Report S2
C

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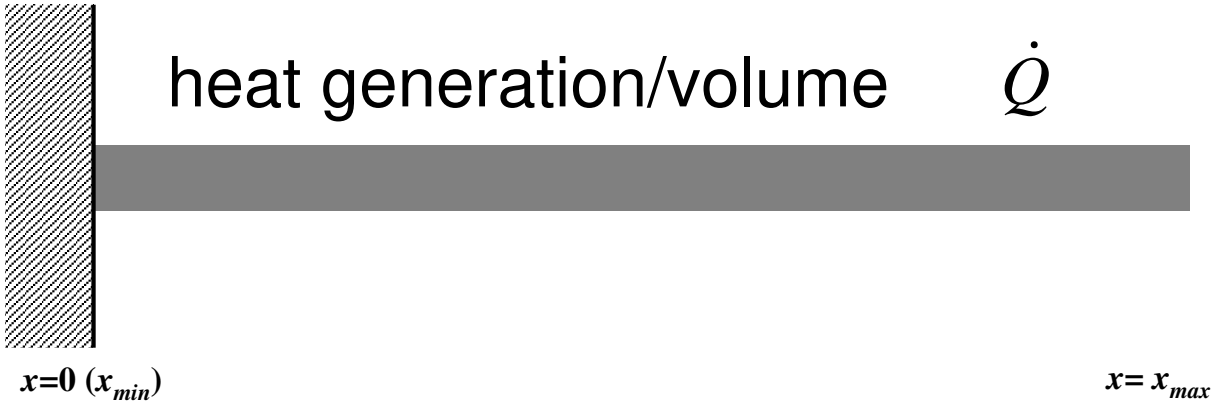
- Overview
- Distributed Local Data
- Program
- Results

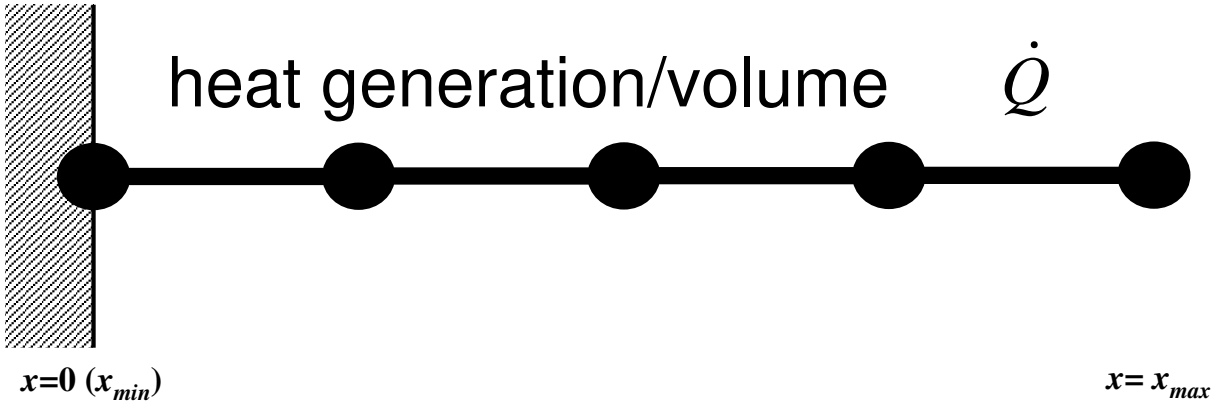
1D Steady State Heat Conduction



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

- 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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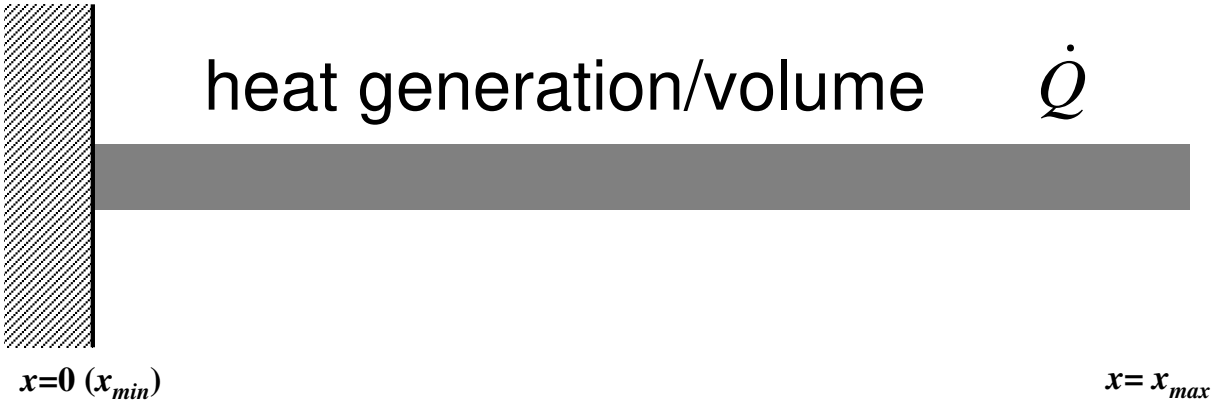
Analytical Solution



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

$$T=0 \;@\; x=0$$

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

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

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

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

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

Report S2 (1/2)

- Parallelize 1D code (1d.f) using MPI
- Read entire element number, and decompose into sub-domains in your program

- Validate the results
  - Answer of Original Code = Answer of Parallel Code
  - Explain why number of iterations does not change, as number of MPI processes changes.
- Measure parallel performance

Report S2 (2/2)

- Deadline: January 26th (Wed), 2022, 17:00@ITC-LMS
- Problem
  - Apply “Generalized Communication Table”
  - Read entire elem. #, decompose into sub-domains in your program
  - Evaluate parallel performance
    - You need huge number of elements, to get excellent performance.
    - Fix number of iterations (e.g. 100), if computations cannot be completed.
- Report
  - Cover Page: Name, ID, and Problem ID (S2) must be written.
  - Less than eight pages including figures and tables (A4).
    - Strategy, Structure of the Program, Remarks
  - Source list of the program (if you have bugs)
  - Output list (as small as possible)

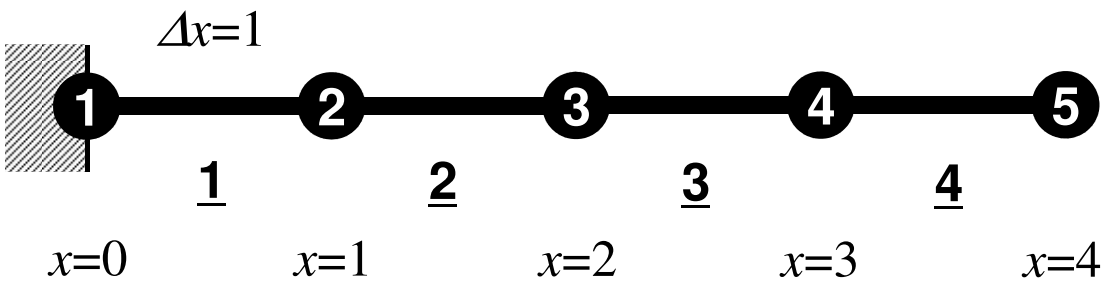
Copy and Compile

Control File: input.dat

Control Data **`input.dat`**

```
1000000
1.0  1.0  1.0  1.0
100
1.e-8
```

`NE` (Number of Elements)
Δx (Length of Each Elem.: `L`) , `Q`, `A`, λ
Number of MAX. Iterations for CG Solver
Convergence Criteria for CG Solver



Element ID
Node ID (Global)

g16.sh: 8-nodes, 256-cores, 16x2x8

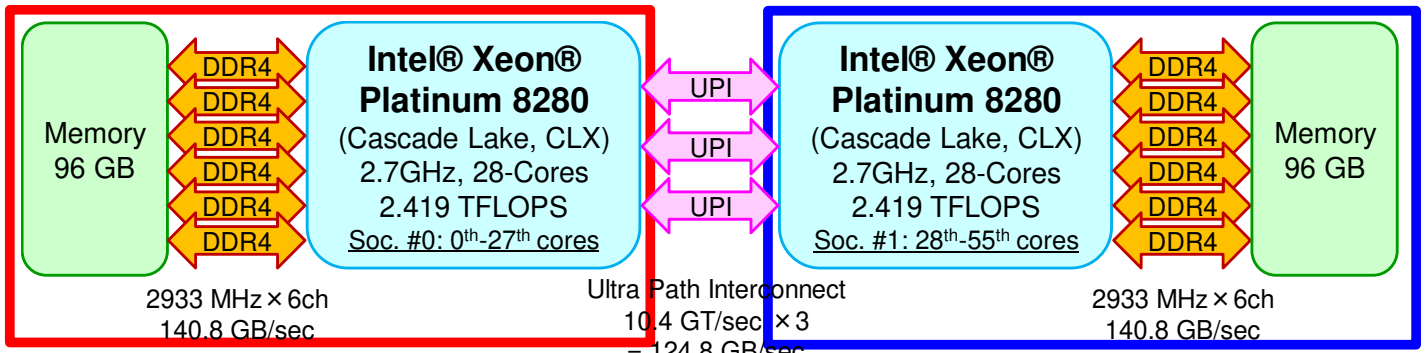
```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=8
#PJM -mpi proc=256
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o test.lst

mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
export I_MPI_PIN_PROCESSOR_LIST=0-15,28-43
mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
```

256/8= 32 cores/node

1da: -O3 + AVX512
1db: -O3 Only

32-cores are randomly selected from 56-cores on the node

32-cores on each socket are assigned.
A little bit more stable



Socket #0: 0th-27th Cores

Socket #1: 28th-55th Cores

g24.sh: 8-nodes, 384-cores, 24x2x8

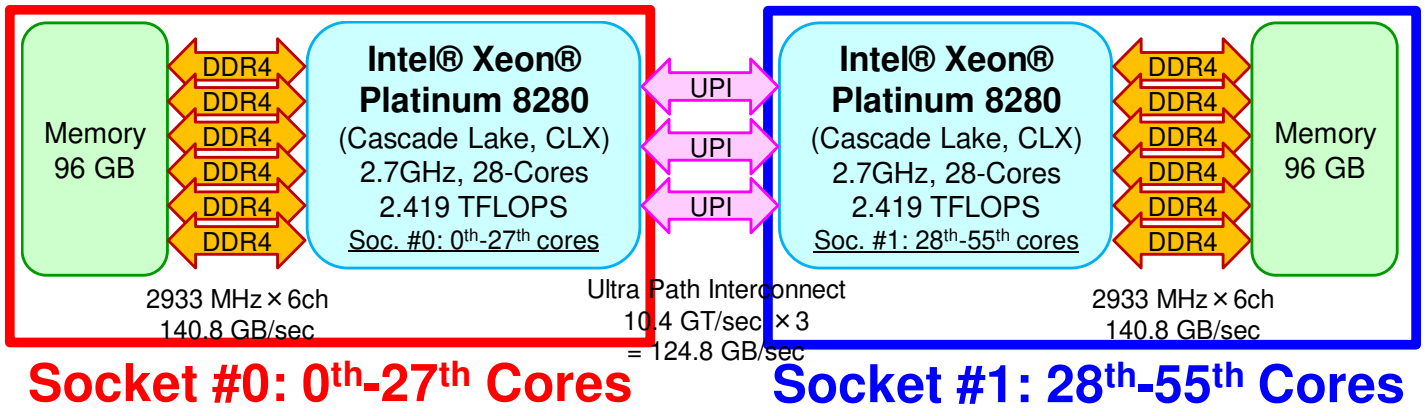
```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=8
#PJM --mpi proc=384
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o test.lst

mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
export I_MPI_PIN_PROCESSOR_LIST=0-23,28-51
mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
```

384/8= 48 cores/node

1da: -O3 + AVX512
1db: -O3 Only

48-cores are randomly selected from 56-cores on the node

24-cores on each socket are assigned.
A little bit more stable

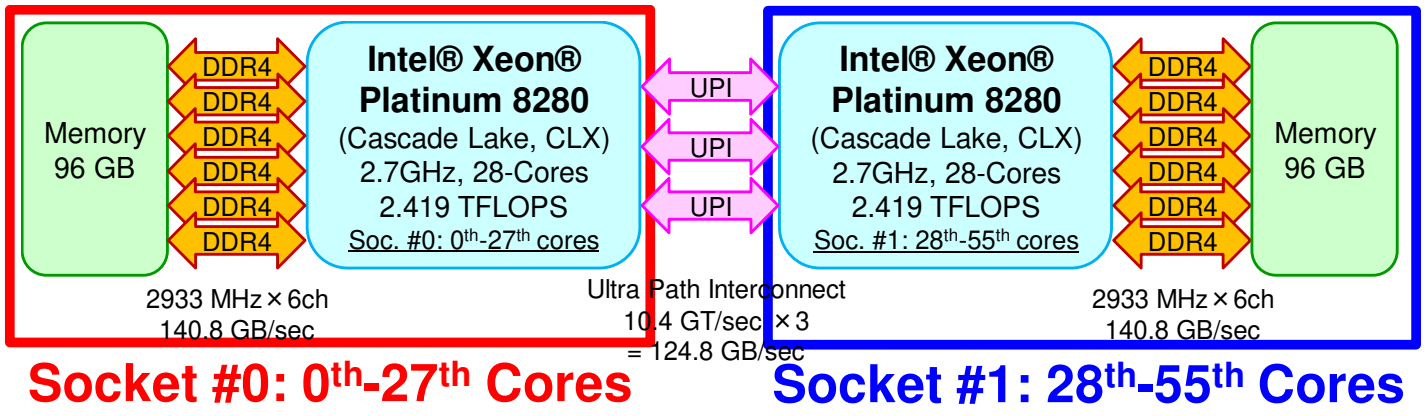


g28.sh: 8-nodes, 448-cores, 28x2x8

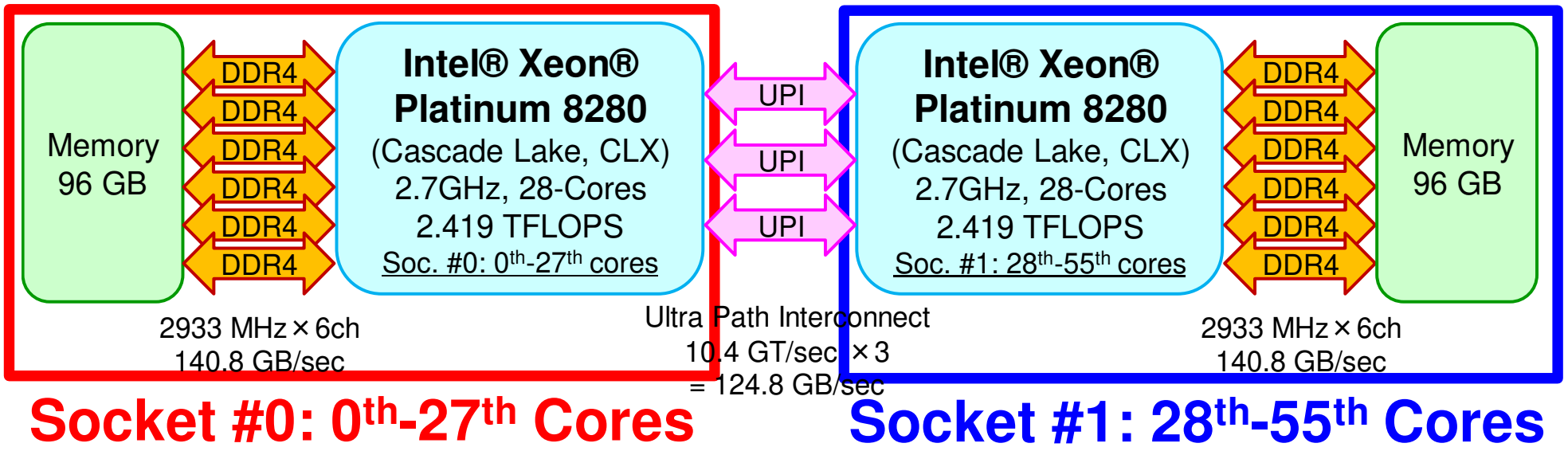
```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=8
#PJM --mpi proc=448
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o test.lst

mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
export I_MPI_PIN_PROCESSOR_LIST=0-55
mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
```

448/8= 56 cores/node

1da: -O3 + AVX512
1db: -O3 Only



NUMA Architecture



- Each Node of Oakbridge-CX (OBCX)
  - 2 Sockets (CPU's) of Intel CLX
  - Each socket has 28 cores
- Each core of a socket can access to the memory on the other socket : NUMA (Non-Uniform Memory Access)
  - `numactl -l` : local memory to be used
  - Sometimes (not always), more stable with this option

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

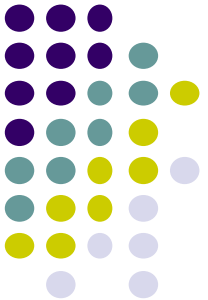
- Not so different from those of original code

- 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

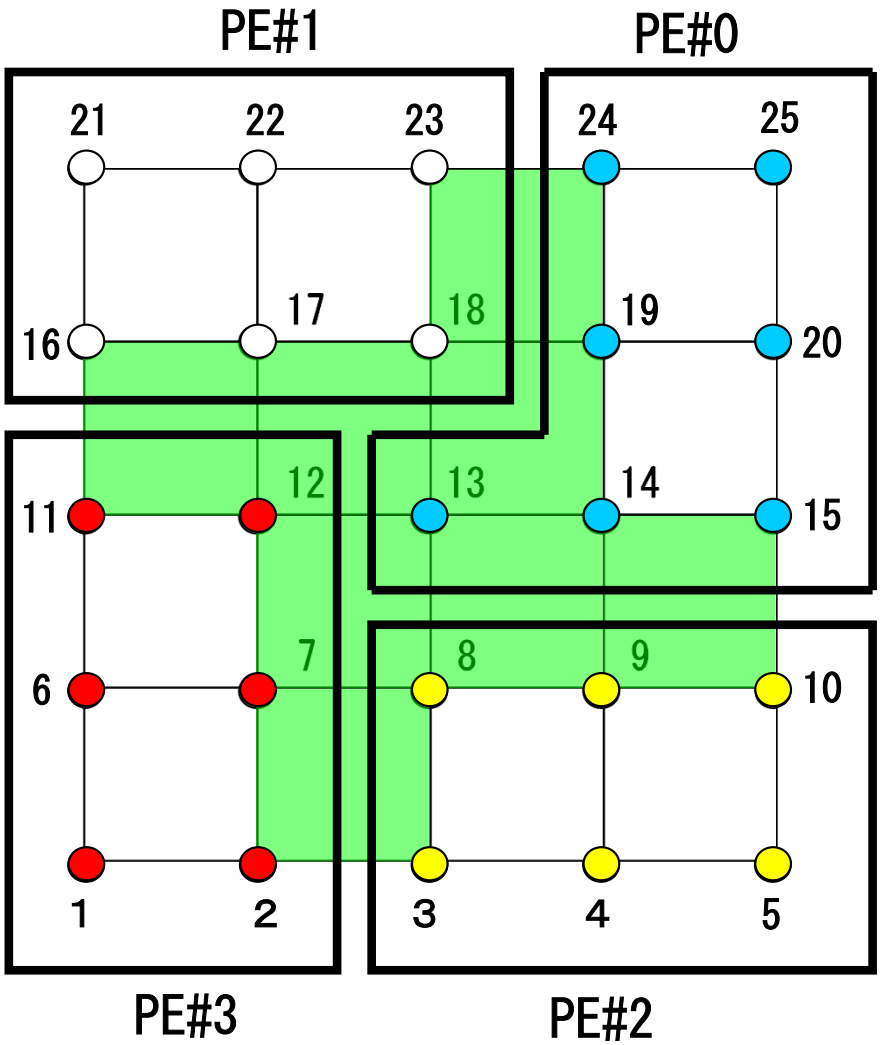


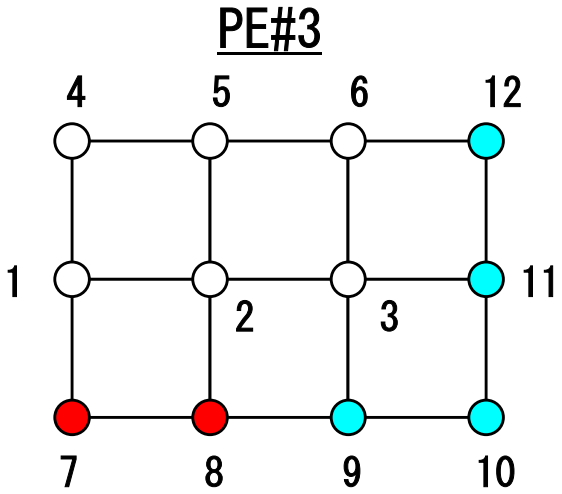
- Node-based partitioning
- Local data includes:
  - Nodes originally assigned to the domain/PE/partition
  - Elements which include above nodes
  - Nodes which are included above elements, and originally NOT-assigned to the domain/PE/partition
- 3 categories for nodes
  - Internal nodes Nodes originally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

