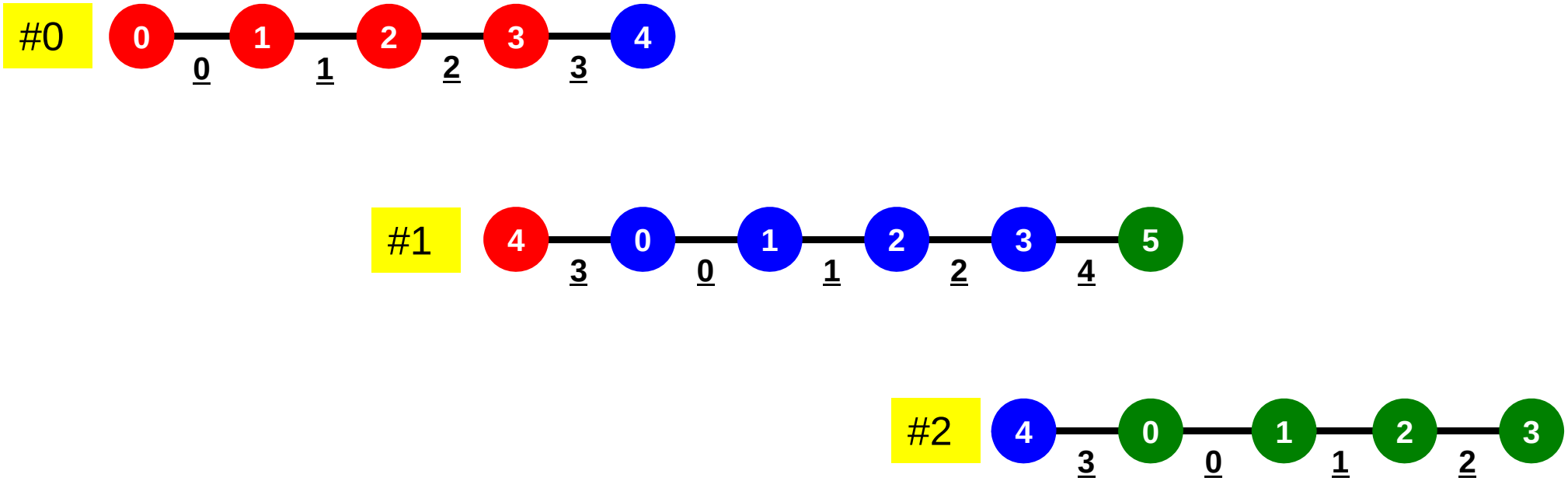


1D FEM: 12 nodes/11 elem's/3 domains



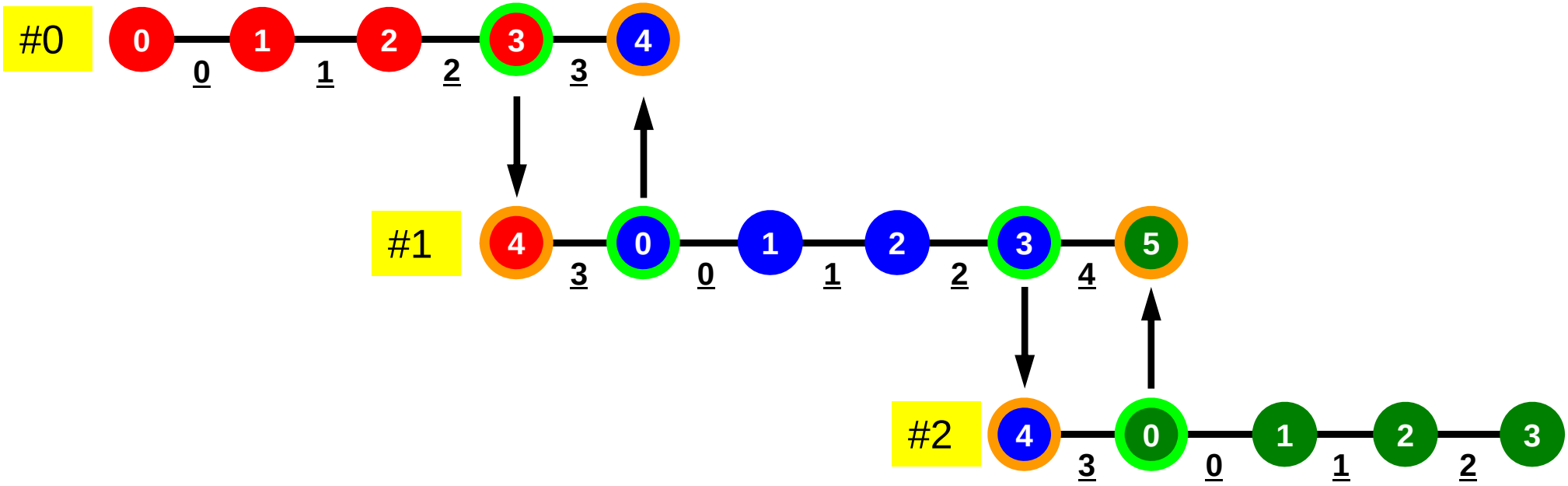
1D FEM: 12 nodes/11 elem’s/3 domains

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

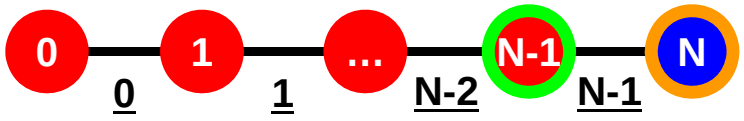


1D FEM: 12 nodes/11 elem's/3 domains

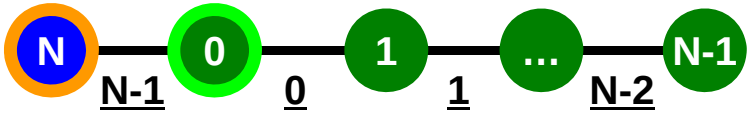
Internal/External Nodes



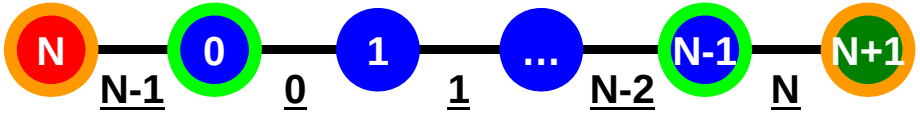
1D FEM: Numbering of Local ID



#0:
N+1 nodes
N elements



#PETot-1:
N+1 nodes
N elements

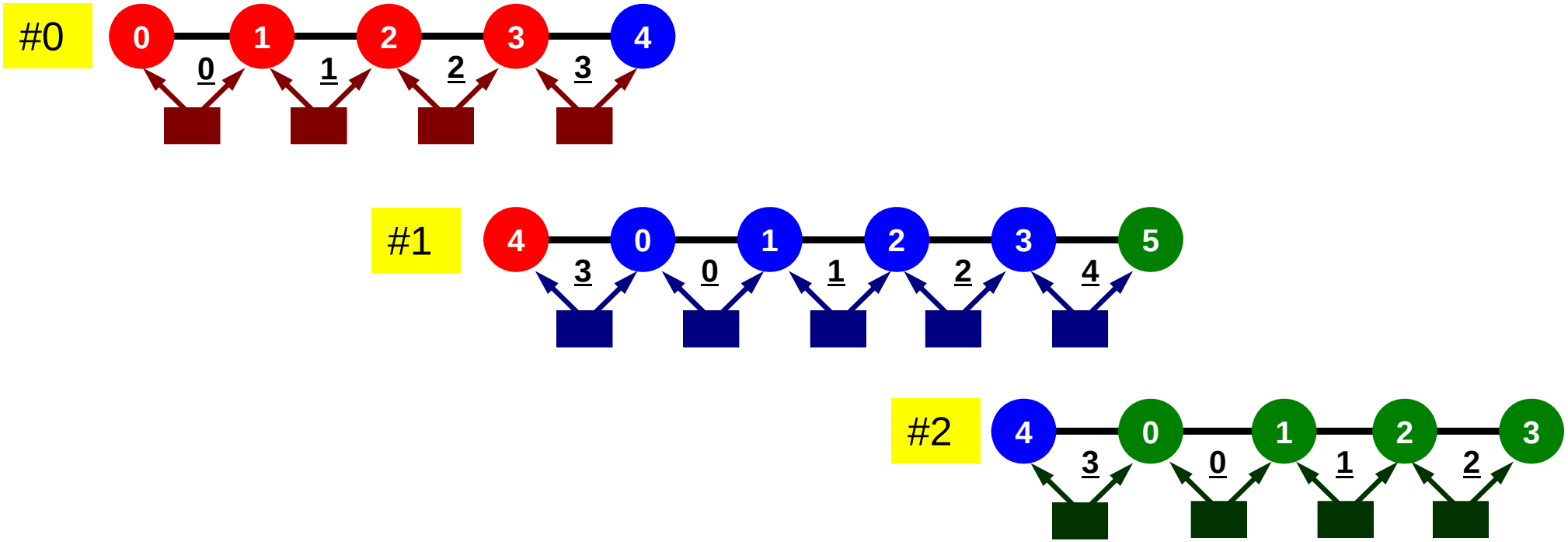


Others (General):
N+2 nodes
N+1 elements

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

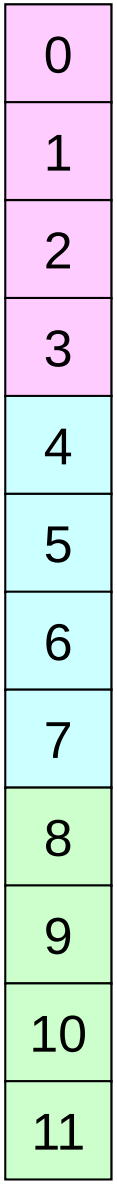
Preconditioning:
Diagonal Scaling
(or Point Jacobi)