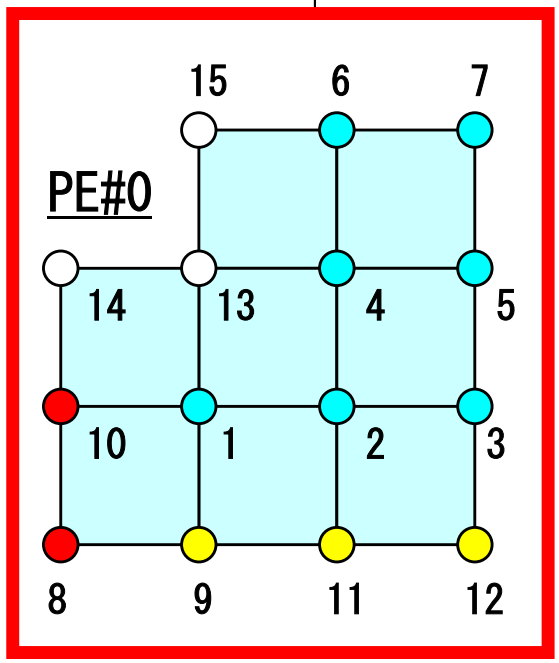
- Global info. is not needed except relationship between domains
  - Property of FEM: local element-by-element operations

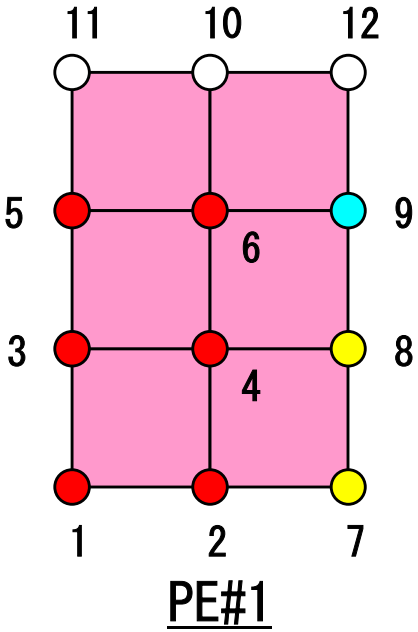
Node-based Partitioning

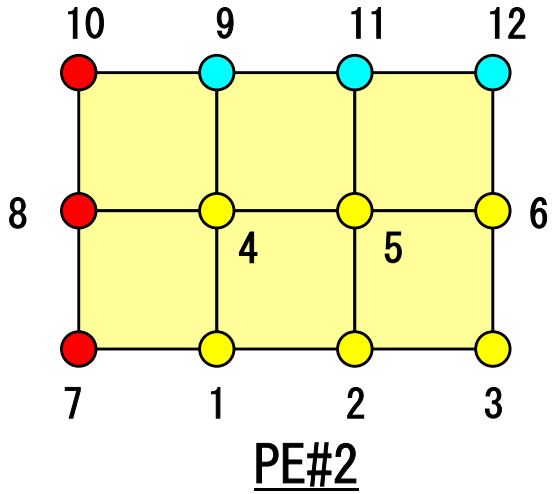
internal nodes - elements - external nodes





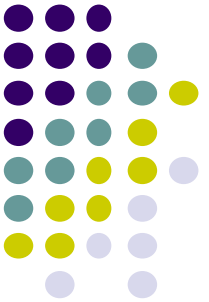




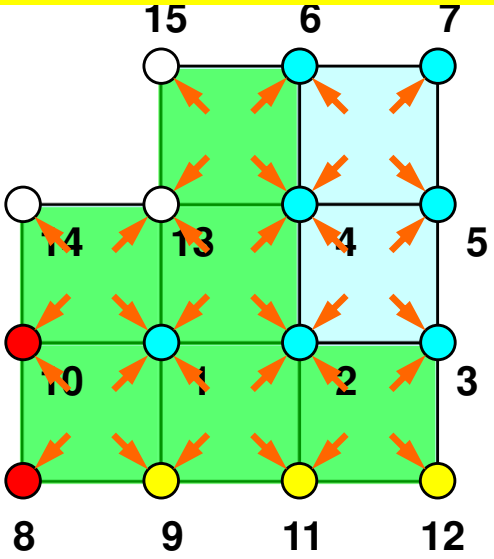


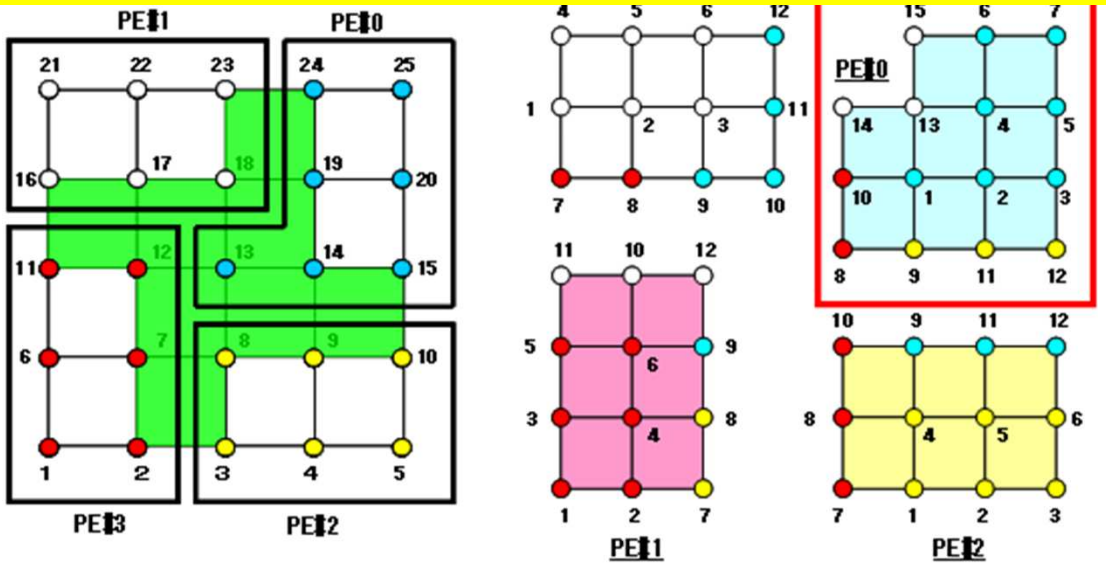
Node-based Partitioning

internal nodes - elements - external nodes

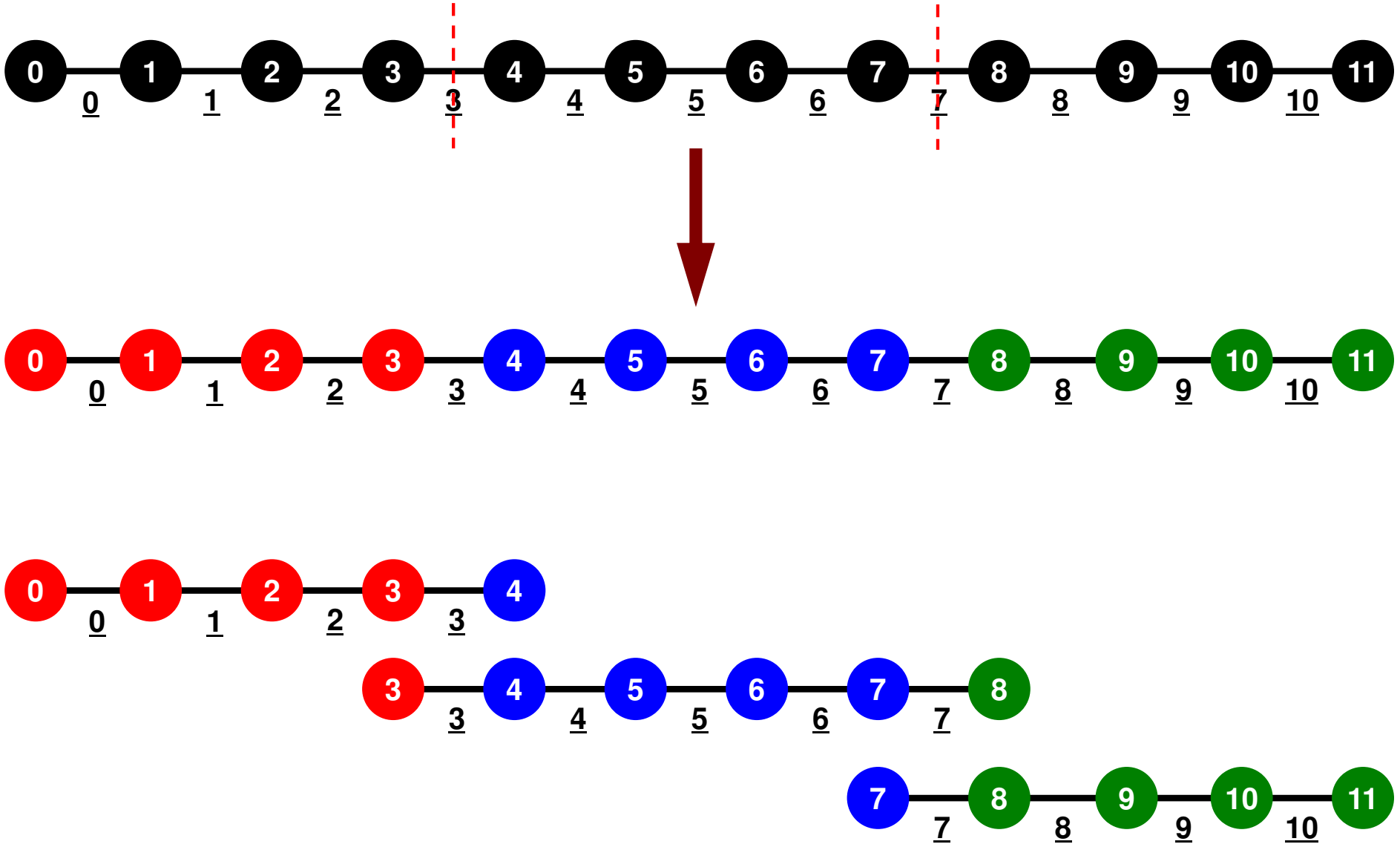


- Partitioned nodes themselves (Internal Nodes)　内点
- Elements which include Internal Nodes　内点を含む要素
- External Nodes included in the Elements　外点
  - in overlapped region among partitions.
- Info of External Nodes are required for completely local element–based operations on each processor.

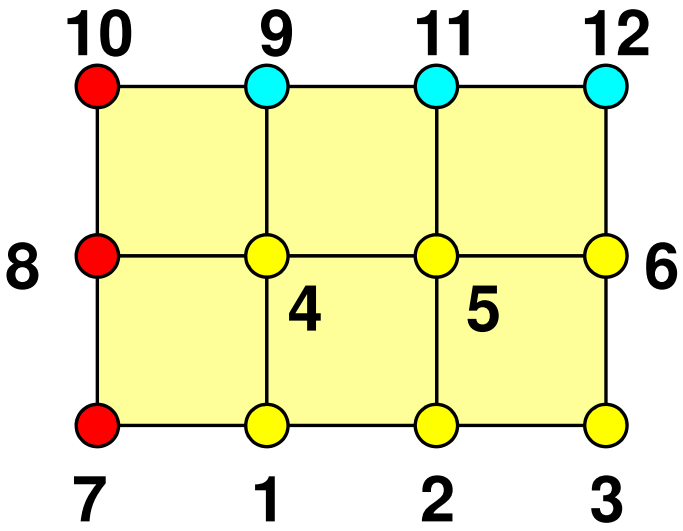




1D FEM: 12 nodes/11 elem's/3 domains



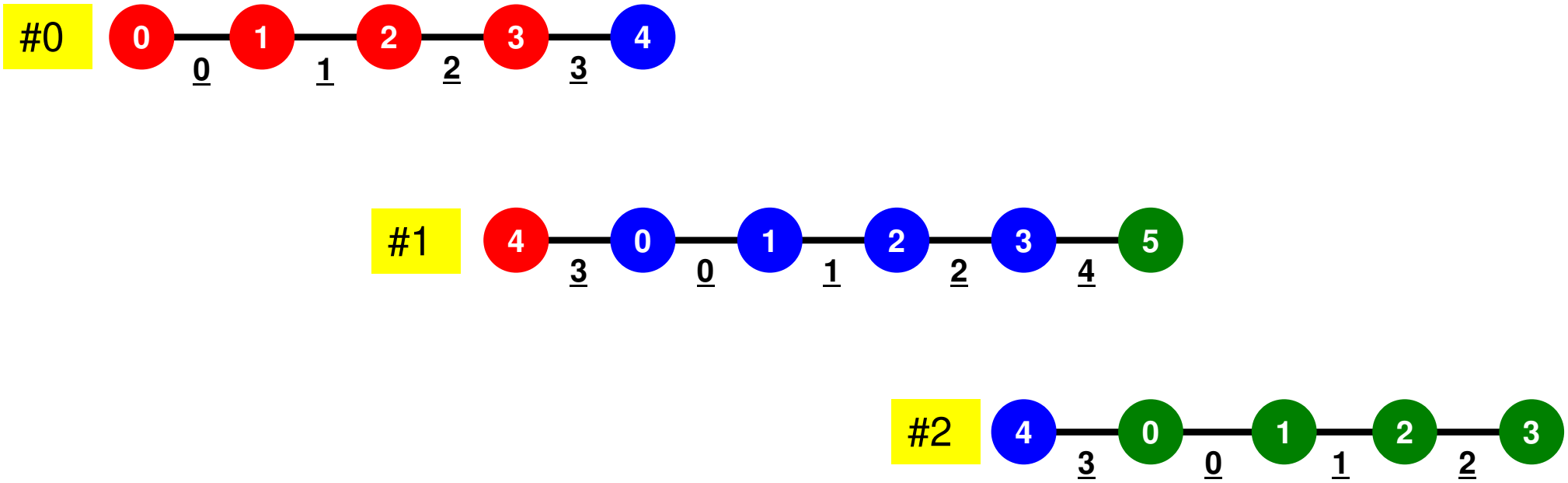
Description of Distributed Local Data



- 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

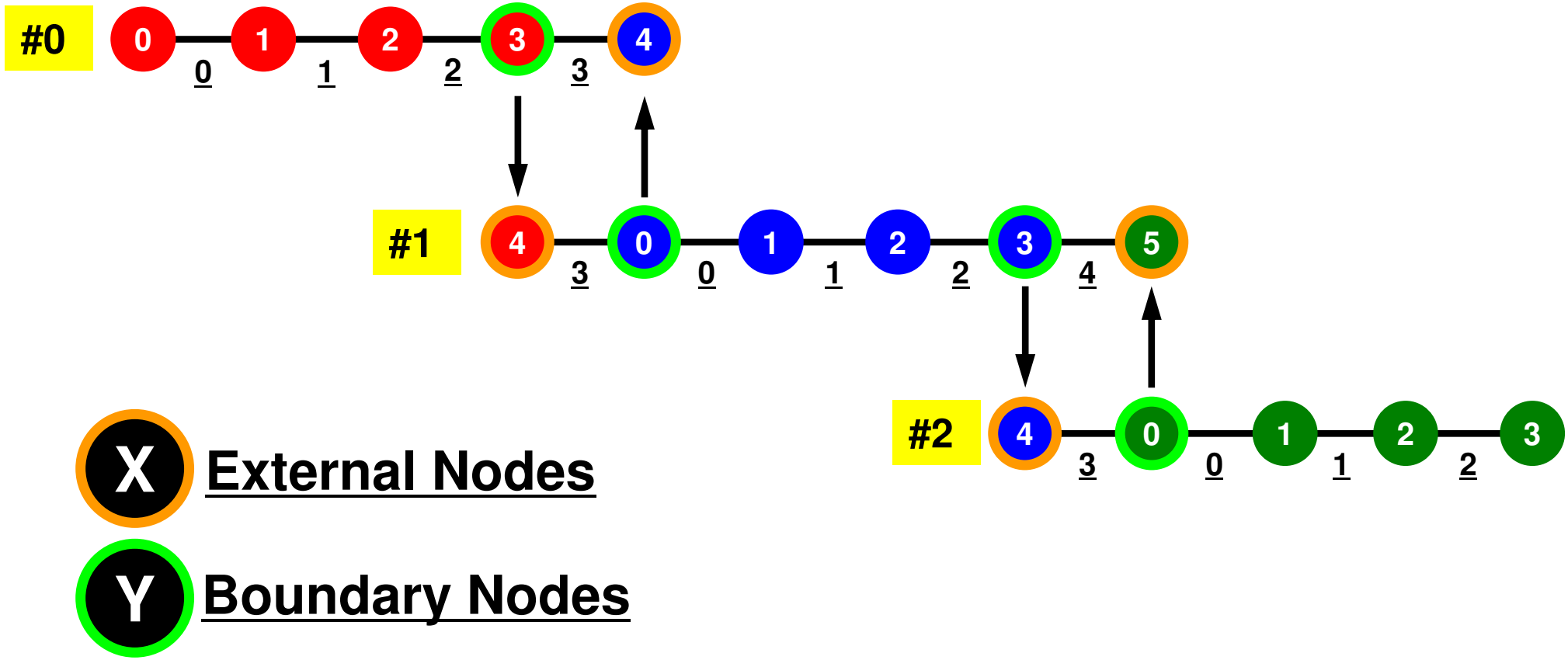
Local ID: Starting from 0 for node and elem at each domain



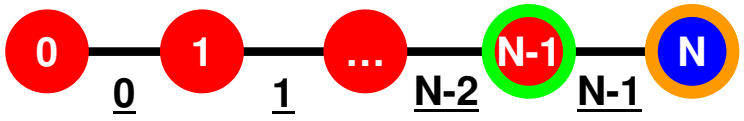
1D FEM: 12 nodes/11 elem's/3 domains

Internal/External/Boundary Nodes

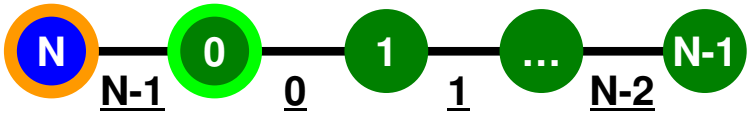
Boundary Nodes: Part of Internal Nodes, and External Nodes of Other Domains