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];
    }
```

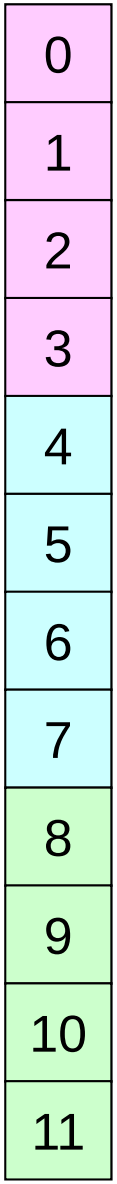
```
/*
//-- {x}= {x} + ALPHA*{p}
//   {r}= {r} - ALPHA*{q}
*/
  for(i=0;i<N;i++){
      U[i]    += Alpha * W[P][i];
      W[R][i] -= Alpha * W[Q][i];
  }
```



Dot Products

Global Summation needed: Communication ?

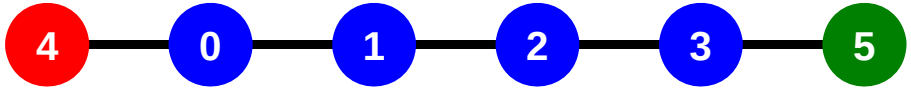
```
/*
//-- ALPHA= RHO / {p}{q}
*/
  C1 = 0.0;
  for(i=0;i<N;i++){
      C1 += W[P][i] * W[Q][i];
  }

  Alpha = Rho / C1;
```



Matrix-Vector Products

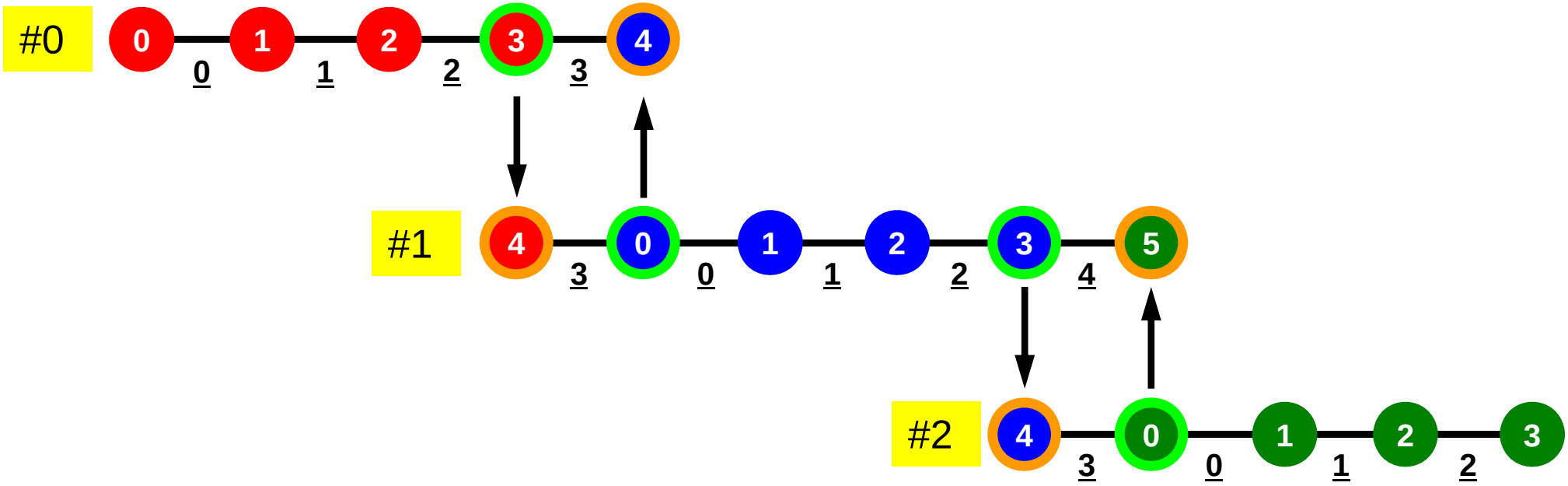
Values at External Points: P-to-P Communication

```
/*
//-- {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]];
          }
      }
```

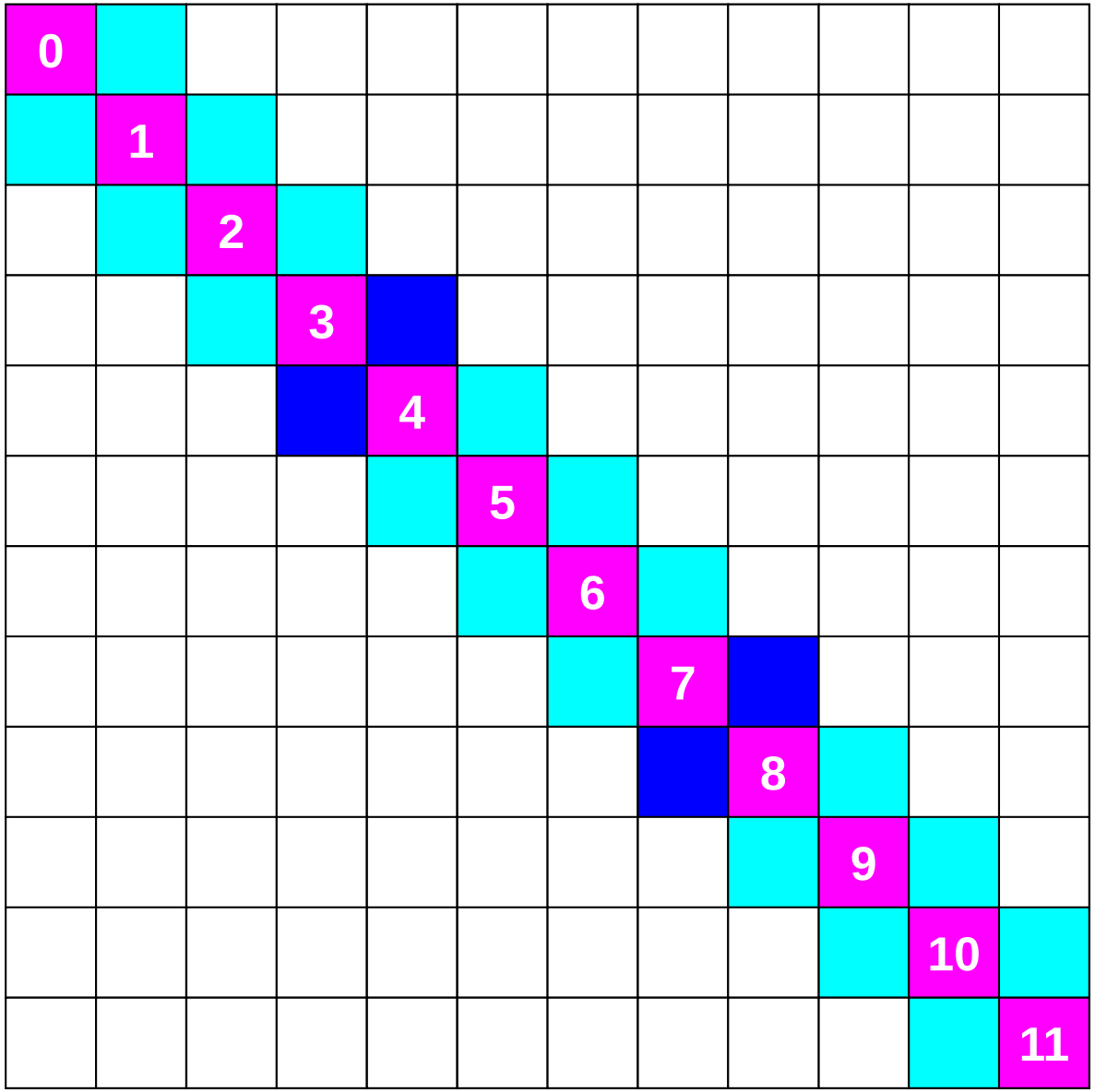


1D FEM: 12 nodes/11 elem's/3 domains

Internal/External Nodes



Mat-Vec Products: Local Op. Possible



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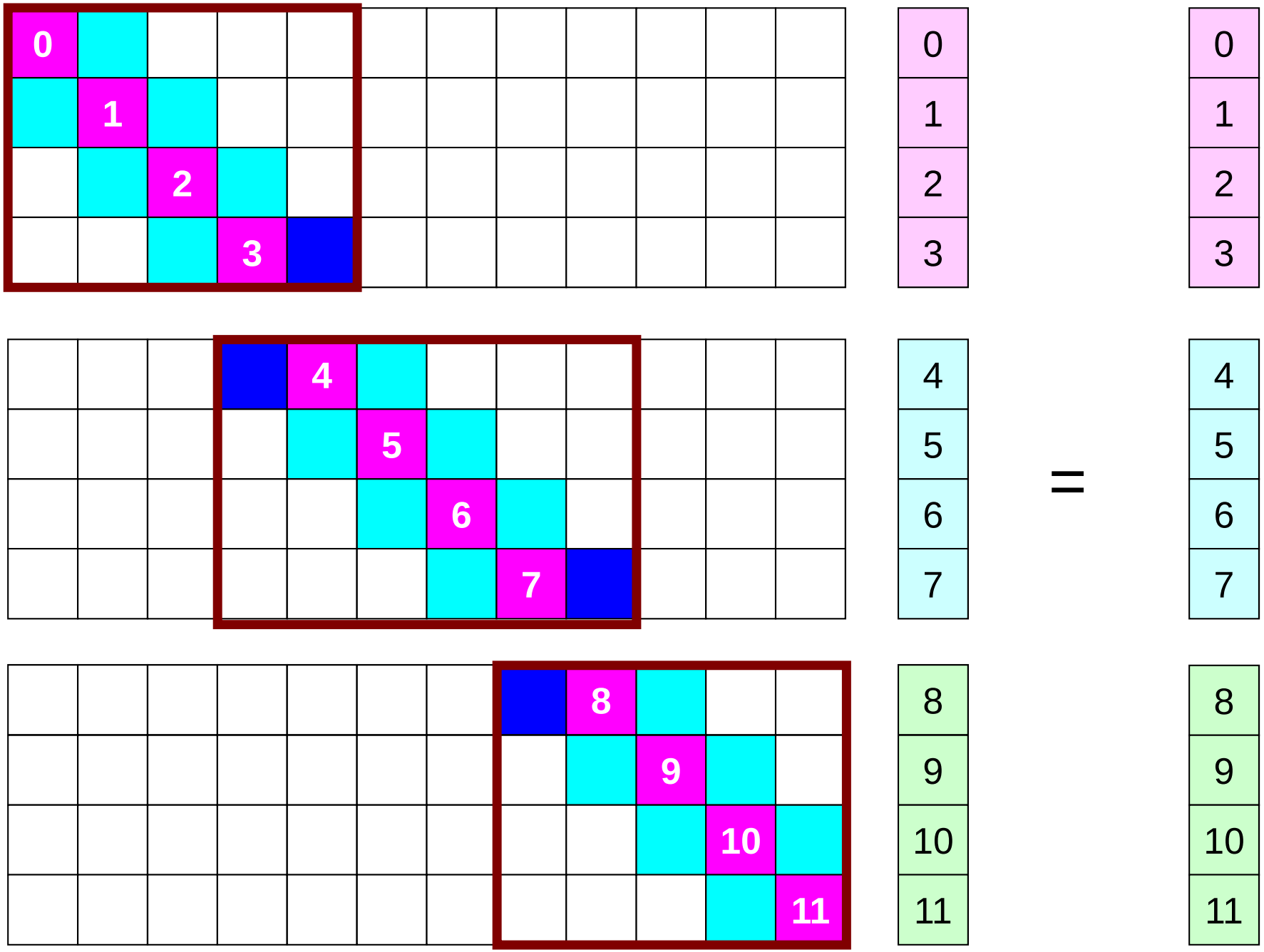
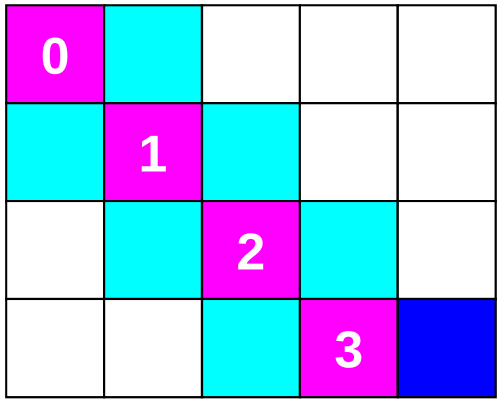
Mat-Vec Products: Local Op. Possible



Mat-Vec Products: Local Op. Possible



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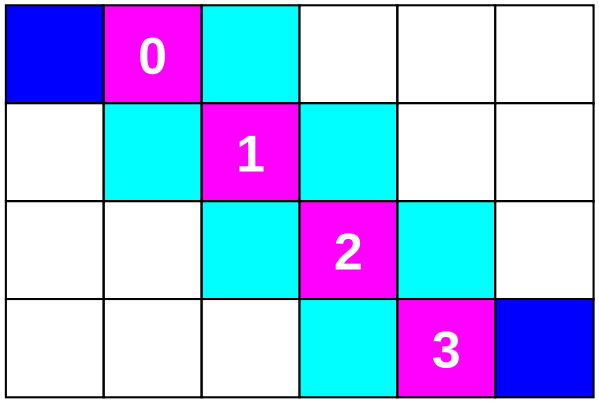

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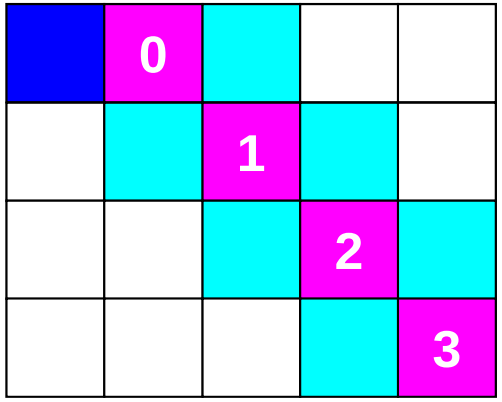

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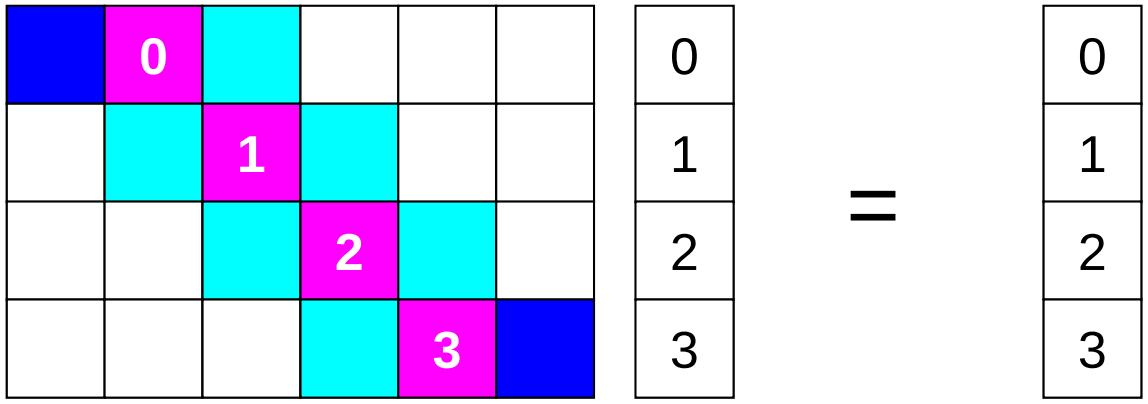
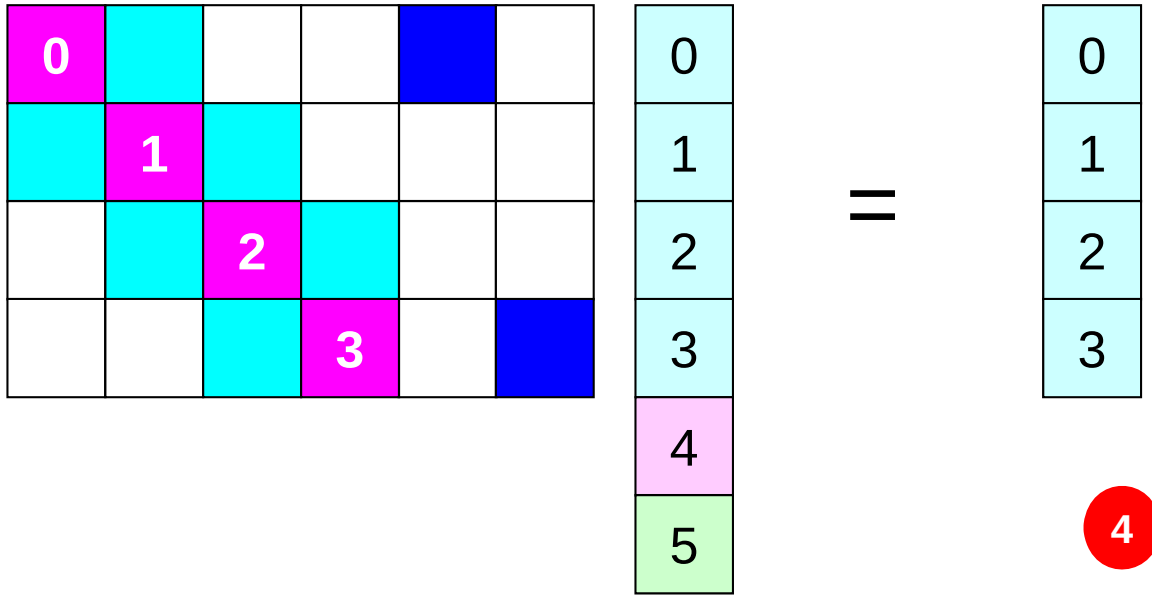
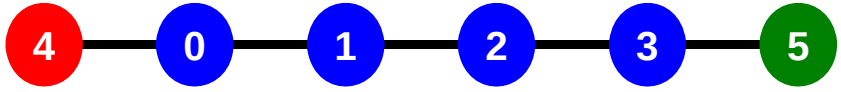
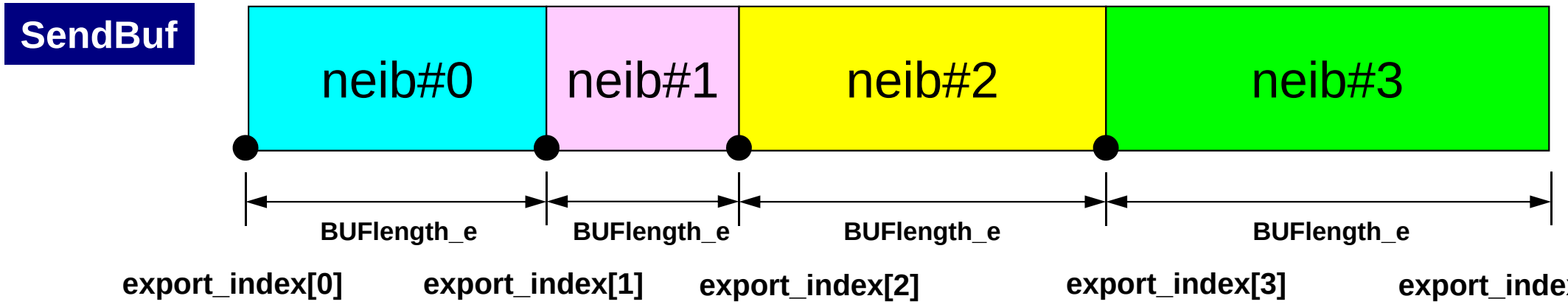
Mat-Vec Products: Local Op. #1







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);
```