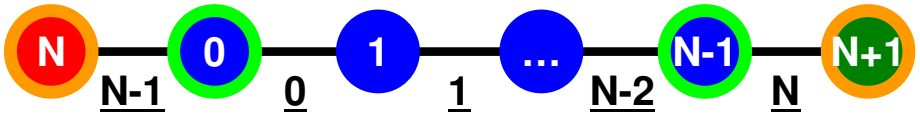
1D FEM: Numbering of Local ID



#0:
N+1 nodes
N elements



#PETot-1:
N+1 nodes
N elements

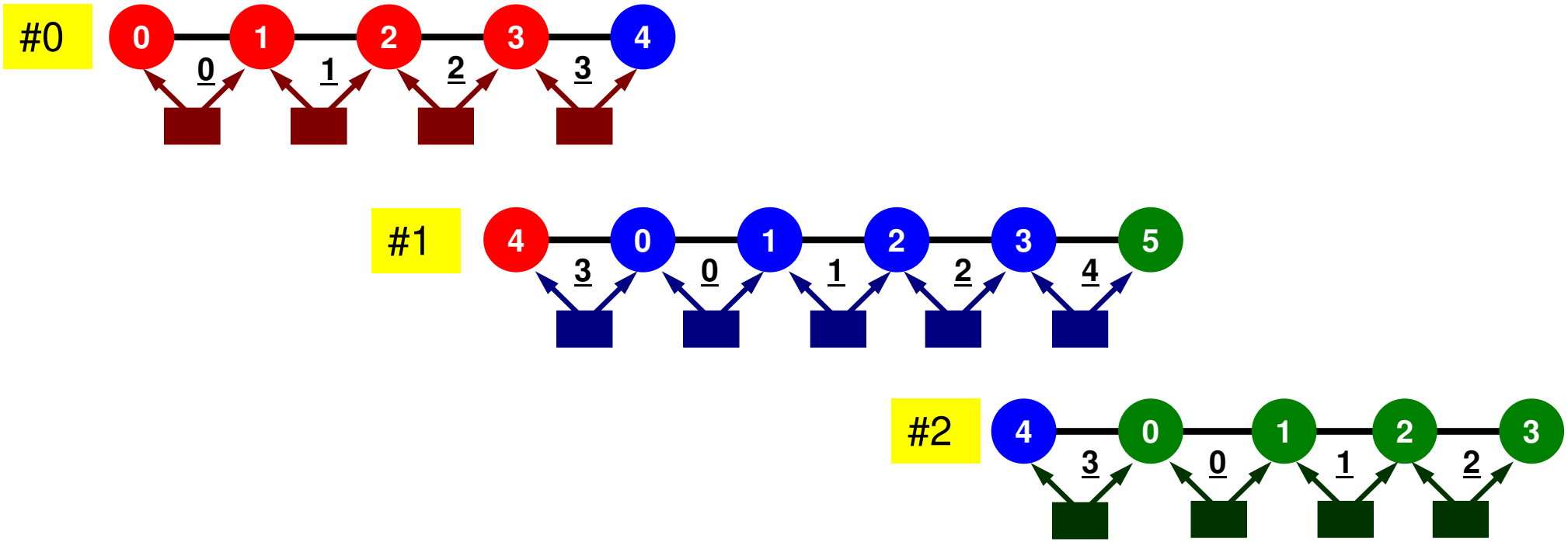


Others (General):
N+2 nodes
N+1 elements

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

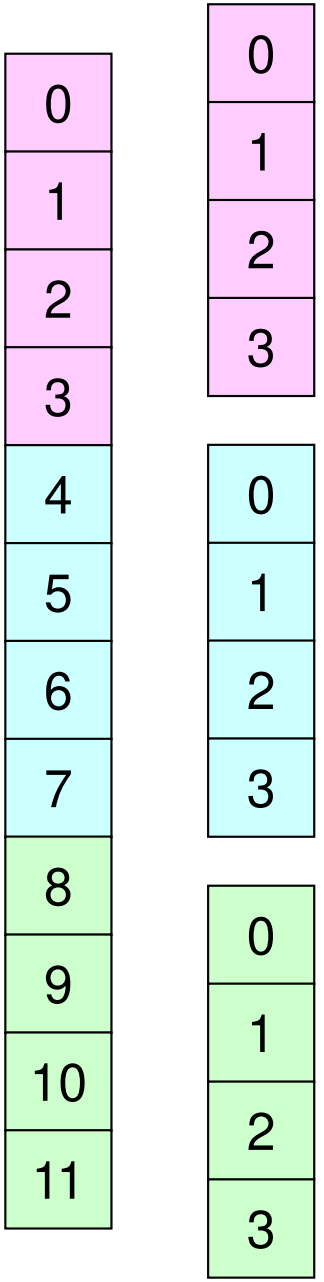
Preconditioning:
Diagonal Scaling
(or Point Jacobi)

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];
    }
```

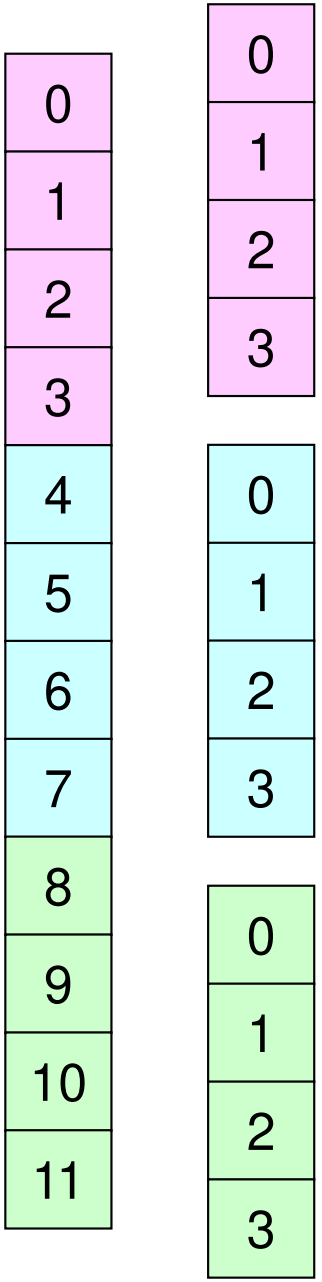
```
/*
//-- {x}= {x} + ALPHA*{p}
//   {r}= {r} - ALPHA*{q}
*/
  for(i=0;i<N;i++){
      U[i]    += Alpha * W[P][i];
      W[R][i] -= Alpha * W[Q][i];
  }
```



Dot Products

Global Summation needed: Communication ?

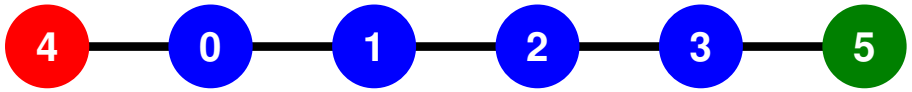
```
/*
//-- ALPHA= RHO / {p}{q}
*/
  C1 = 0.0;
  for(i=0;i<N;i++){
      C1 += W[P][i] * W[Q][i];
  }