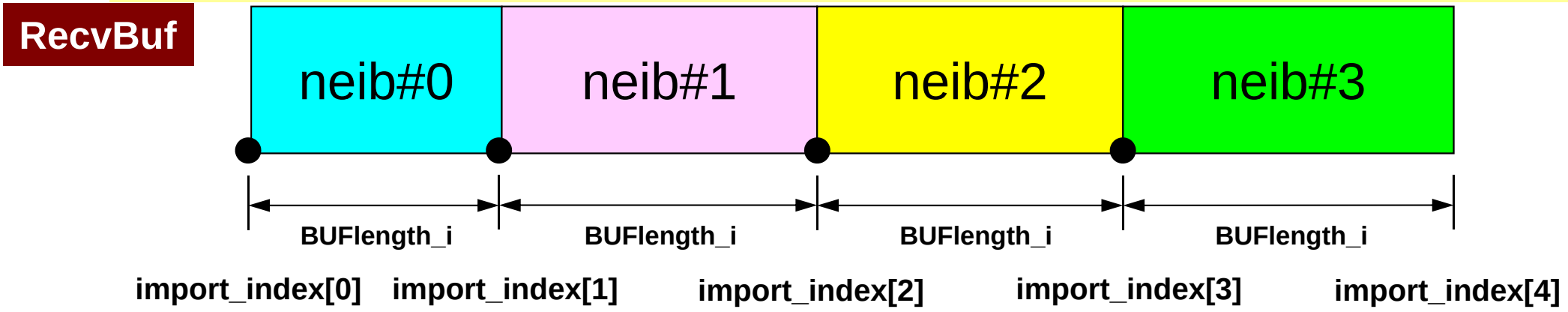
Copied to sending buffers

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

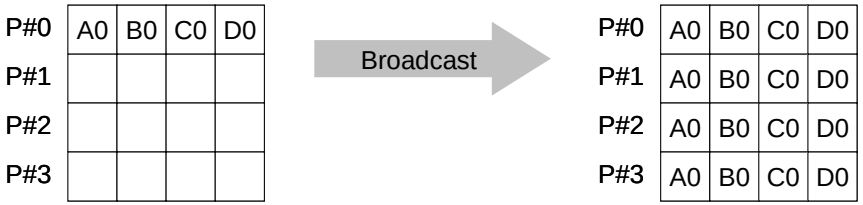
```
/*
// +-------+
// | INIT. |
// +-------+
//=== */

/*
//-- 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

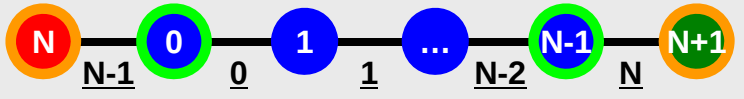
Program: 1d.c (3/11)
Distributed Local Mesh

```
/*
//-- 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

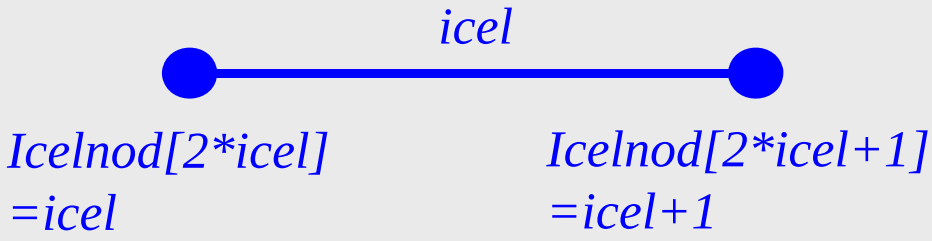
Program: 1d.c (3/11)
Distributed Local Mesh, Uniform Elements

```
/*
//-- 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)

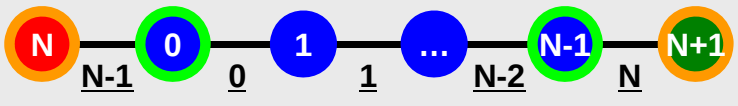
Initialization of Arrays, Elements-Nodes

```
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

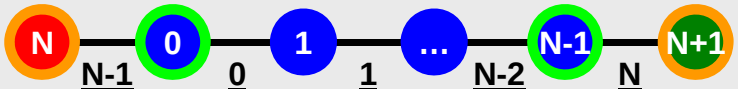
Program: 1d.c (5/11)

"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

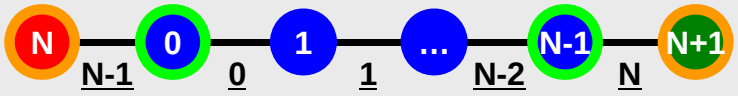
Program: 1d.c (6/11)

”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



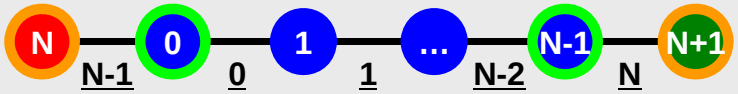
Others (General):
N+2 nodes
N+1 elements

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

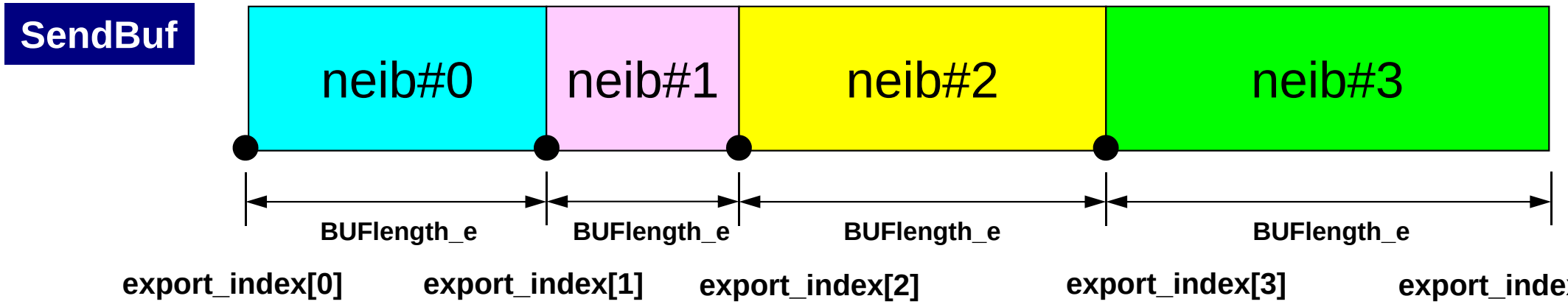
- **MPI_Waitall** blocks until all comm's, associated with **request** in the array, complete. It is used for synchronizing **MPI_Isend** and **MPI_Irecv** in this class.
- At sending phase, contents of sending buffer cannot be modified before calling corresponding **MPI_Waitall**. At receiving phase, 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

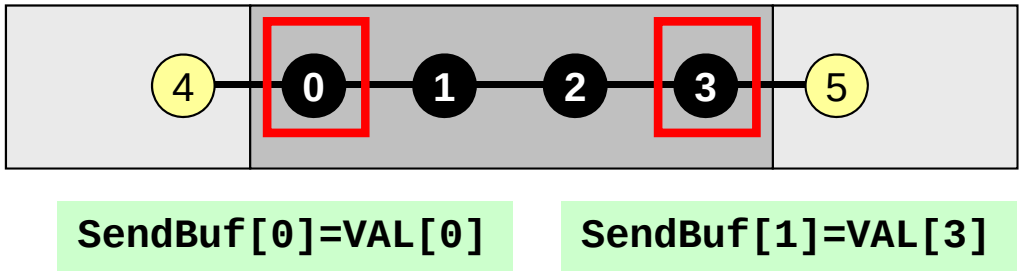


export_item (export_index[neib]:export_index[neib+1]-1) are sent to neib-th neighbor

```
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

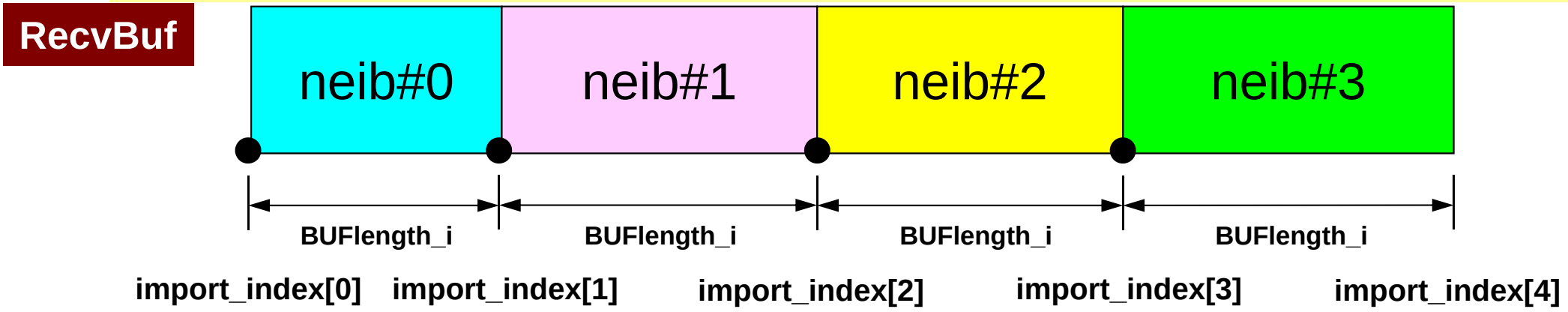
- Neighbors
  - NeibPETot , NeibPE[neib]
- Message size for each neighbor
  - import_index[neib], neib= 0, NeibPETot-1
- ID of **external** points
  - import_item[k], k= 0, import_index[NeibPETot]-1
- Messages from each neighbor
  - RecvBuf[k], k= 0, import_index[NeibPETot]-1

RECV: MPI_Isend/Irecv/Waitall

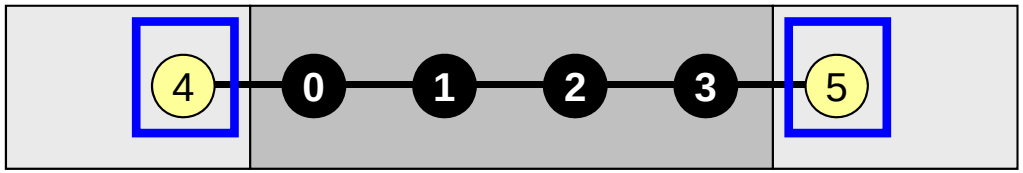
```
for (neib=0; neib<NeibPETot; neib++){
   tag= 0;
   iS_i= import_index[neib];
   iE_i= import_index[neib+1];
   BUFlength_i= iE_i - iS_i

   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



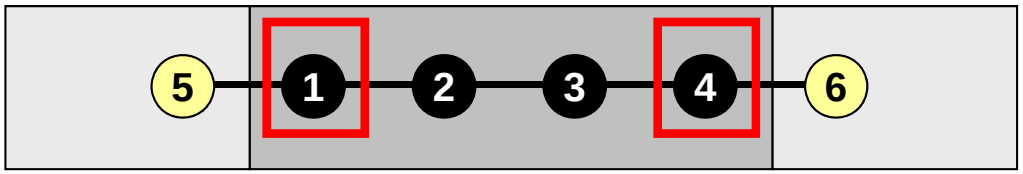
RECV/Import: 1D Problem



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

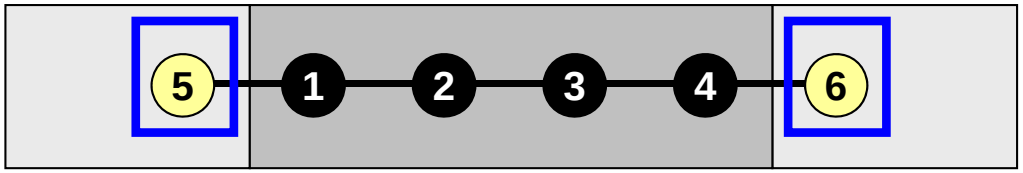
- Neighbors
  - NeibPETot, NeibPE[neib]
    - NeibPETot=2, NeibPE[0]= my_rank-1, NeibPE[1]= my_rank+1
- Message size for each neighbor
  - import_index[neib], neib= 0, NeibPETot-1
    - import_index[0]=0, import_index[1]= 1, import_index[2]= 2
- ID of **external** points
  - import_item[k], k= 0, import_index[NeibPETot]-1
    - 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)

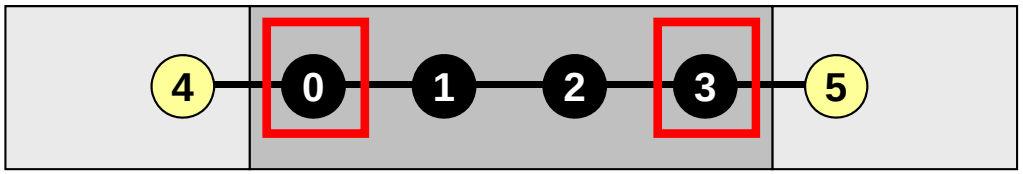


BUF(5)=RECVbuf(1)

BUF(6)=RECVbuf(2)

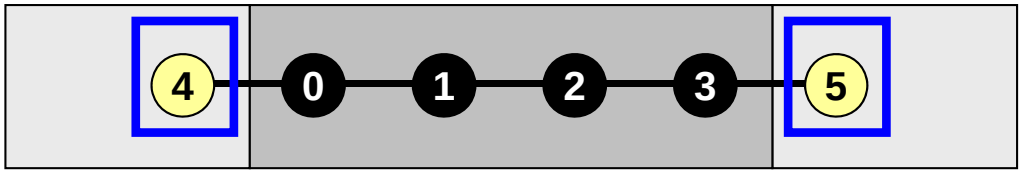
```
NEIBPETOT= 2
NEIBPE(1)= my_rank - 1
NEIBPE(2)= my_rank + 1

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]

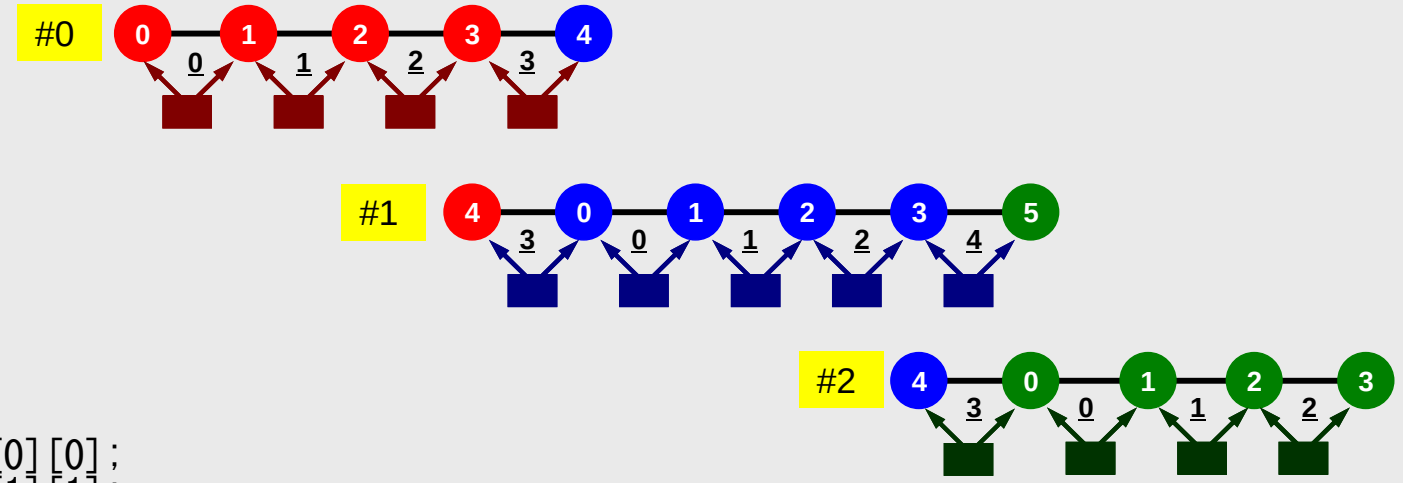
BUF[5]=RECVbuf[1]

```
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

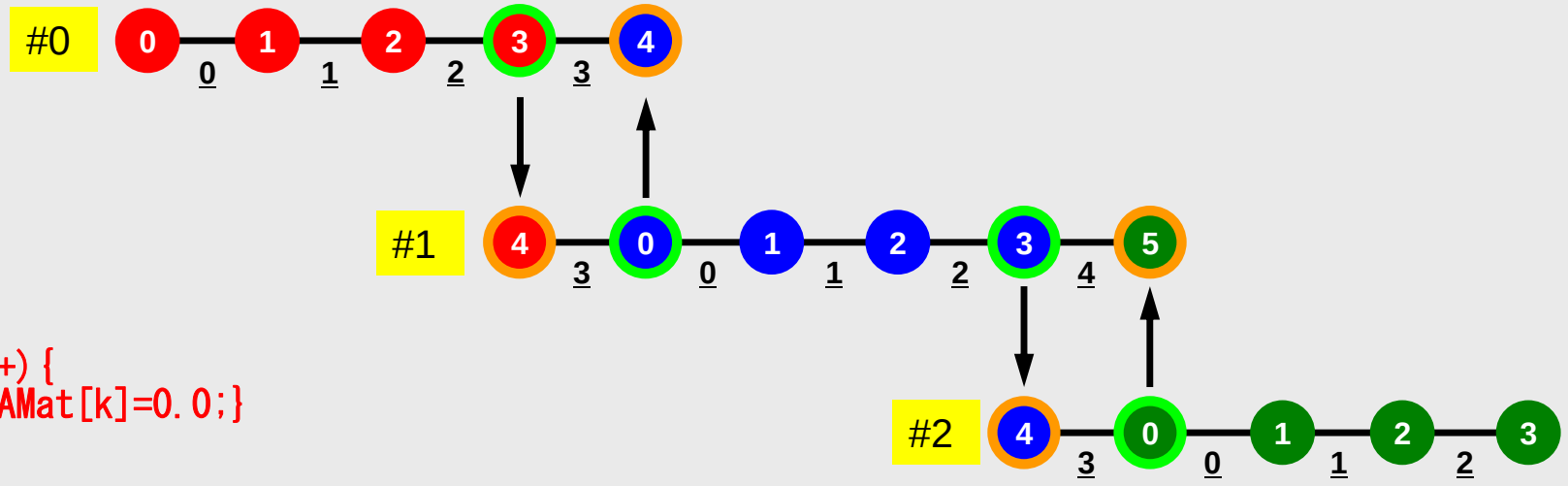
```
/*
// +-----------------+
// | MATRIX assemble |
// +-----------------+
*/
    for(icel=0;icel<NE;icel++){
      in1= Icelnod[2*icel];
      in2= Icelnod[2*icel+1];
      DL = dX;

      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;
    }
```



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}

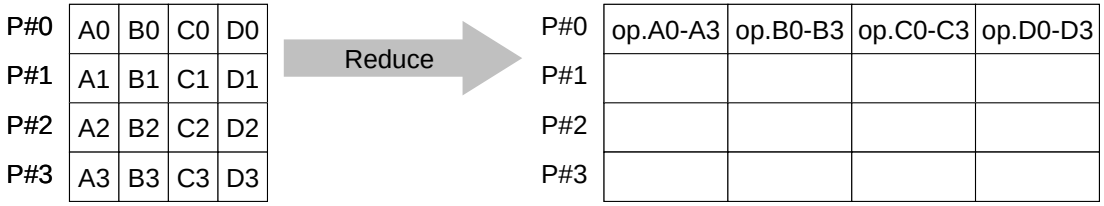
```
MPI_Waitall(NeibPETot, RequestSend, StatSend);

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)
```