  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]];
          }
      }
```



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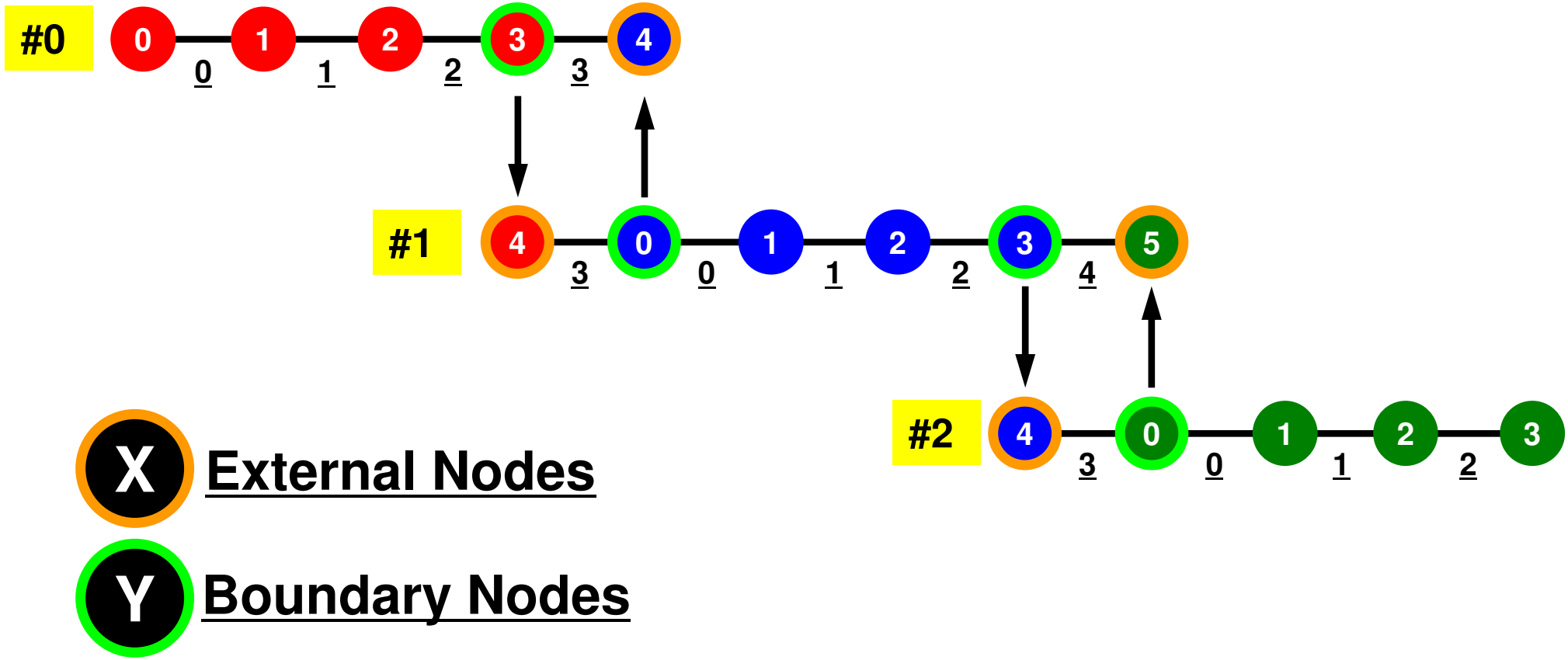
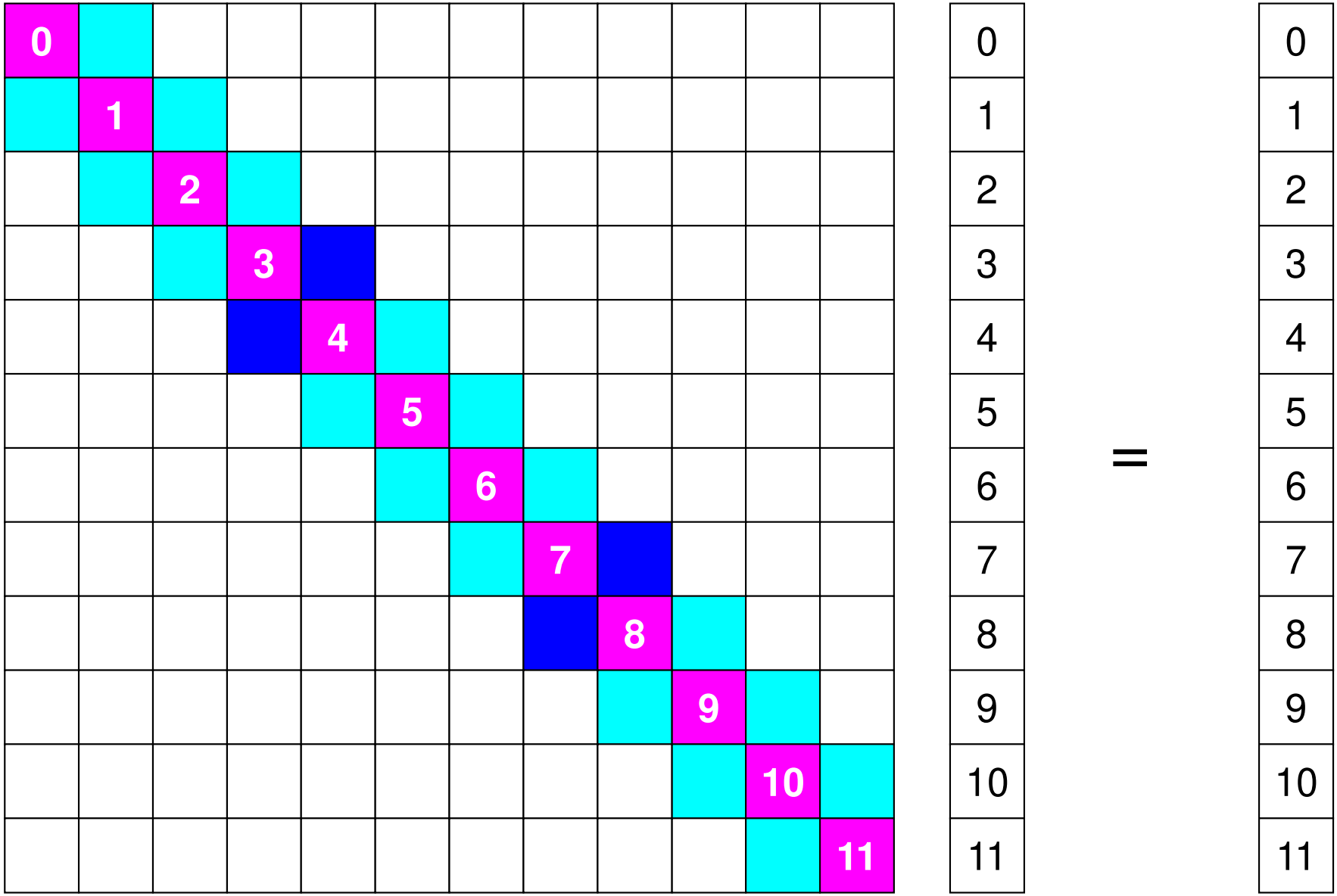
Internal/External/Boundary Nodes

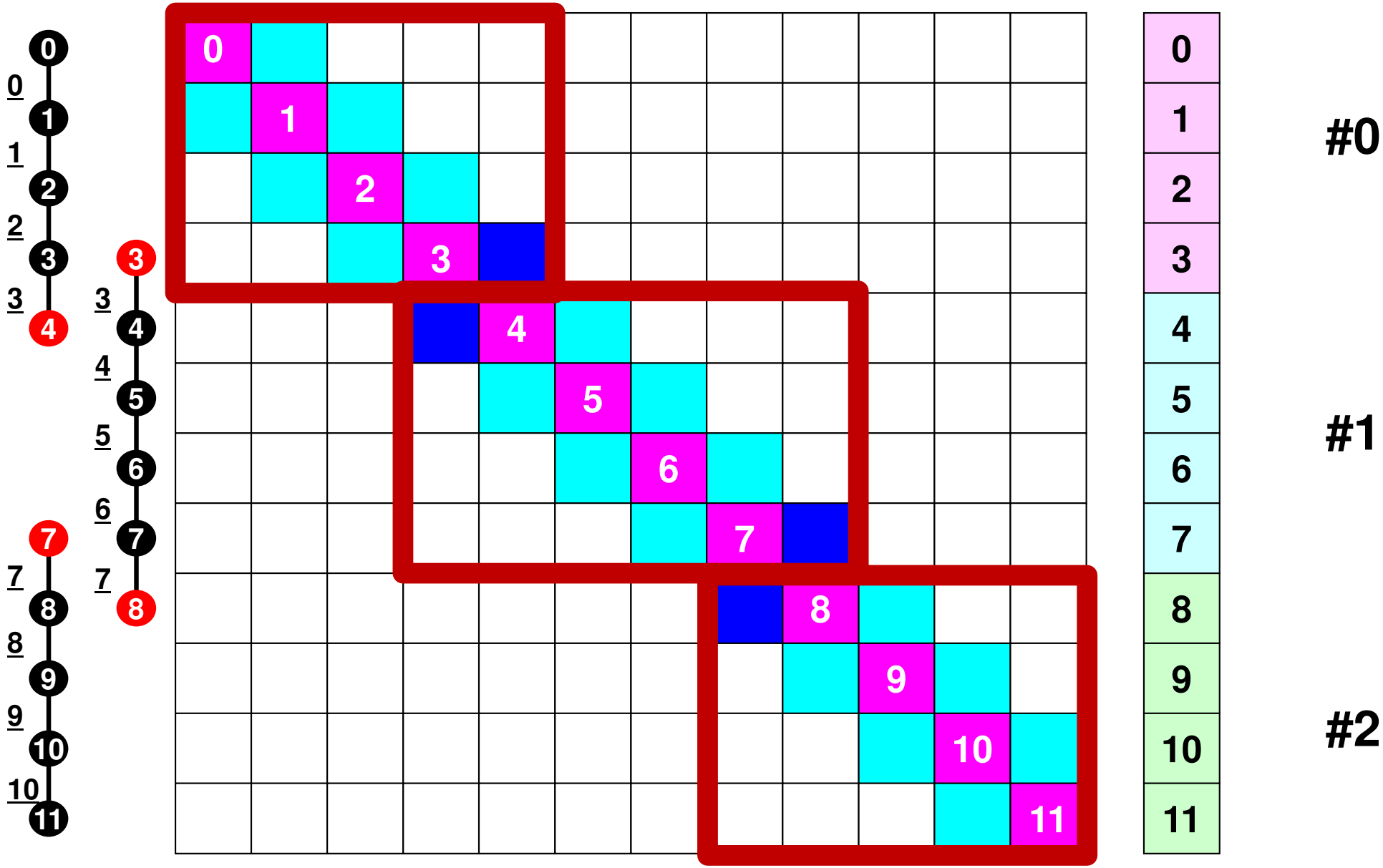
Boundary Nodes: Part of Internal Nodes, and External Nodes of Other Domains



Mat-Vec Products: Local Op. Possible



Because the matrix is sparse, the union of the local matrices forms the global matrix !



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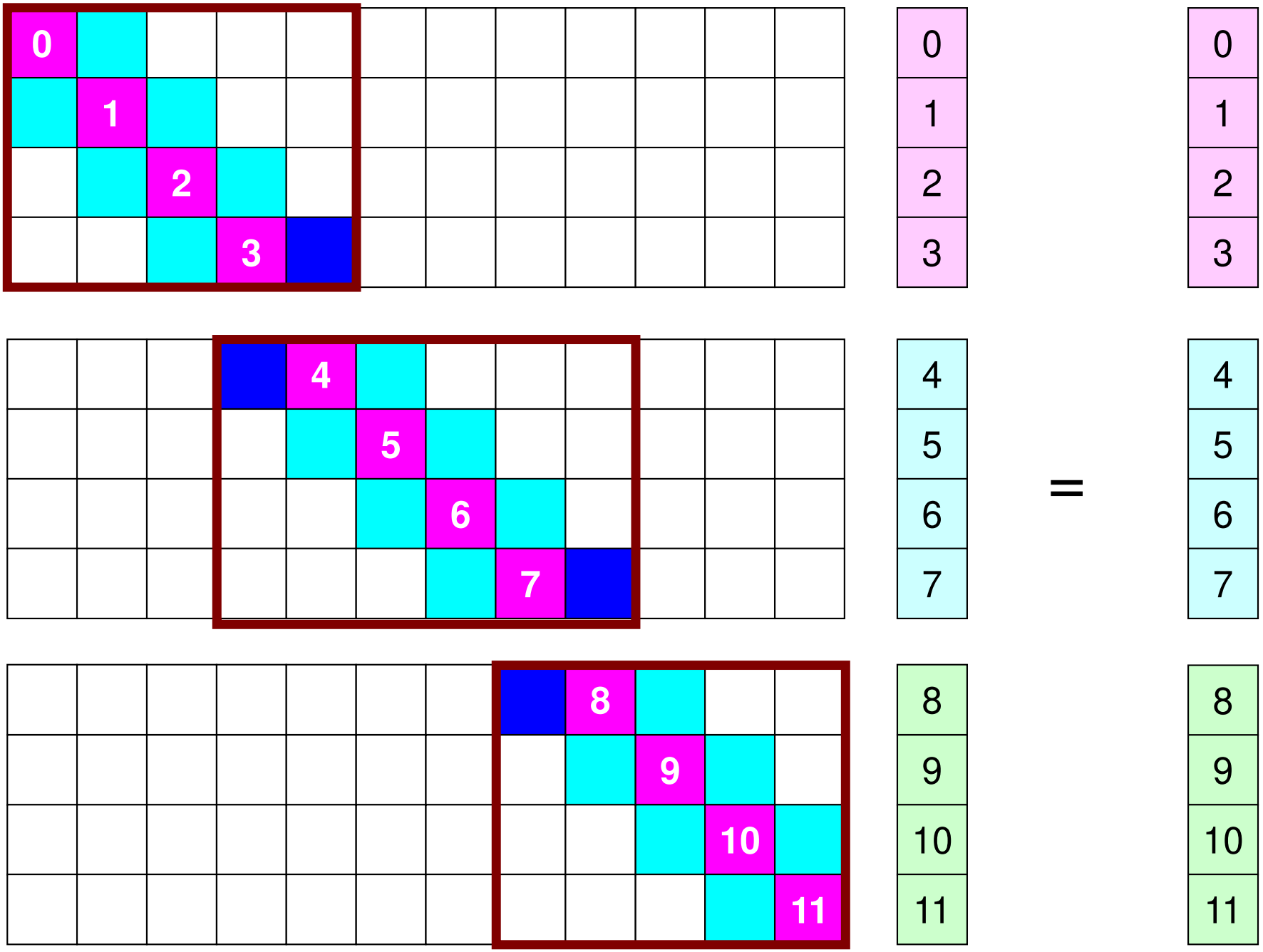

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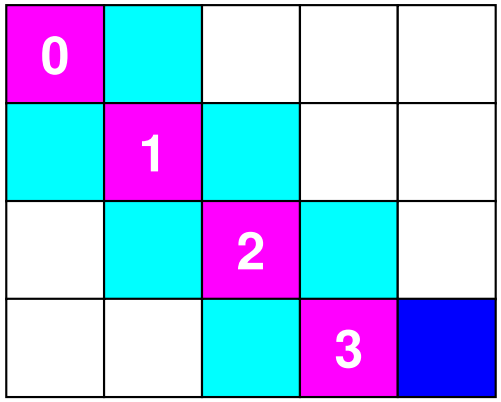
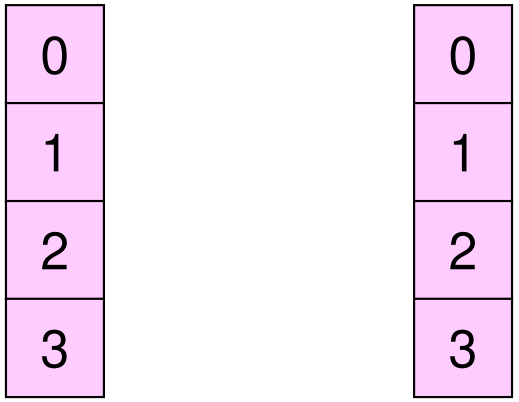
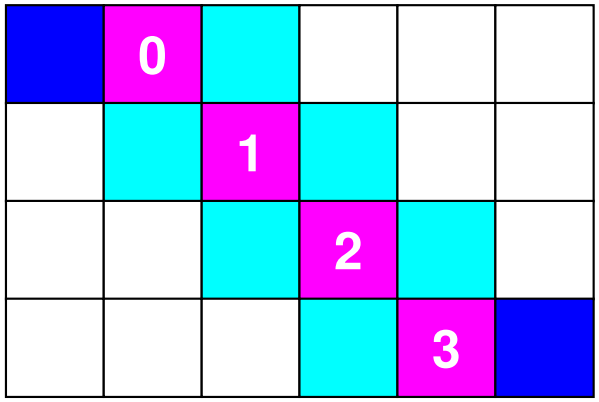
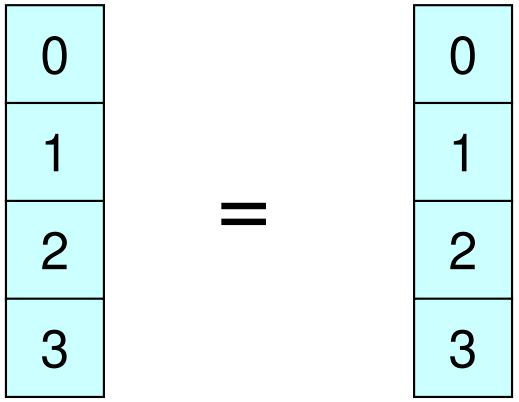
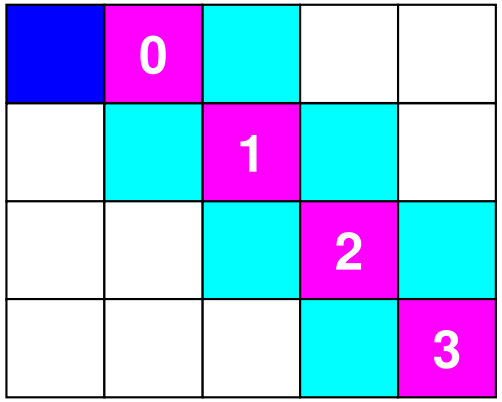
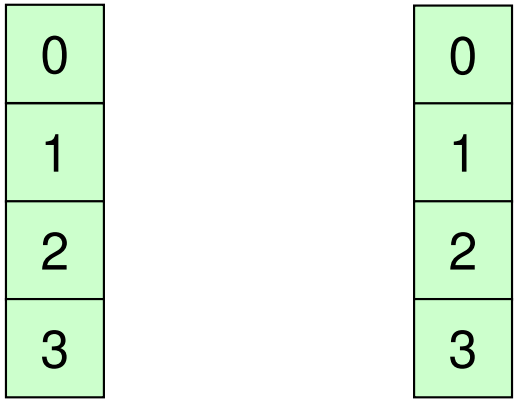




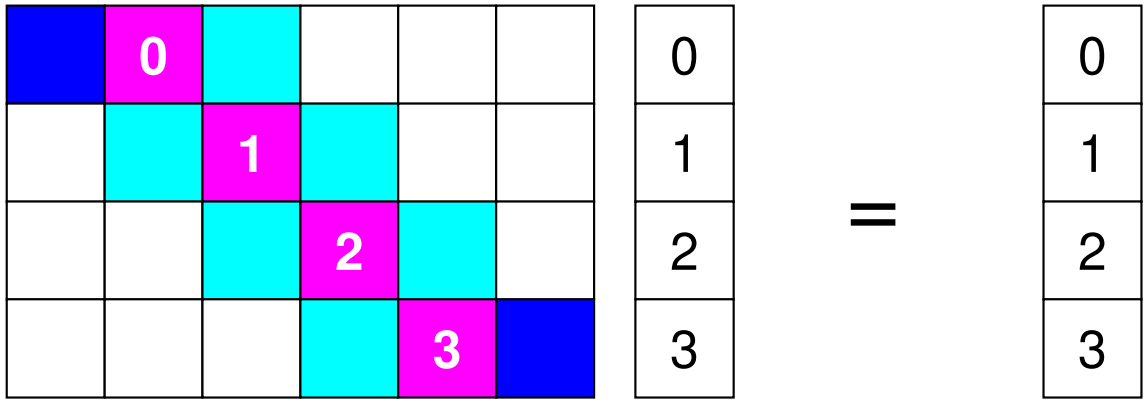


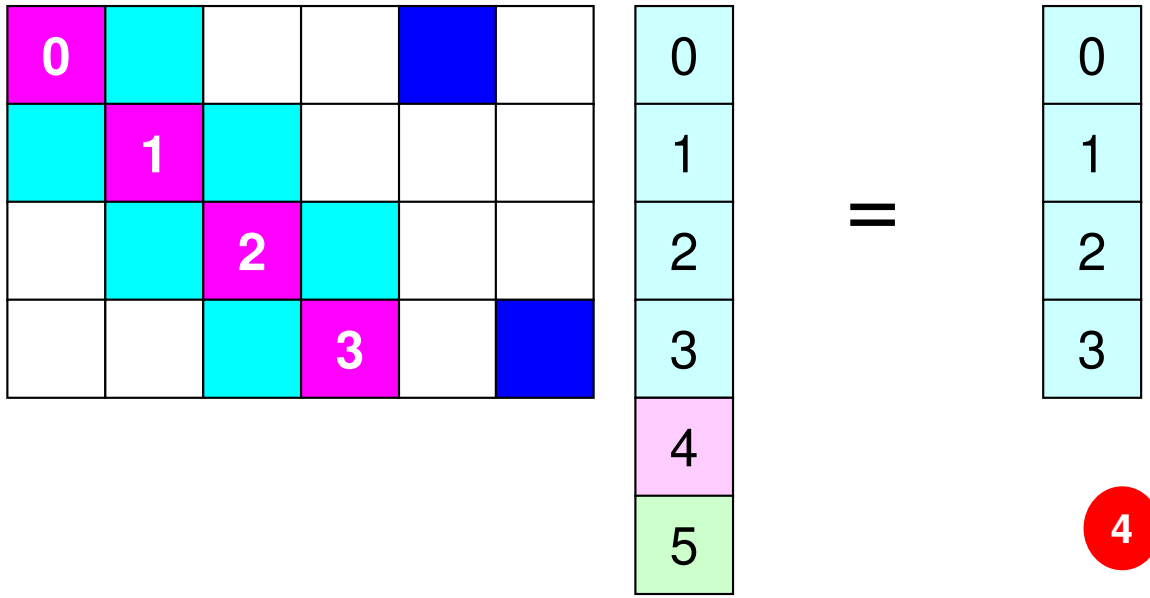


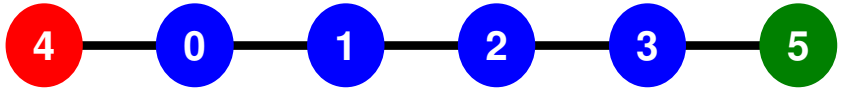




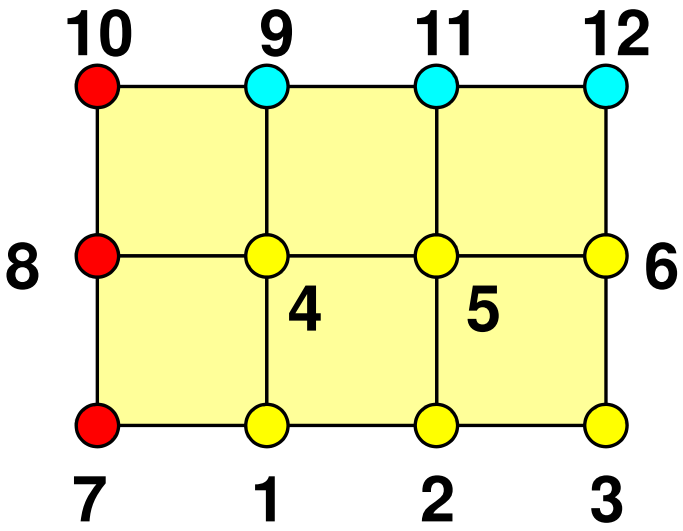
Mat-Vec Products: Local Op. #1







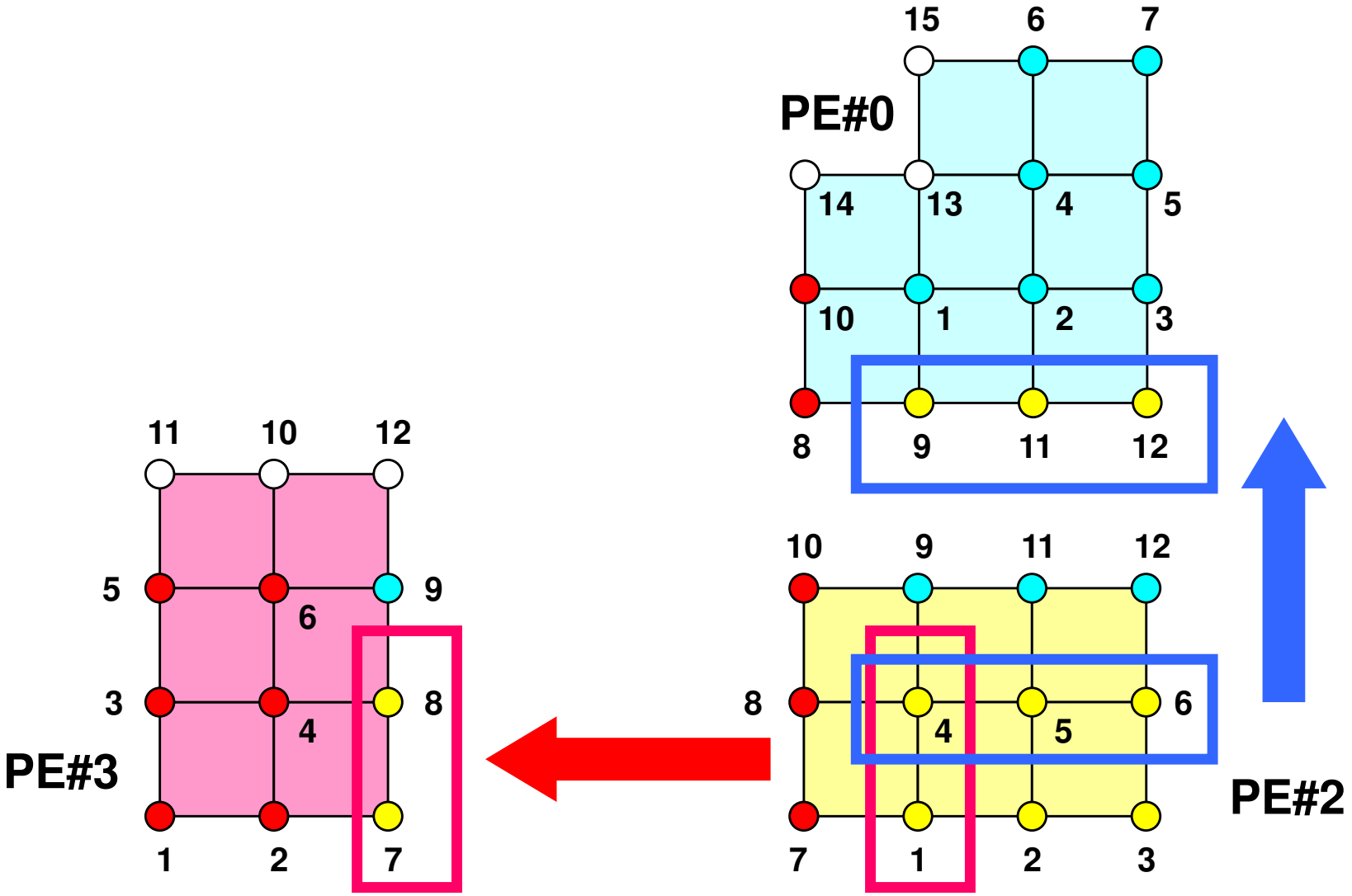
Description of Distributed Local Data



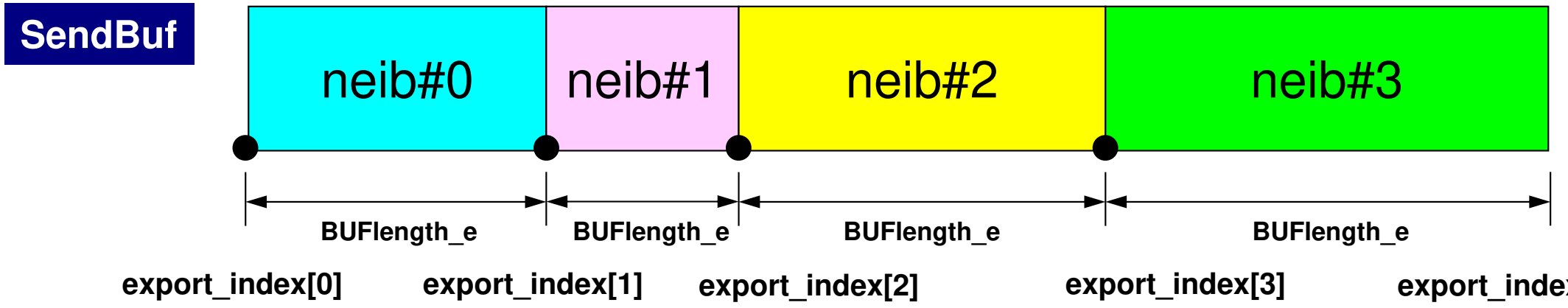
- Internal/External Points
  - Numbering: Starting from internal pts, then external pts after that
- Neighbors
  - Shares overlapped meshes
  - Number and ID of neighbors
- External Points
  - From where, how many, and which external points are received/imported ?
- Boundary Points
  - To where, how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



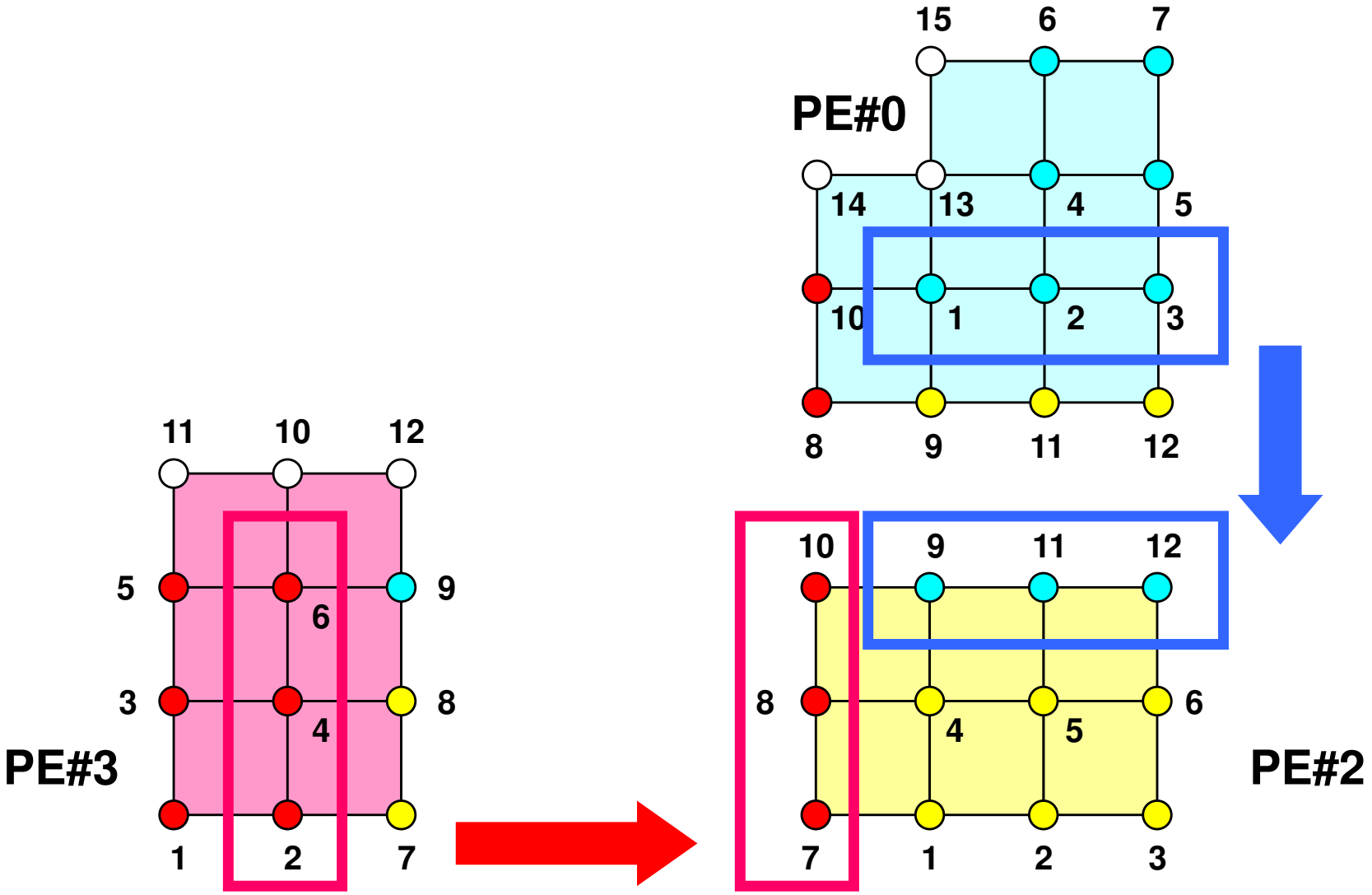
export_item (export_index[neib]:export_index[neib+1]-1) are sent to neib-th neighbor

```
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”

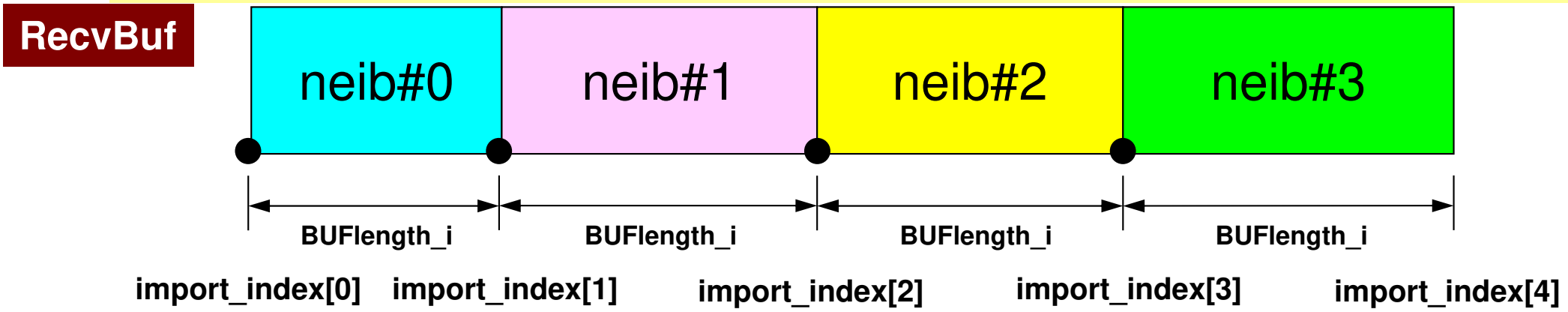


RECV: MPI_Isend/Irecv/Waitall

```
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);
```

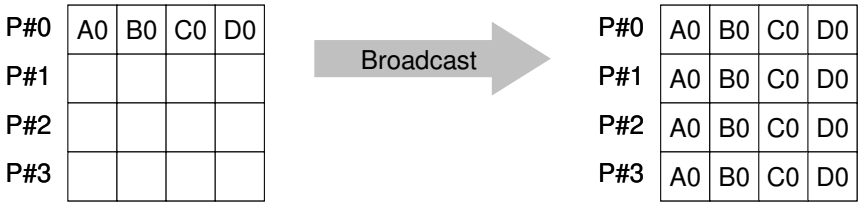
Program: 1d.c (2/11)
Control Data

```
/*
// +-------+
// | 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.

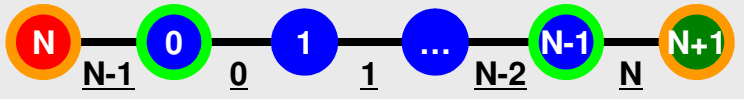
    C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc.
  - **`root`** int I rank of root process
  - **`comm`** MPI_Comm I communicator

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

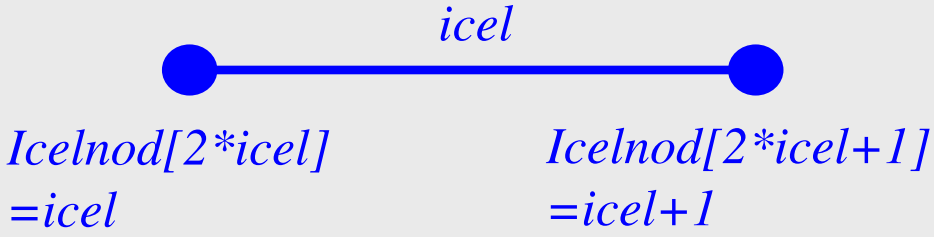
Program: 1d.c (3/11)
Distributed Local Mesh, Uniform Elements

```
/*
//-- 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));
    IceInod= 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)

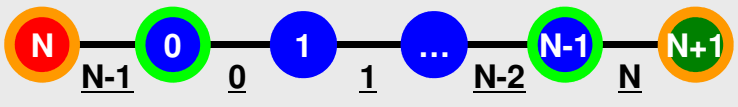
Initialization of Arrays, Elements-Nodes

```
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

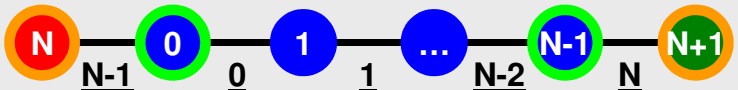
Program: 1d.c (5/11)

"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

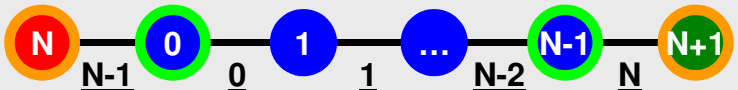
Program: 1d.c (6/11)

”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



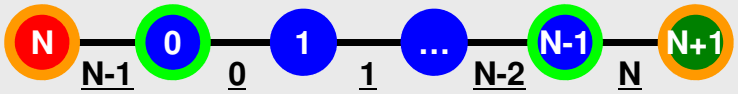
Others (General):
N+2 nodes
N+1 elements

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

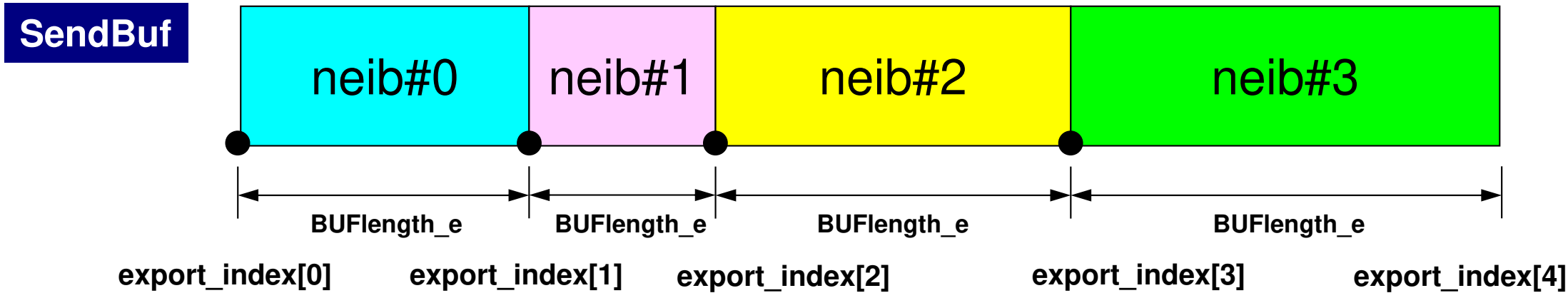
- **MPI_Waitall** blocks until all comm's, associated with **request** in the array, complete. It is used for synchronizing **MPI_Isend** and **MPI_Irecv** in this class.
- At sending phase, contents of sending buffer cannot be modified before calling corresponding **MPI_Waitall**. At receiving phase, 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[NeibPETot]
- Message size for each neighbor
  - export_index[NeibPETot+1]
- ID of **boundary** points
  - export_item[export_index[NeibPETot]]
- Messages to each neighbor
  - SendBuf[export_index[NeibPETot]]

SEND: MPI_Isend/Irecv/Waitall

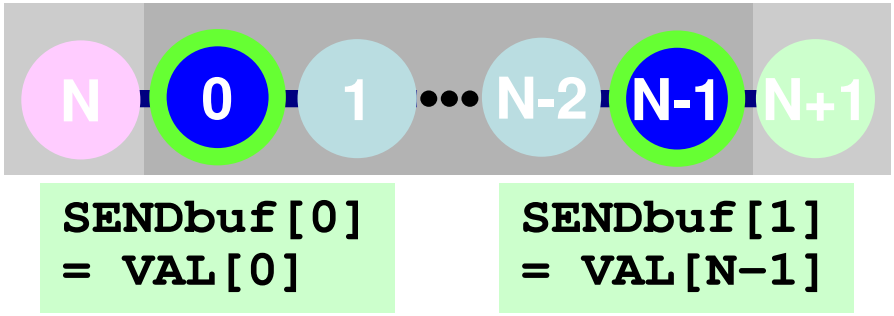


export_item (export_index[neib]:export_index[neib+1]-1) are sent to neib-th neighbor

```
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

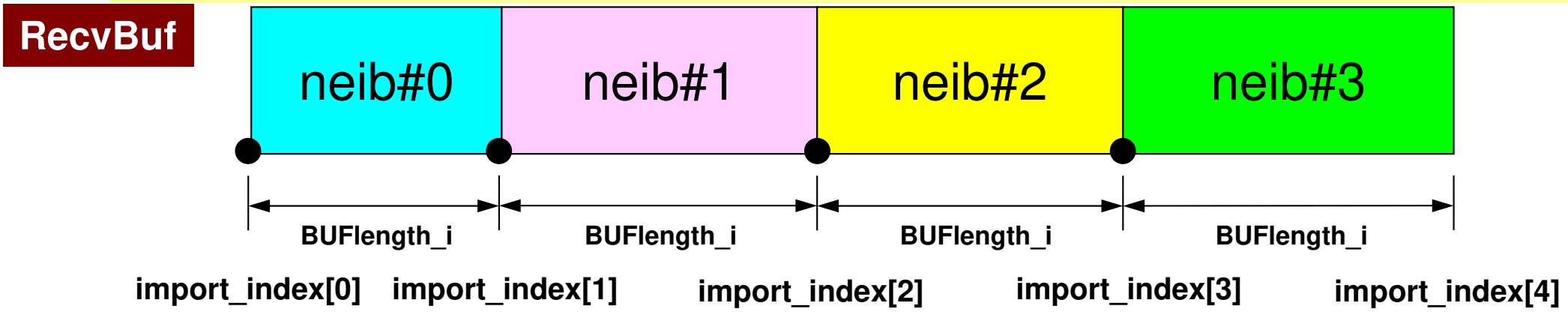
- Neighbors
  - NeibPETot, NeibPE[NeibPETot]
- Message size for each neighbor
  - import_index [NeibPETot+1]
- ID of **external** points
  - import_item [import_index[NeibPETot]]
- Messages from each neighbor
  - import_item [import_index[NeibPETot]]

RECV: MPI_Isend/Irecv/Waitall

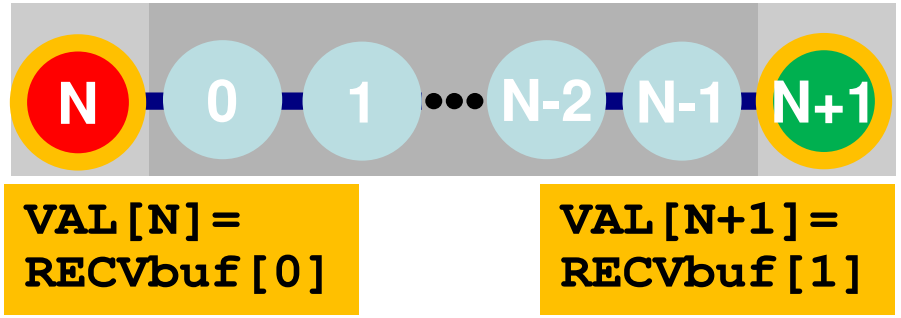
```
for (neib=0; neib<NeibPETot; neib++){
   tag= 0;
   iS_i= import_index[neib];
   iE_i= import_index[neib+1];
   BUFlength_i= iE_i - iS_i

   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

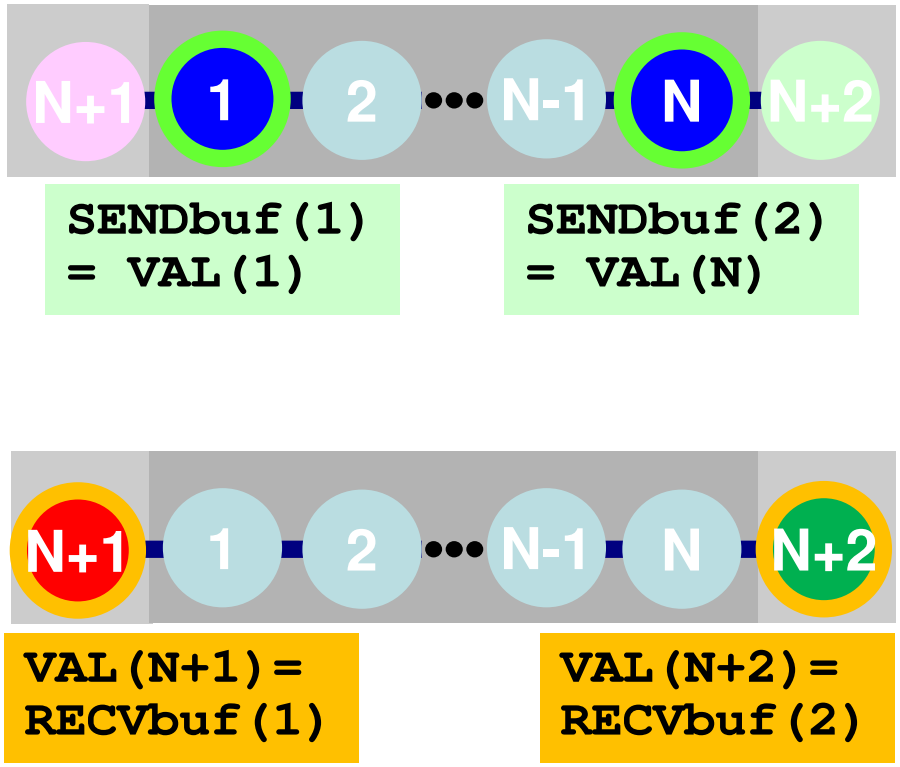


RECV/Import: 1D Problem



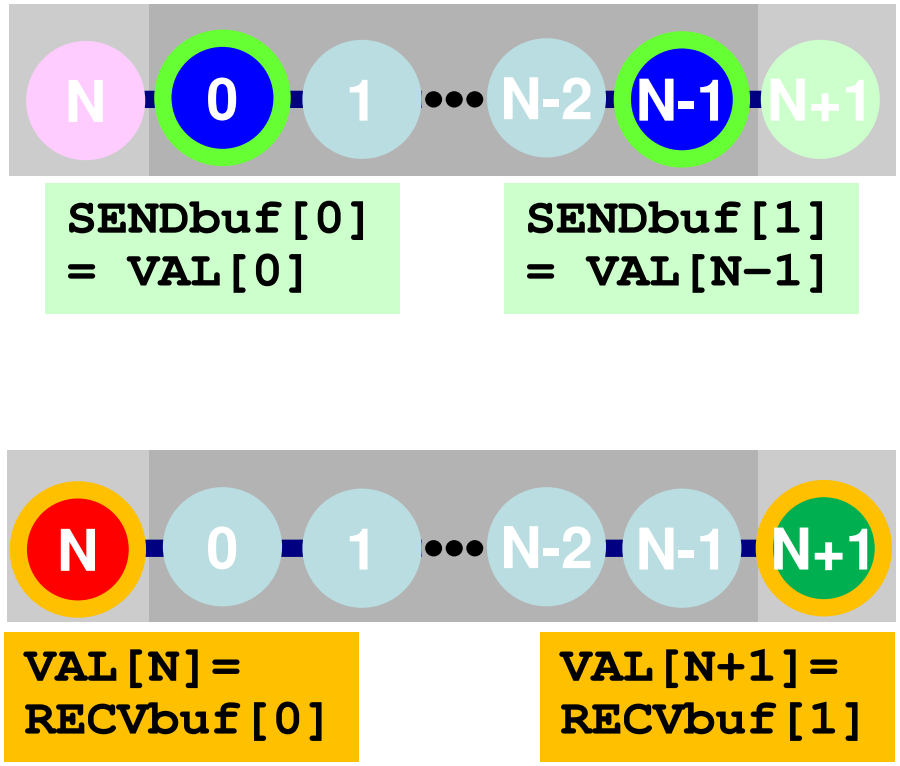
- Neighbors
  - NeibPETot, NeibPE[NeibPETot]
    - NeibPETot=2, NeibPE[0]= my_rank-1, NeibPE[1]= my_rank+1
- Message size for each neighbor
  - import_index [NeibPETot+1]
    - import_index[0]=0, import_index[1]= 1, import_index[2]= 2
- ID of **external** points
  - import_item [import_index[NeibPETot+1]]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

Generalized Comm. Table: Fortran