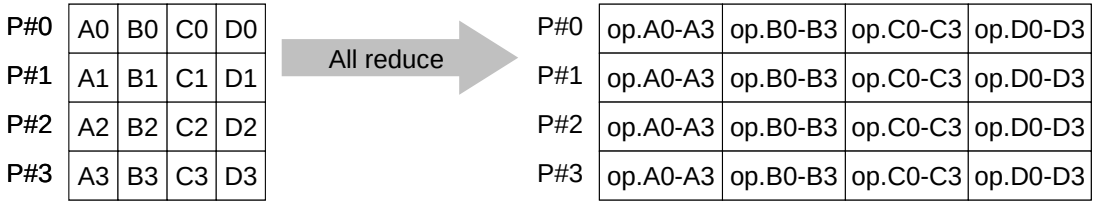
```
real(kind=8):: X0, XSUM

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

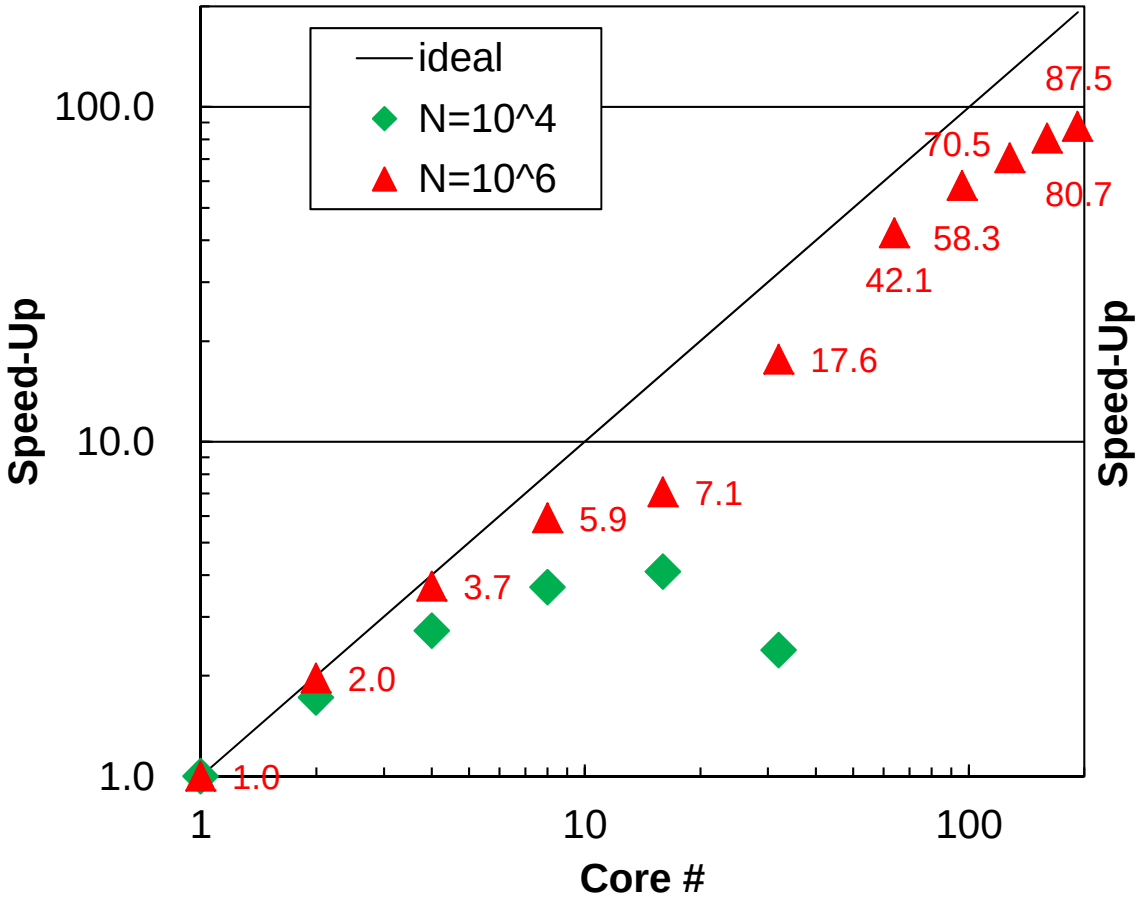
```
/*
//-- OUTPUT
*/
    printf("¥n%s¥n", "### TEMPERATURE");
    for(i=0;i<N;i++){
      printf("%3d%8d%16.6E¥n", MyRank, i+1, PHI[i]);
    }

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

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

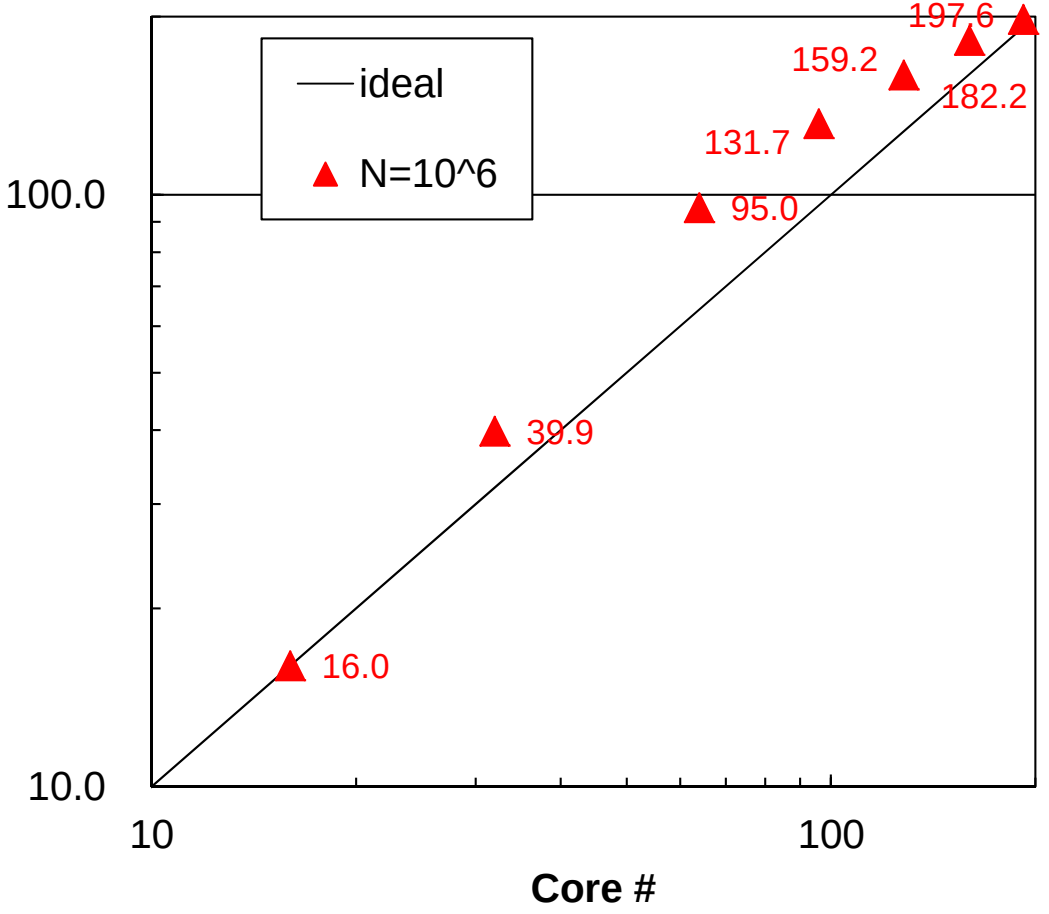
Results for CG Solver

Time for 100 Iterations in $N=10^6$ case

based on a core



based on a node (16 cores)



Performance is lower than ideal one

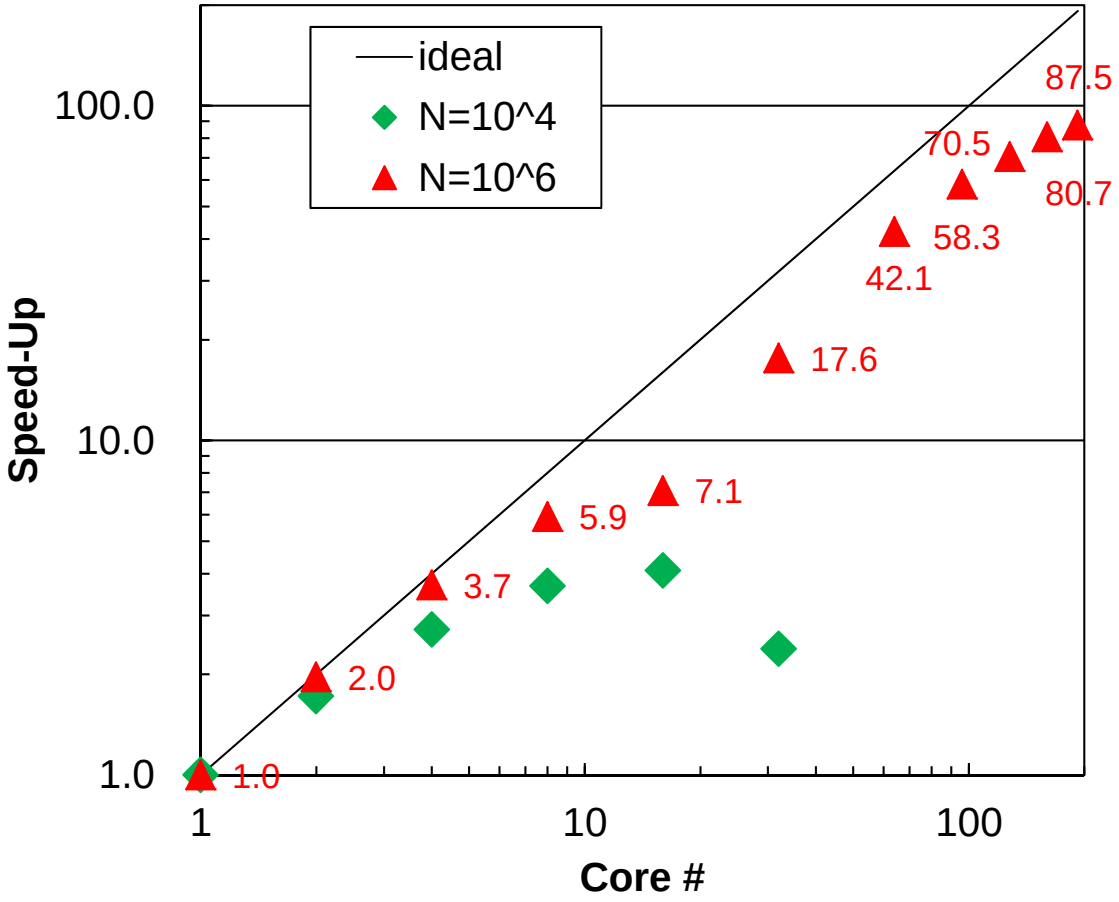
- Time for MPI communication
  - Time for sending data
  - Communication bandwidth between nodes
  - Time is proportional to size of sending/receiving buffers
- Time for starting MPI
  - latency
  - does not depend on size of buffers
    - depends on number of calling, increases according to process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

Performance is lower than ideal one (cont.)

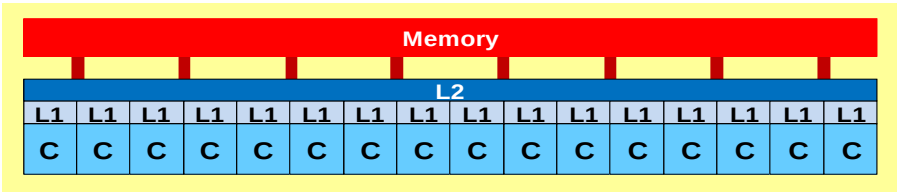
- If computation time is relatively small (N is small in S1-3), these effects are not negligible.
  - If the size of messages is small, effect of “latency” is significant.