```
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

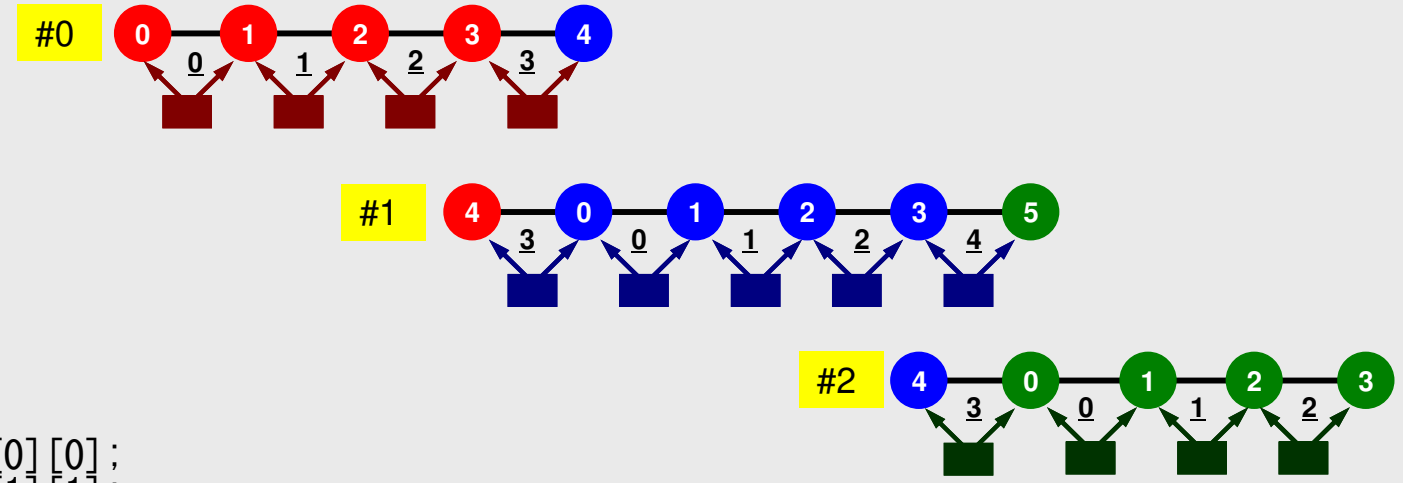



```
NEIBPETOT= 2
NEIBPE[0]= my_rank - 1
NEIBPE[1]= my_rank + 1

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

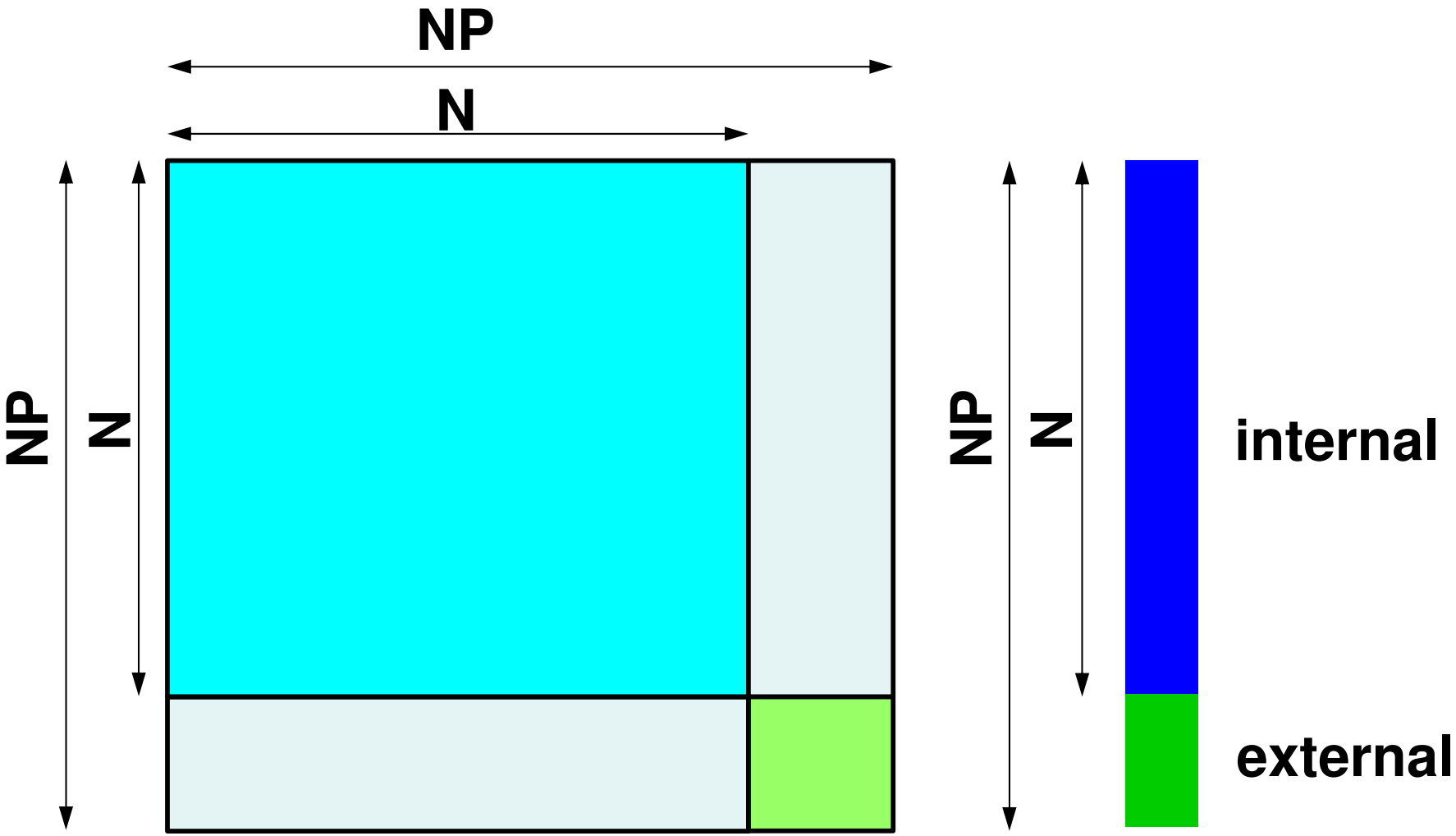
Program: 1d.c (8/11)

Matrix Assembling, NO changes from 1-CPU code

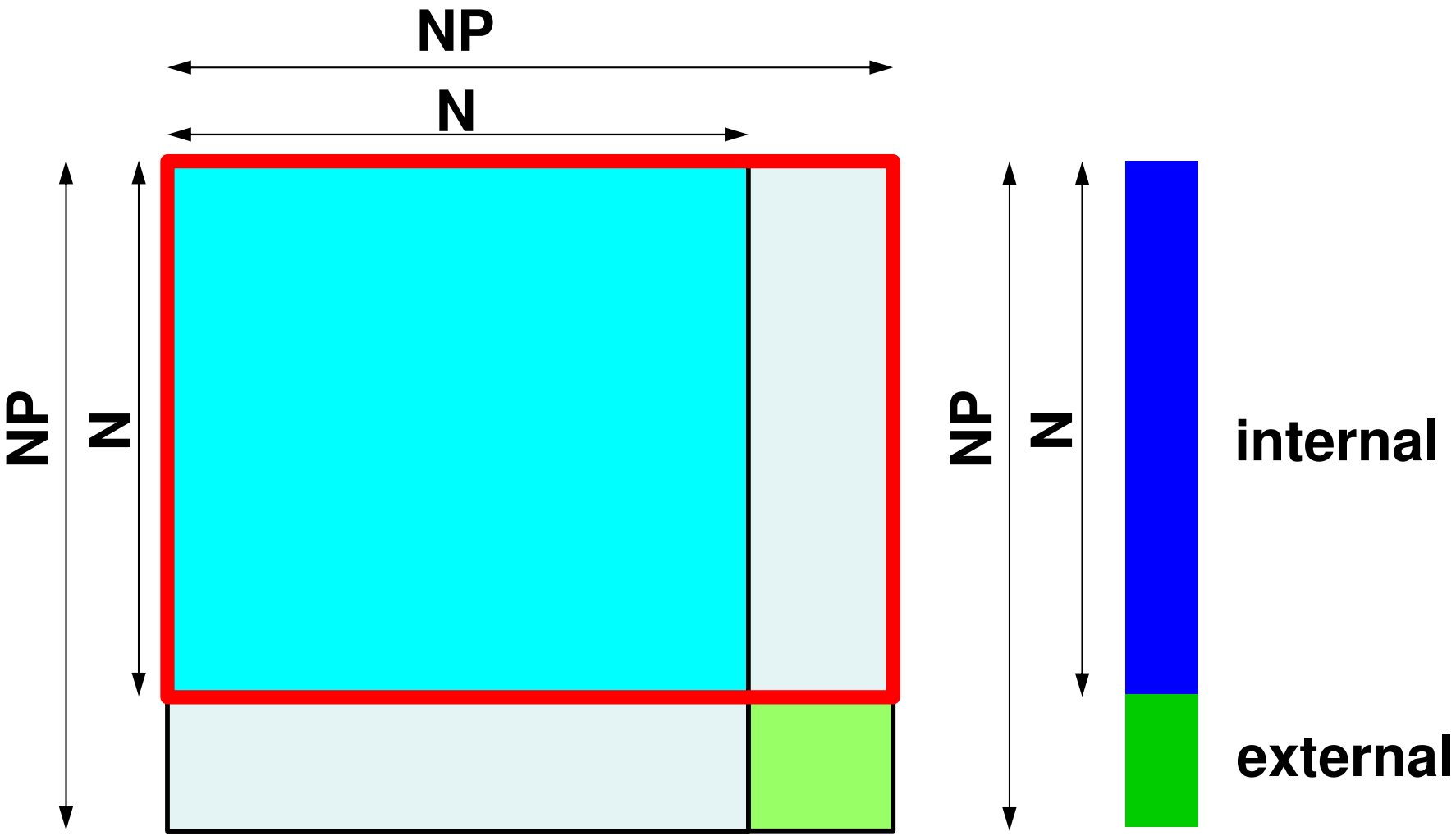
```
/*
// +-----------------+
// | MATRIX assemble |
// +-----------------+
*/
    for(icel=0;icel<NE;icel++){
      in1= Icelnod[2*icel];
      in2= Icelnod[2*icel+1];
      DL = dX;

      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



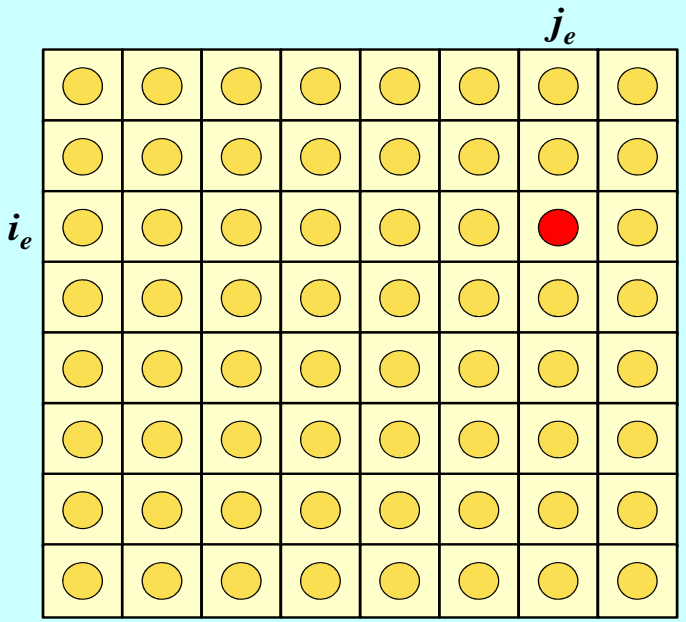
We really need these parts:



MAT_ASS_MAIN: Overview

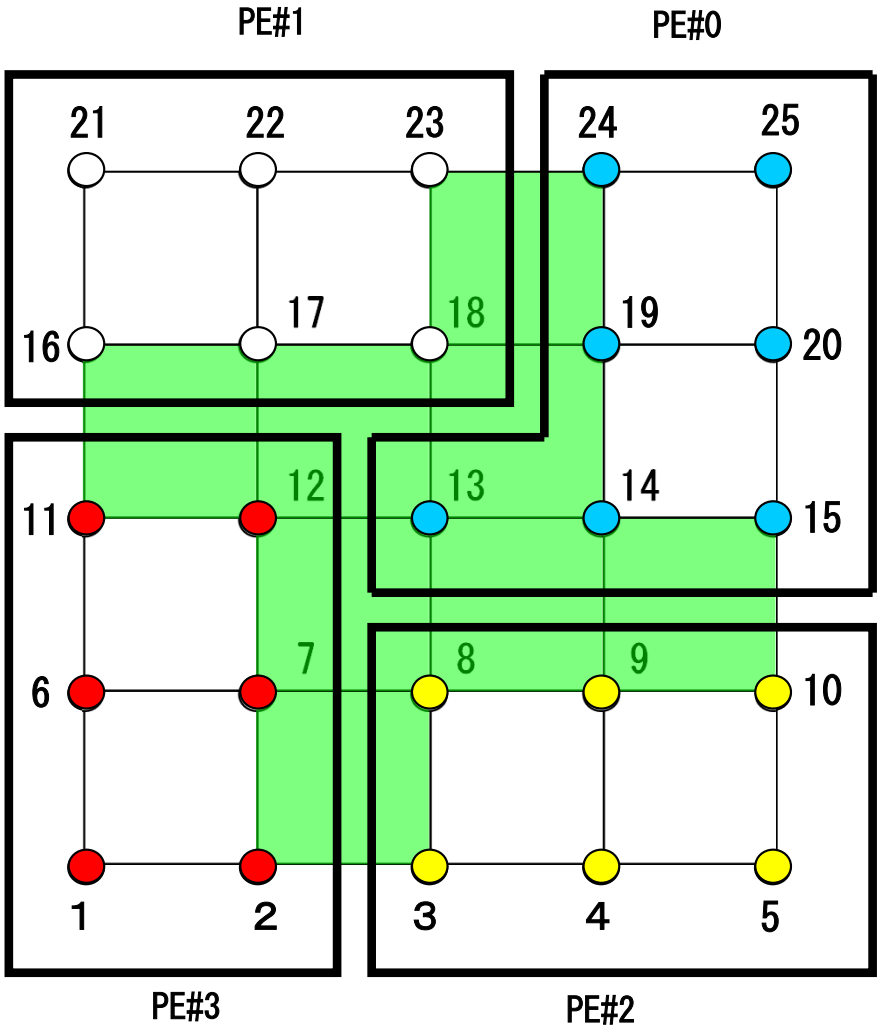
```
do kpn= 1, 2          Gaussian Quad. points in ζ-direction
  do jpn= 1, 2        Gaussian Quad. points in η-direction
    do ipn= 1, 2      Gaussian Quad. Pointe in ξ-direction
      Define Shape Function at Gaussian Quad. Points (8-points)
      Its derivative on natural/local coordinate is also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

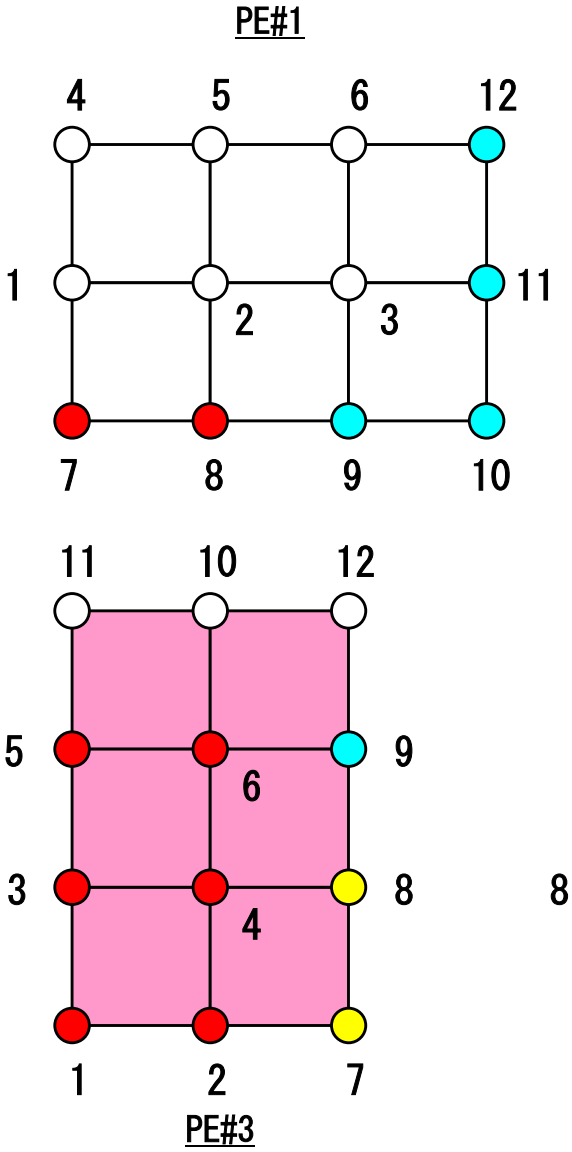
```
do icel= 1, ICELTOT    Loop for Element
  Jacobian and derivative on global coordinate of shape functions at
  Gaussian Quad. Points are defined according to coordinates of 8 nodes. (JACOBI)