Performance is not so good... between 1-16 cores

based on performance at a single core



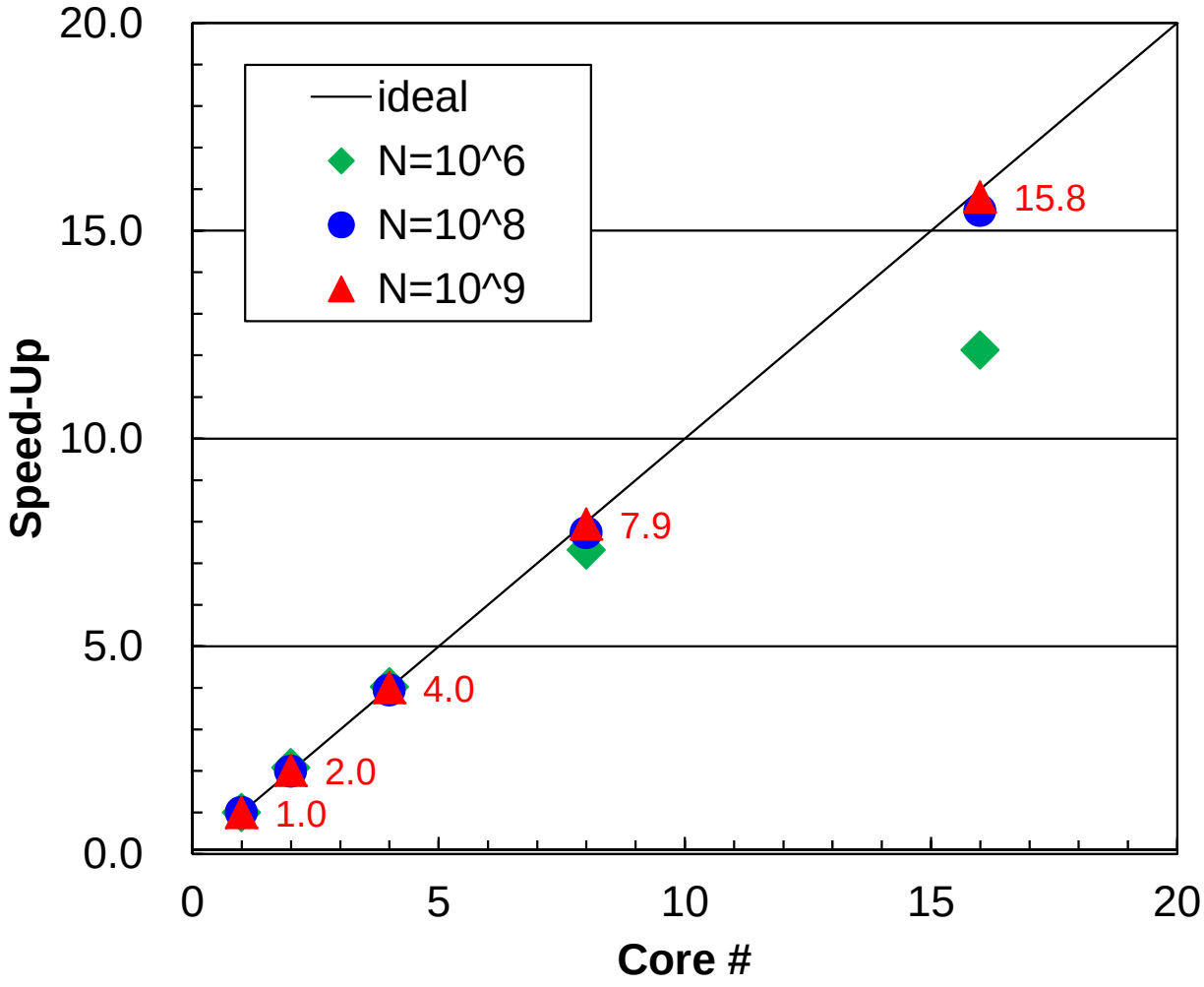
- x 7.1 at 16 cores, because of memory contention
  - STREAM
  - NOT mainly because of communication overhead



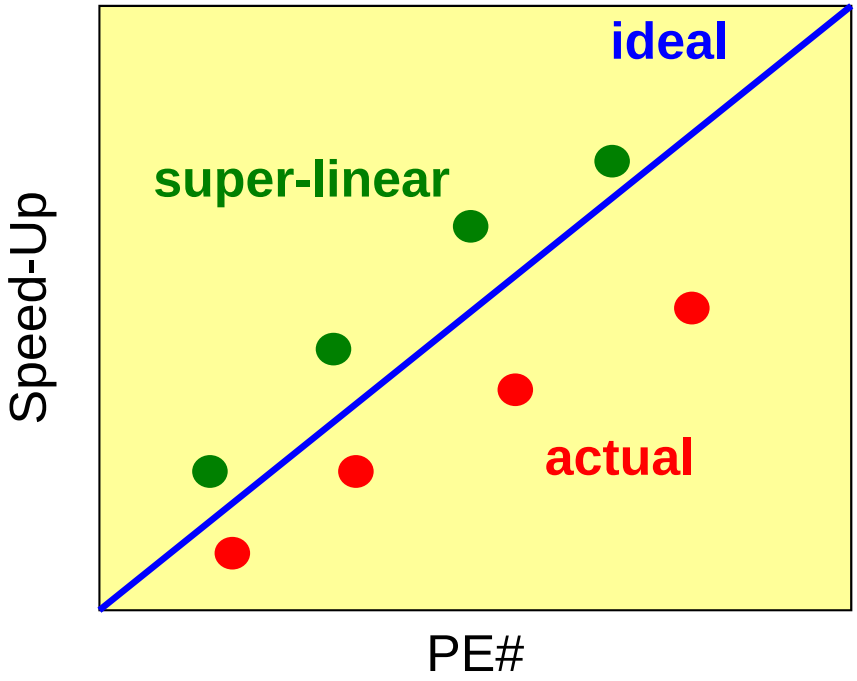
Not so significant in S1-3

- ◆ : N=10^6, ● : 10^8, ▲ : 10^9, — : Ideal
- Based on performance at a single core (sec.)

- Trapezoidal rule: requirement for memory is very small (no arrays), NON memory-bound application