  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
```



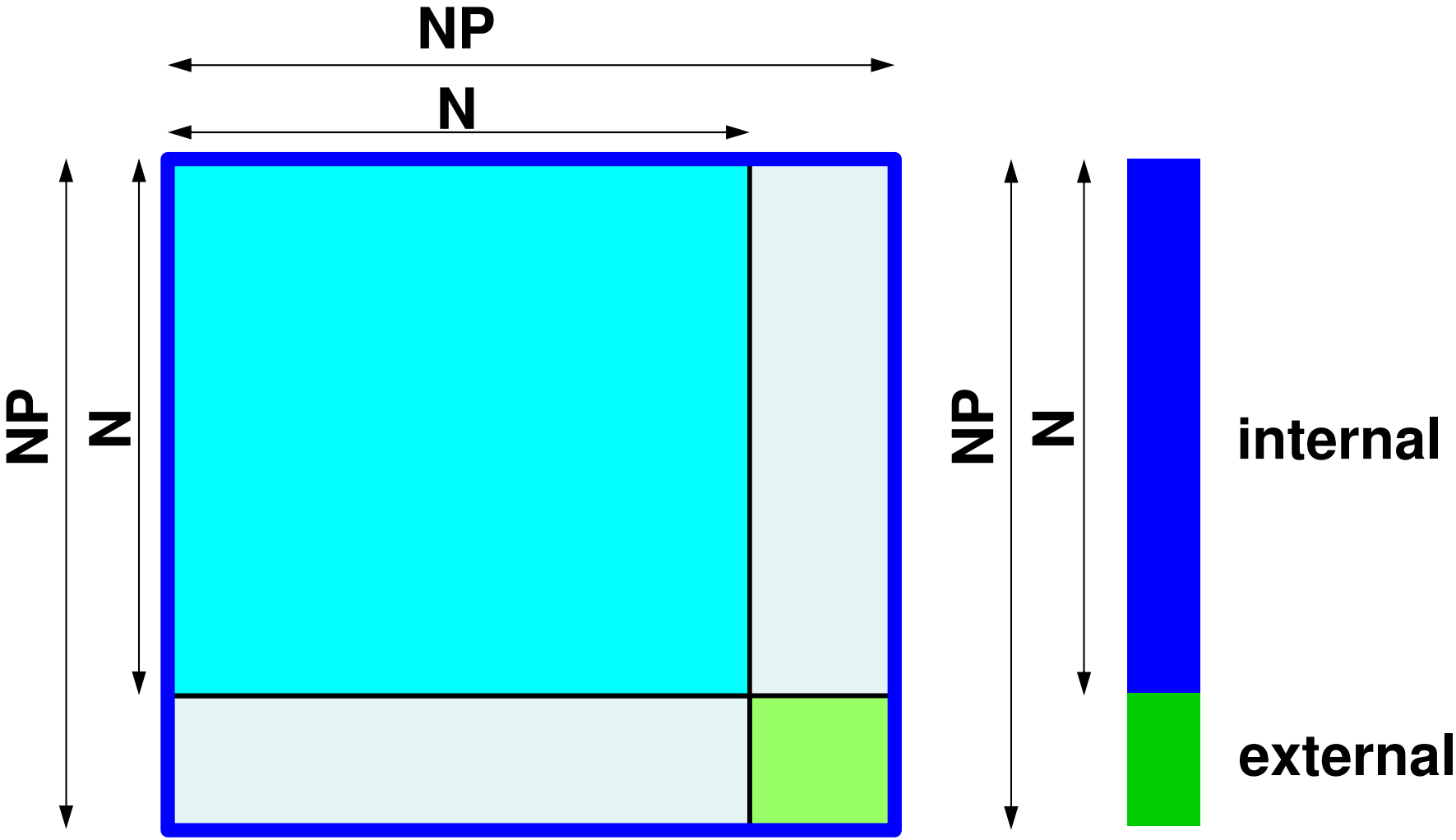
MAT_ASS_MAIN visits all elements

including overlapped elements with external nodes

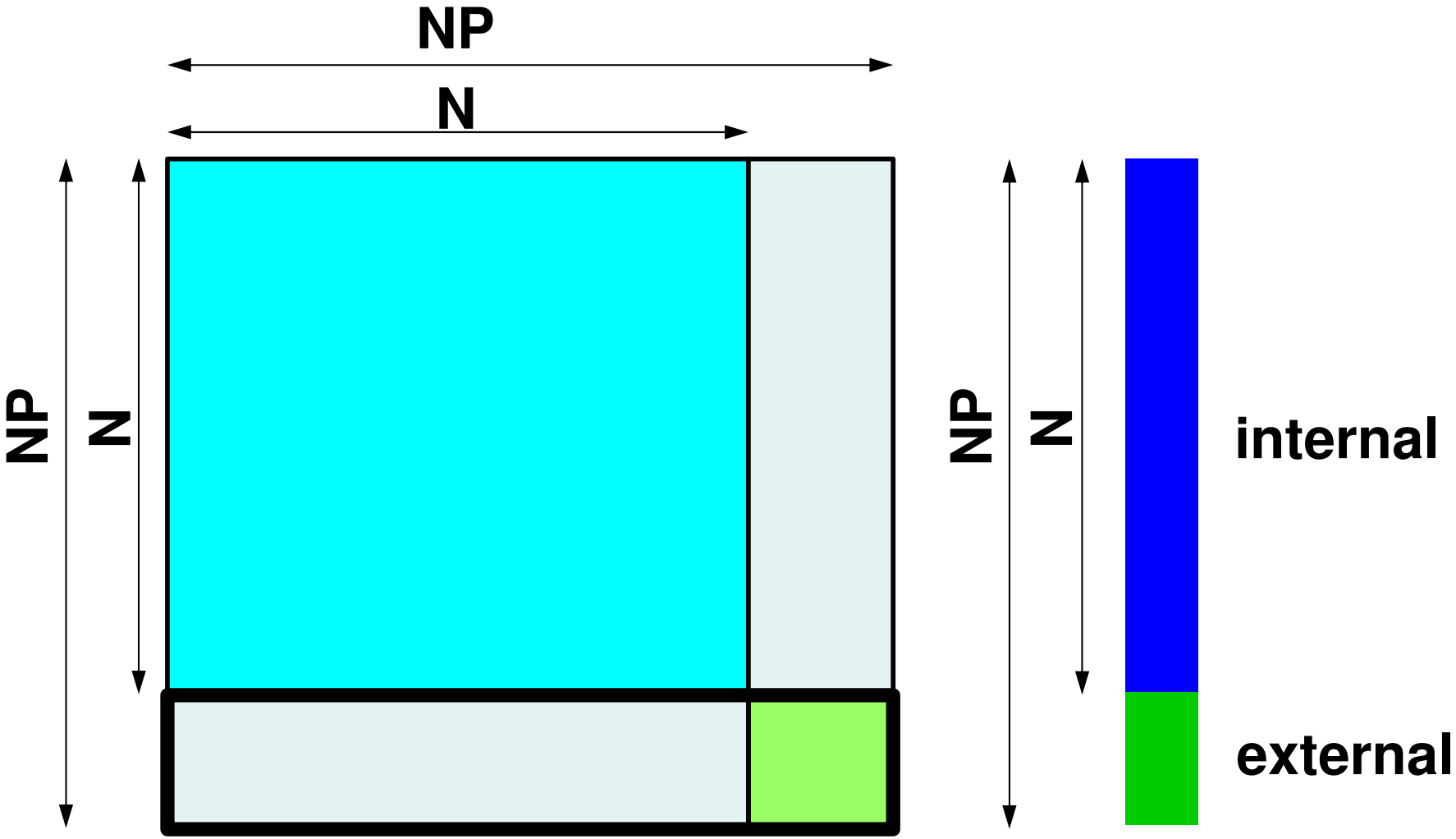




Therefore, we have this matrix



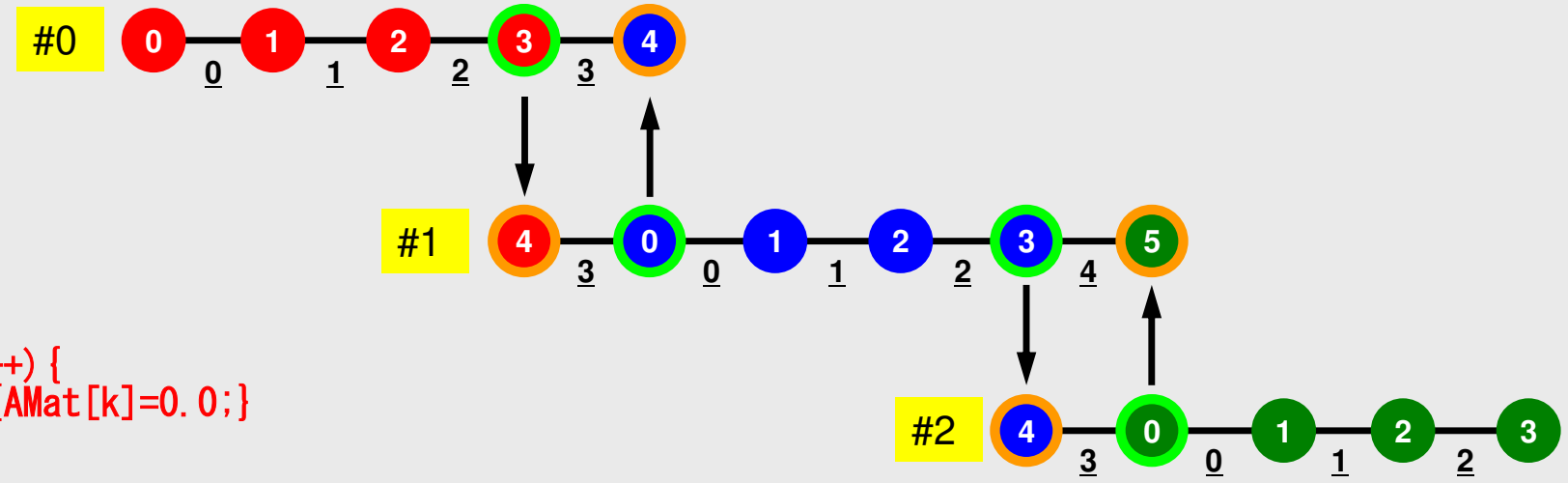
But components of this part are not complete, and not used in computation



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]= PHI[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}

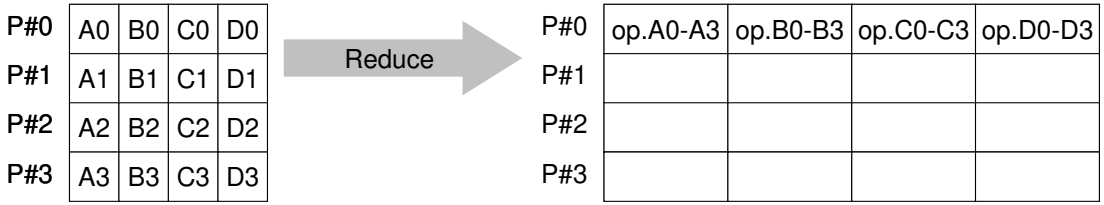
```
MPI_Waitall(NeibPETot, RequestSend, StatSend);

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)
```

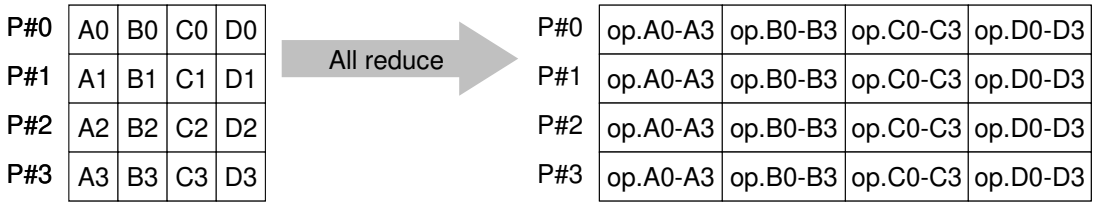
```
real(kind=8):: X0, XSUM

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**

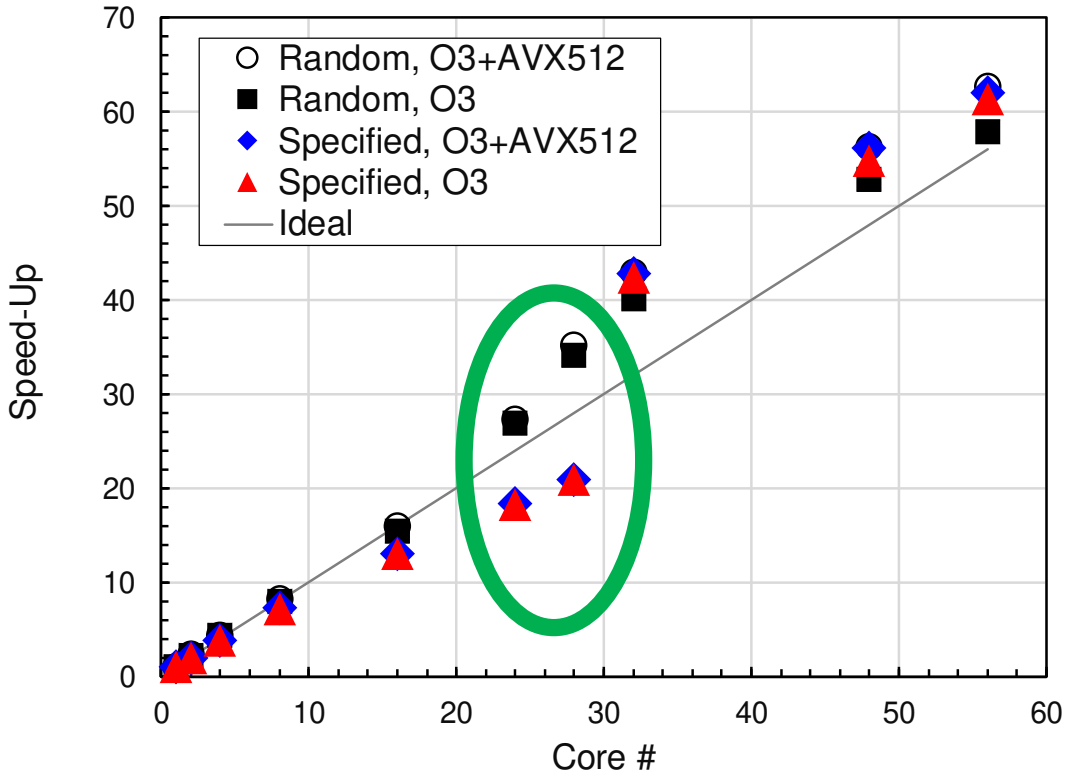
Results: Time for CG Solver, N=10^6

Time for 1,000 iterations, Strong Scaling

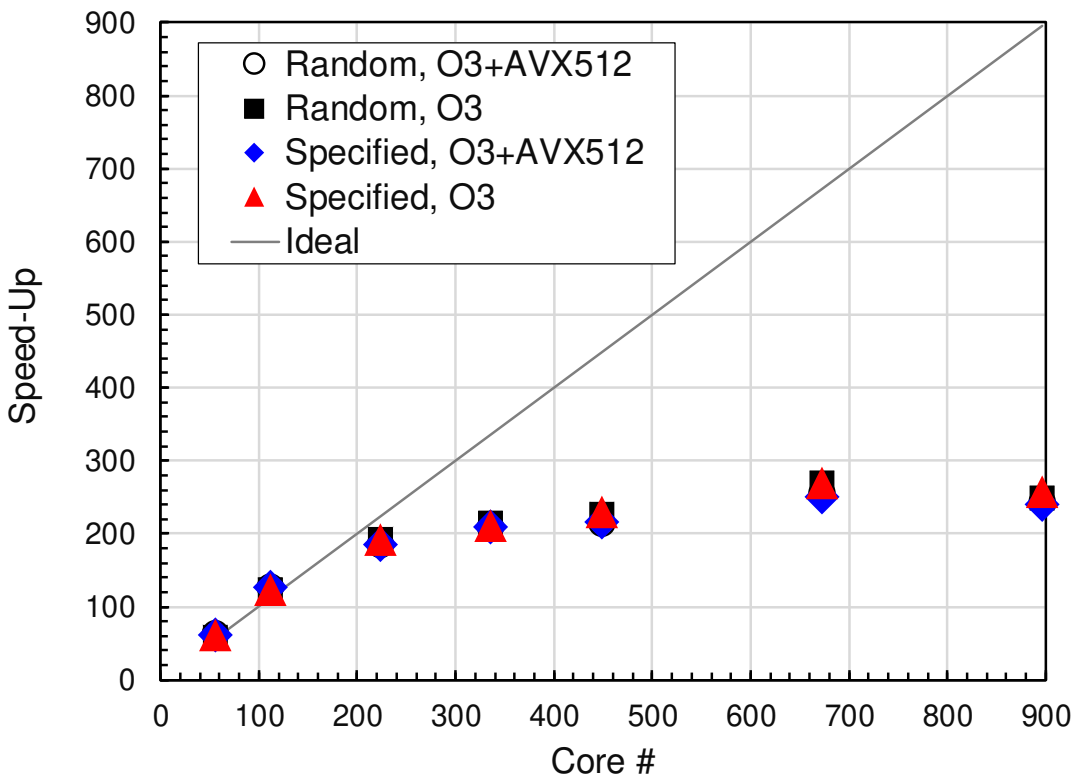
All 56 cores are used if number of nodes is more than 1

Perf. at a single core= 1.00, 5 measurements, Best Case

up to 1 node, 56cores



up to 16 nodes, 896 cores



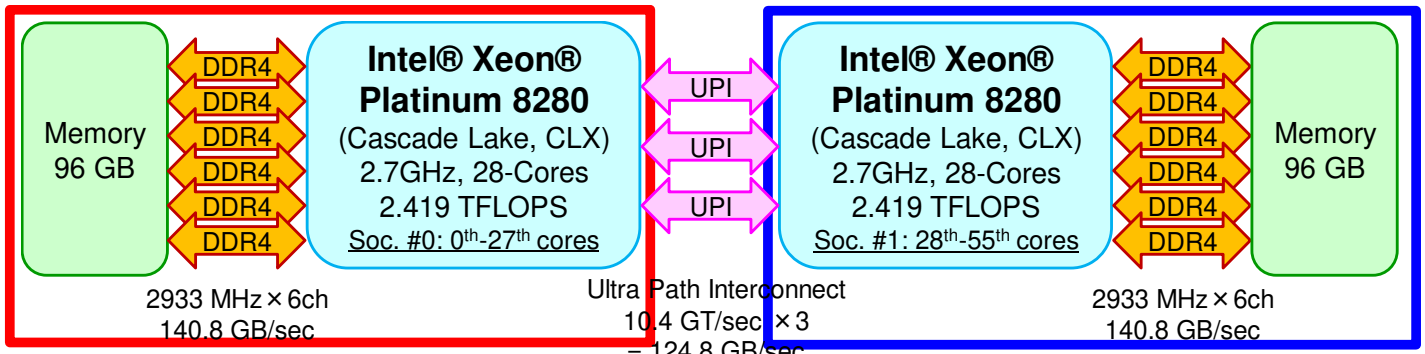
1-node, 24-cores

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=24
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o test.lst

mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
export I_MPI_PIN_PROCESSOR_LIST=0-23
mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
```

1da: -O3 + AVX512
1db: -O3 Only

24-cores are randomly selected from 56-cores on the node
RANDOM

24-cores on Socket #0 are assigned.
SPECIFIED



Socket #0: 0th-27th Cores

Socket #1: 28th-55th Cores

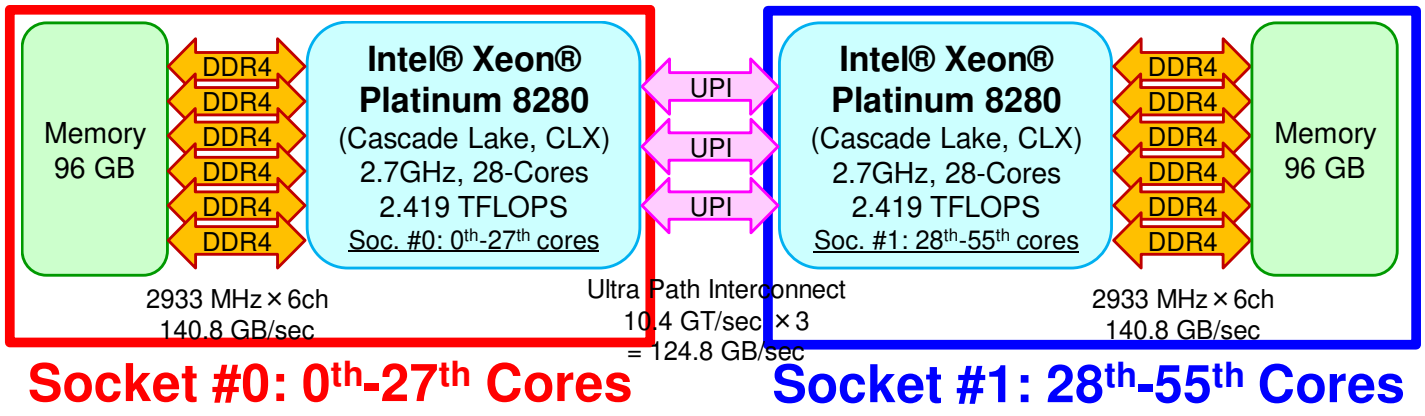
1-node, 28-cores

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=28
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o test.lst

mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
export I_MPI_PIN_PROCESSOR_LIST=0-27
mpiexec.hydra -n ${PJM_MPI_PROC} ./1da
mpiexec.hydra -n ${PJM_MPI_PROC} ./1db
```