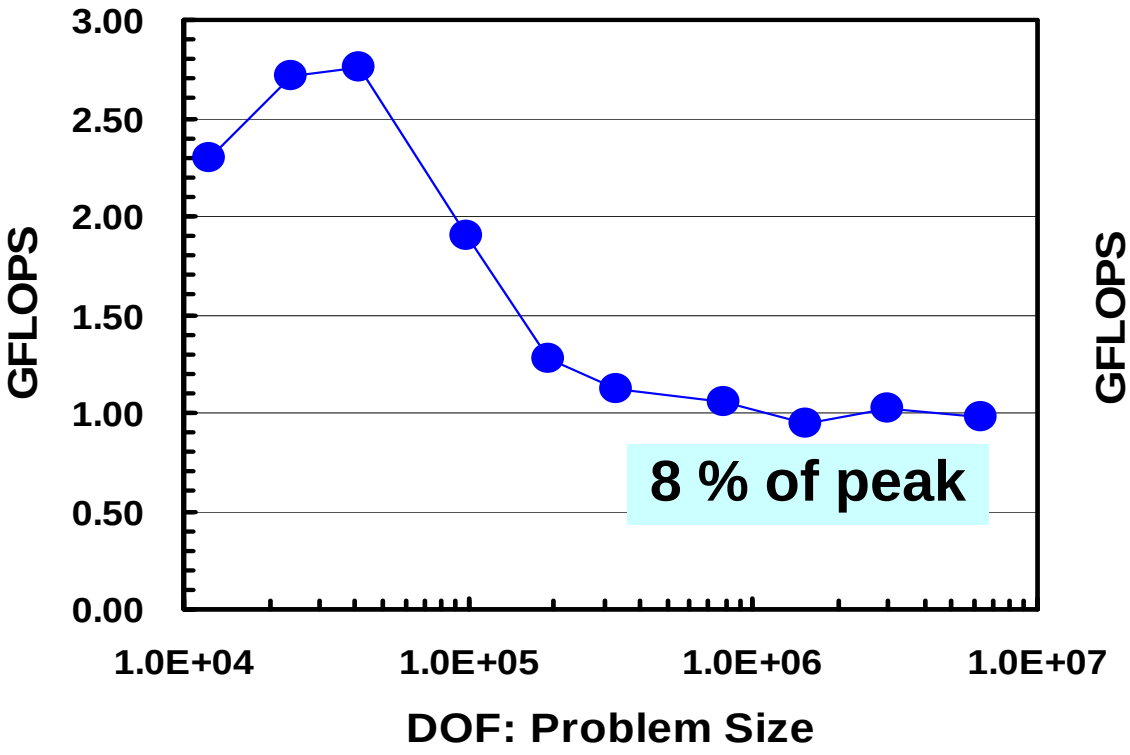


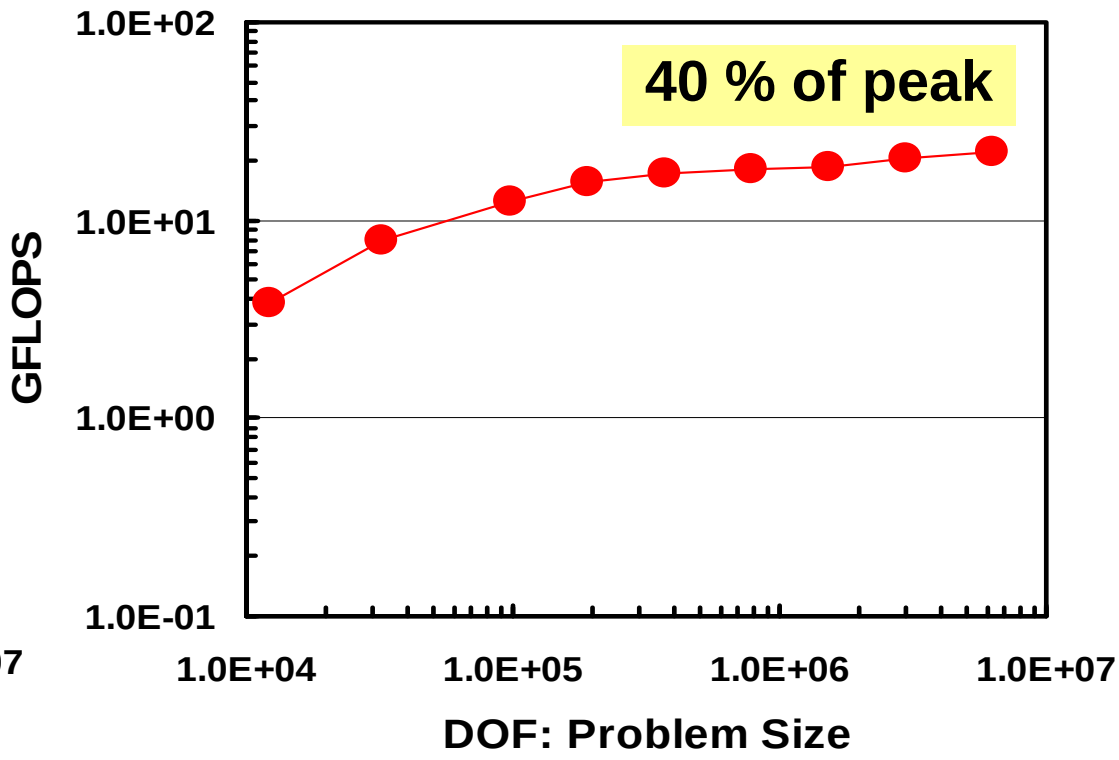
Super-Linear in Strong Scaling



- 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

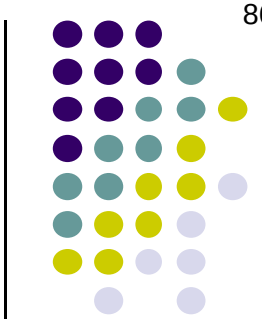
Typical Behaviors



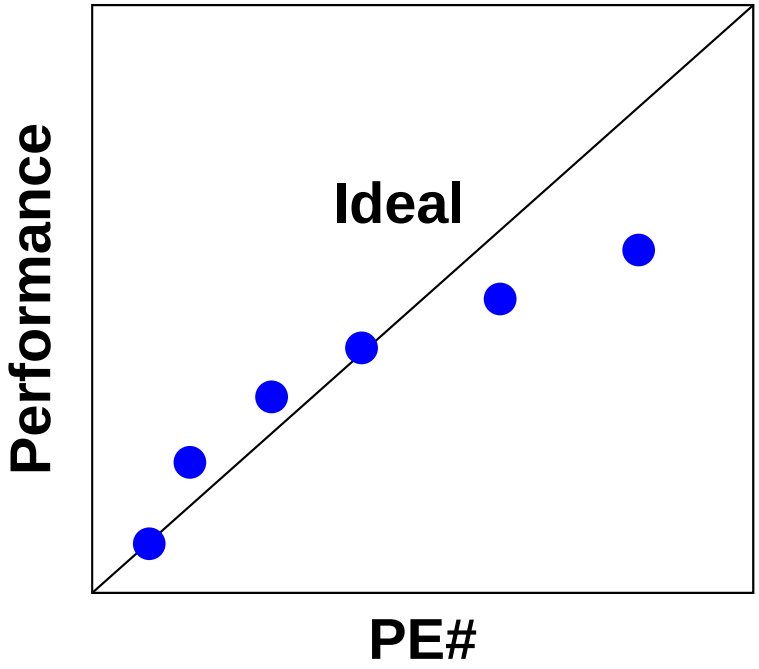


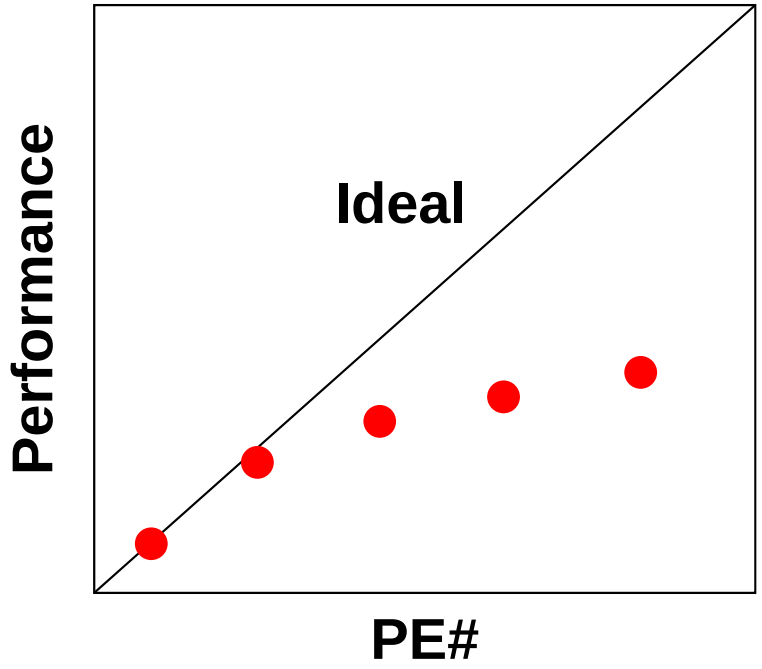
IBM-SP3:
Higher performance for small problems, effect of cache

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



Strong Scaling



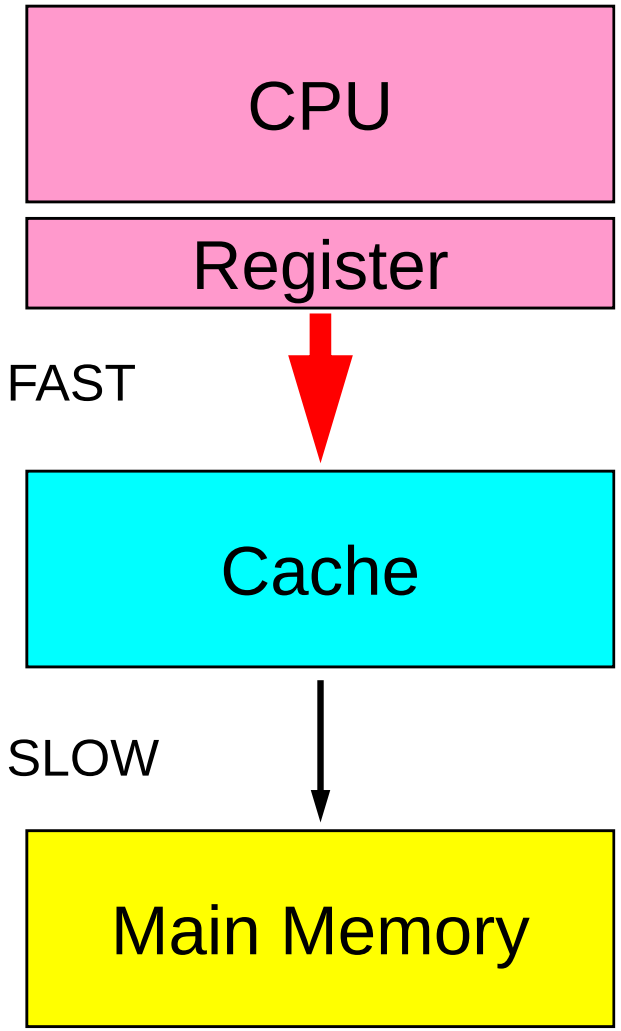


IBM-SP3:
"Super-linear" happens if number of PE is not so large. Performance is getting worse due to communication overhead if PE number is larger.

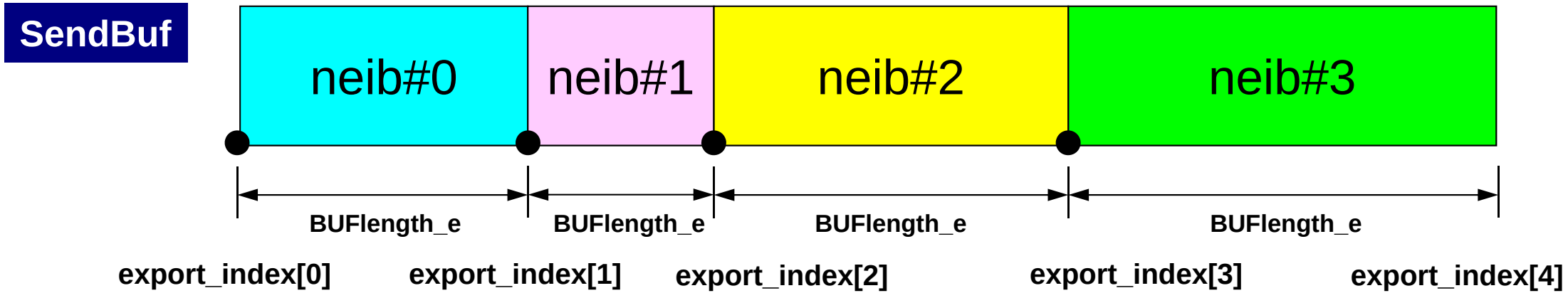
Earth Simulator:
Performance is getting worse due to communication overhead and smaller loop length if PE number is larger.

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);
```

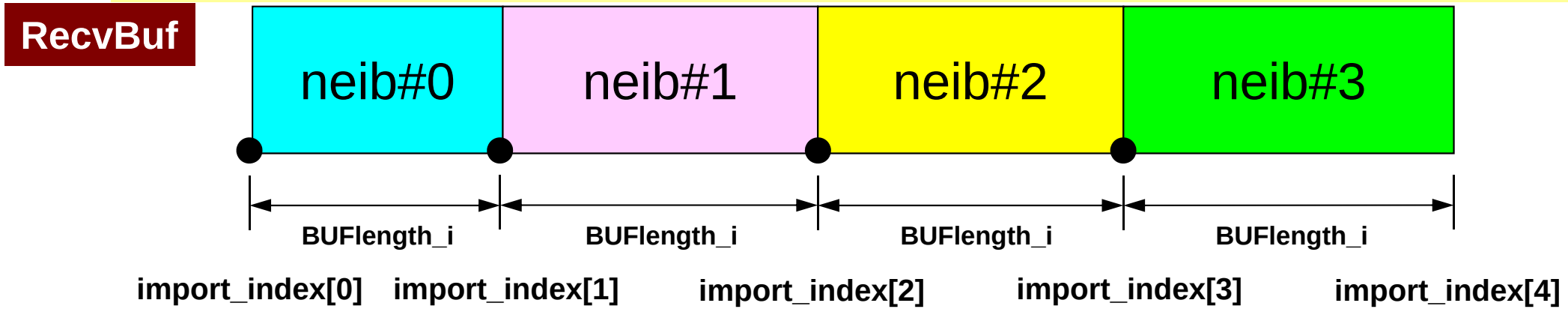
Copied to sending buffers

Memory Copy is expensive (1/2)

```
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



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