1da: -O3 + AVX512
1db: -O3 Only

28-cores are randomly selected from 56-cores on the node
RANDOM

28-cores on Socket #0 are assigned.
SPECIFIED



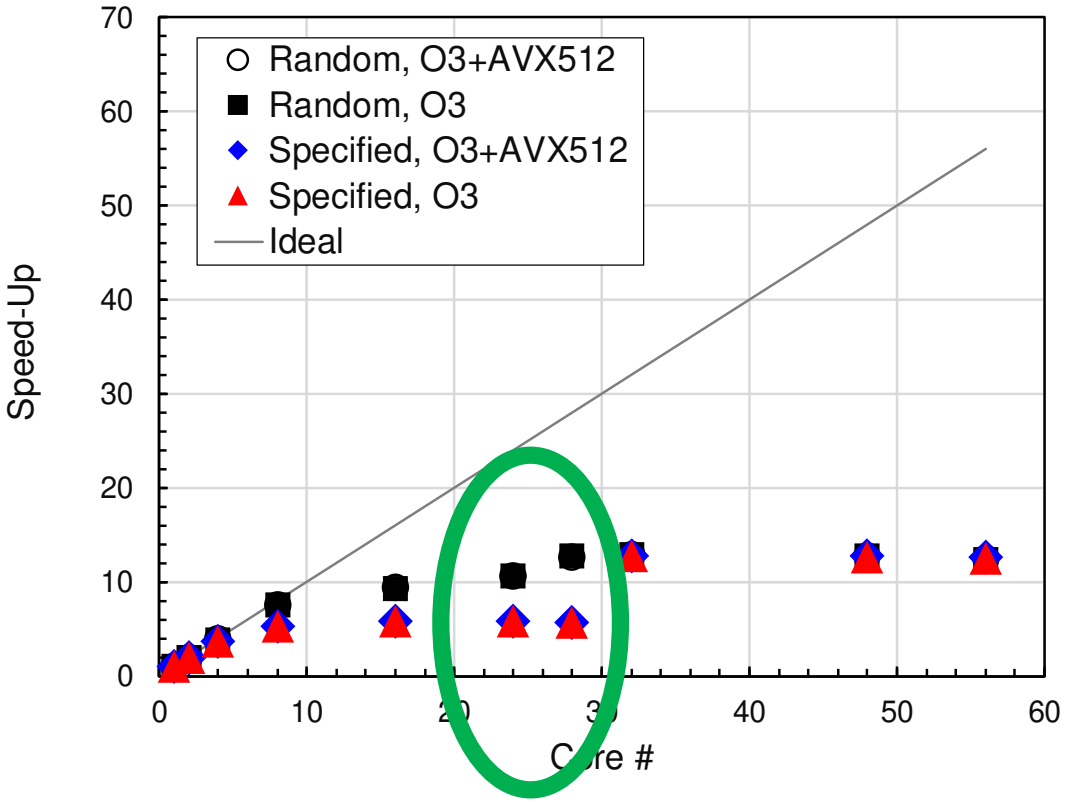
Results: Time for CG Solver, N=10^7

Time for 200 iterations, Strong Scaling

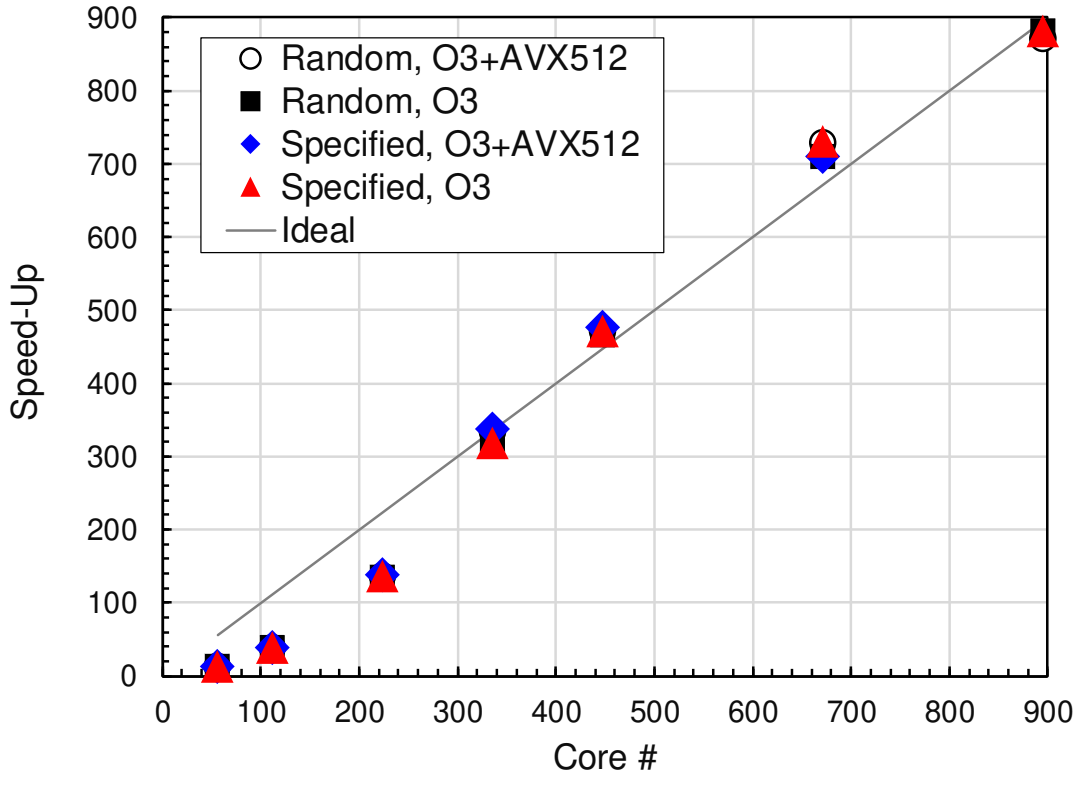
All 56 cores are used if number of nodes is more than 1

Perf. at a single core= 1.00, 5 measurements, Best Case

up to 1 node, 56cores



up to 16 nodes, 896 cores

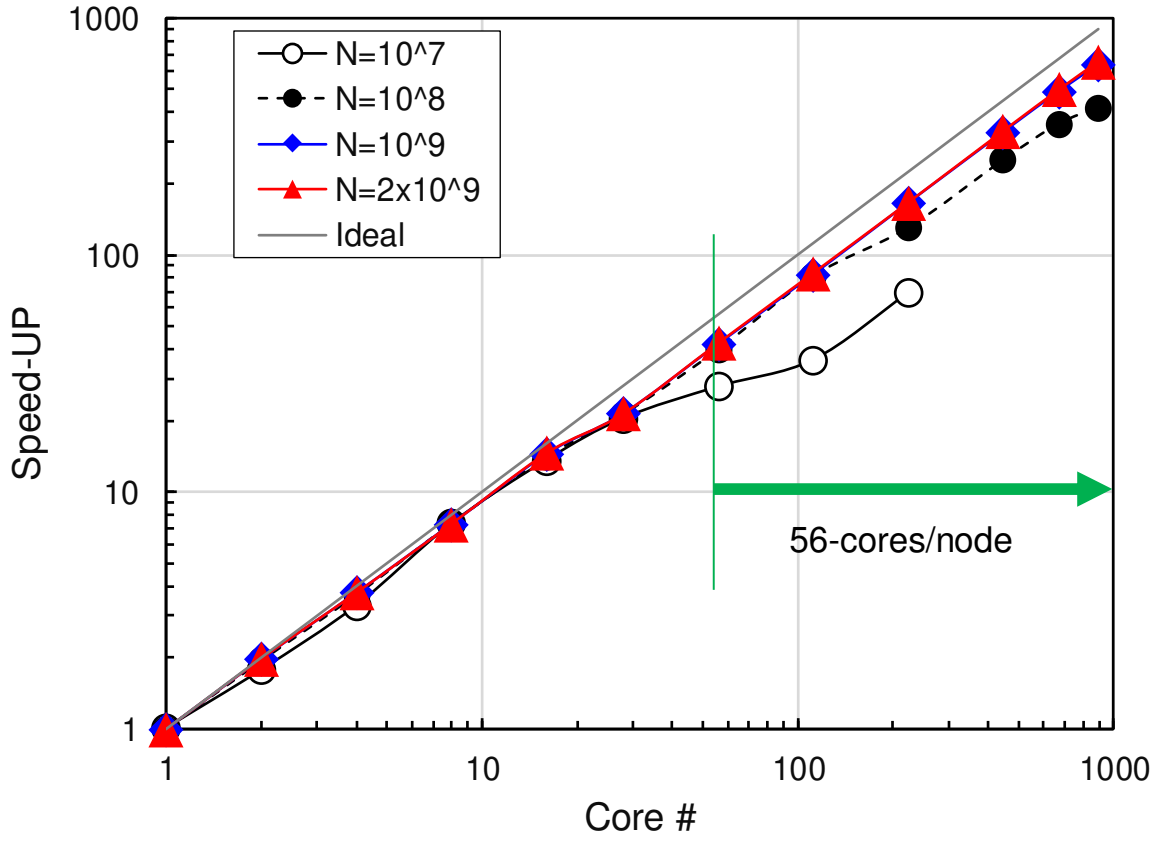


Performance is lower than ideal one

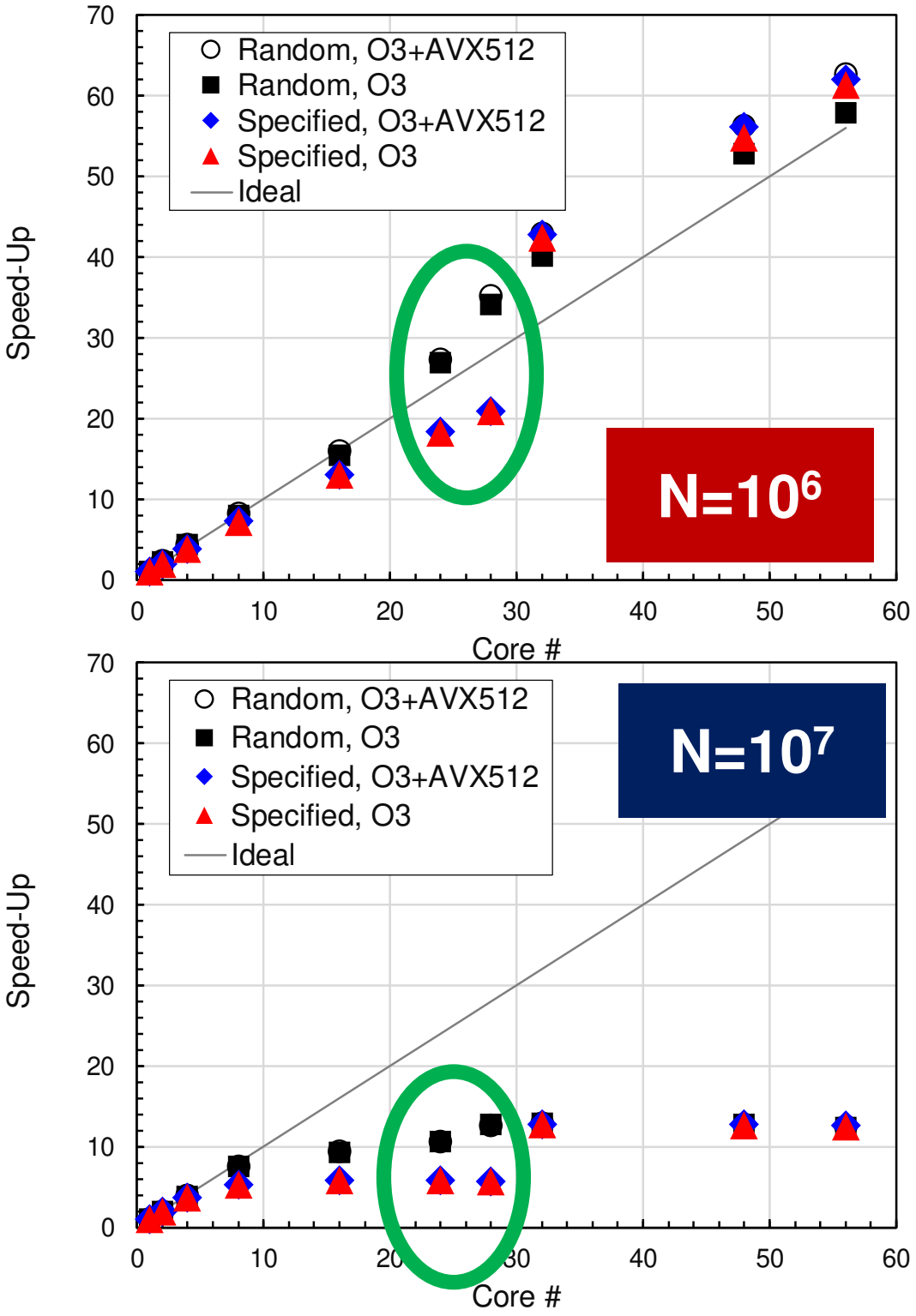
- Time for MPI communication
  - Time for sending data
  - Communication bandwidth between nodes
  - Time is proportional to size of sending/receiving buffers
- Time for starting MPI
  - latency
  - does not depend on size of buffers
    - depends on number of calling, increases according to process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

Performance is lower than ideal one (cont.): S1-3

- 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.



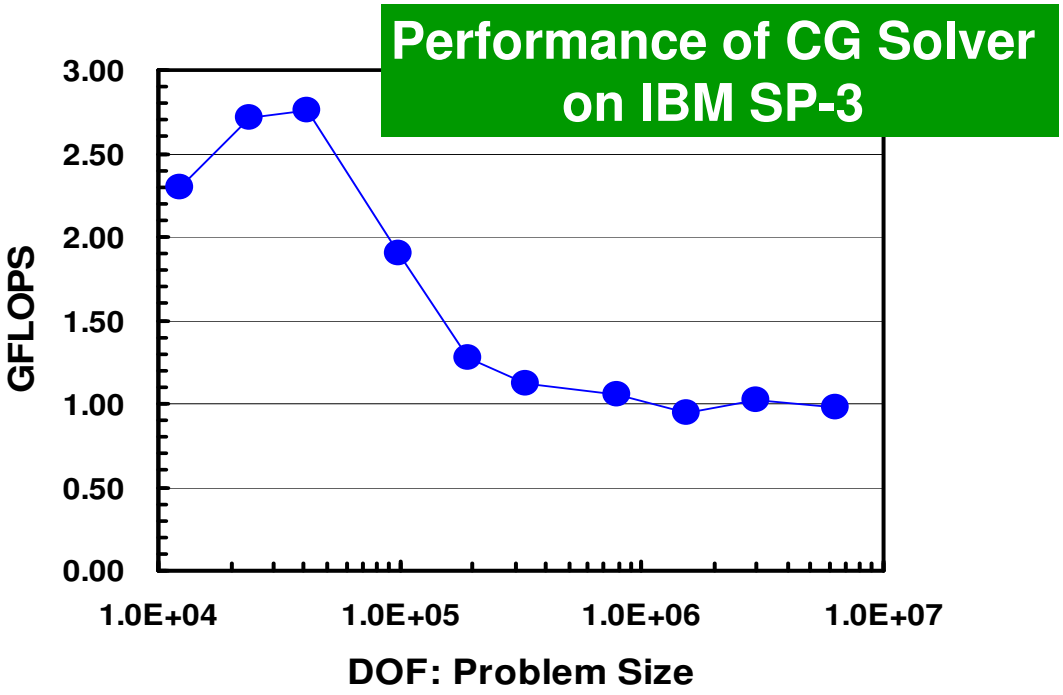
Up to 56 cores (single node)

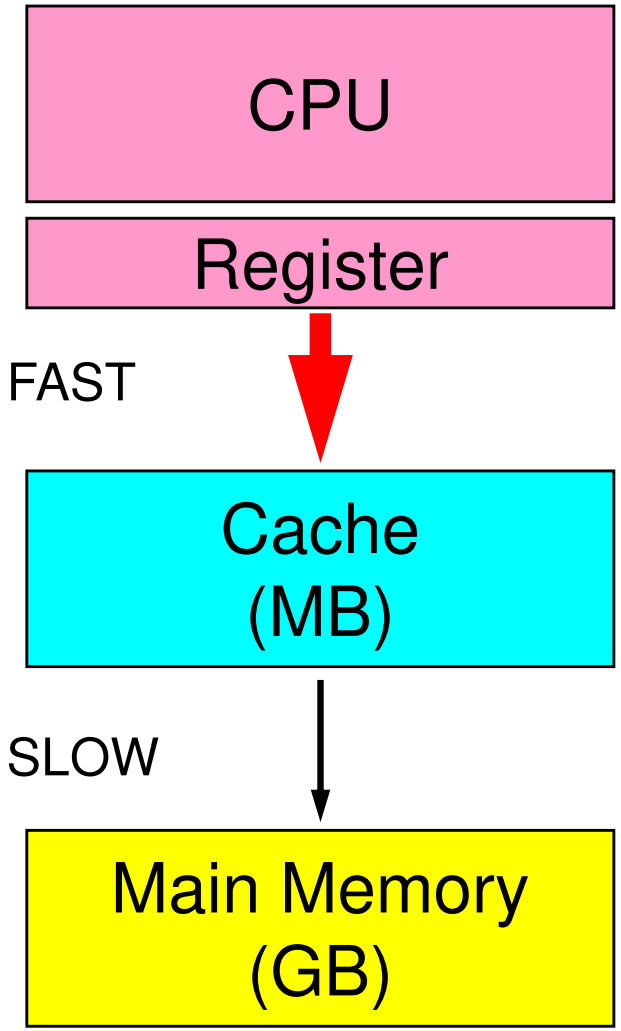


- in a single node (< 56 cores), performance of small cases ($N=10^6$) are rather better.
- Effect of memory contention/saturation (not communication)
- Memory throughput on each soc. is constant for 8+ cores (Stream)
- If problem size is small, cache can be well-utilized. Therefore, effect of memory bandwidth is small.
- Memory/cache of two sockets may be more efficiently utilized in "Random"

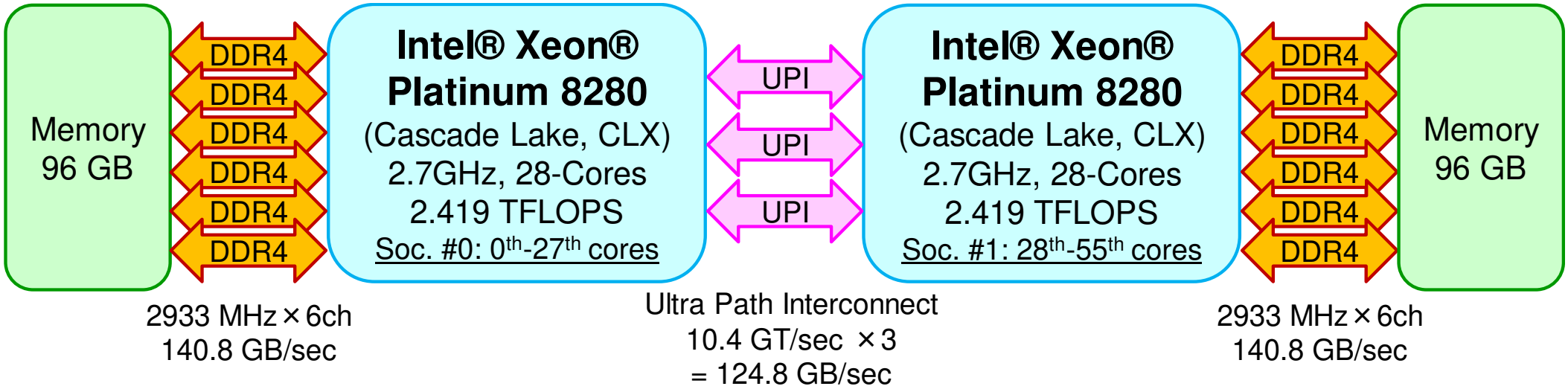
If problem size is small, cache can be well-utilized

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

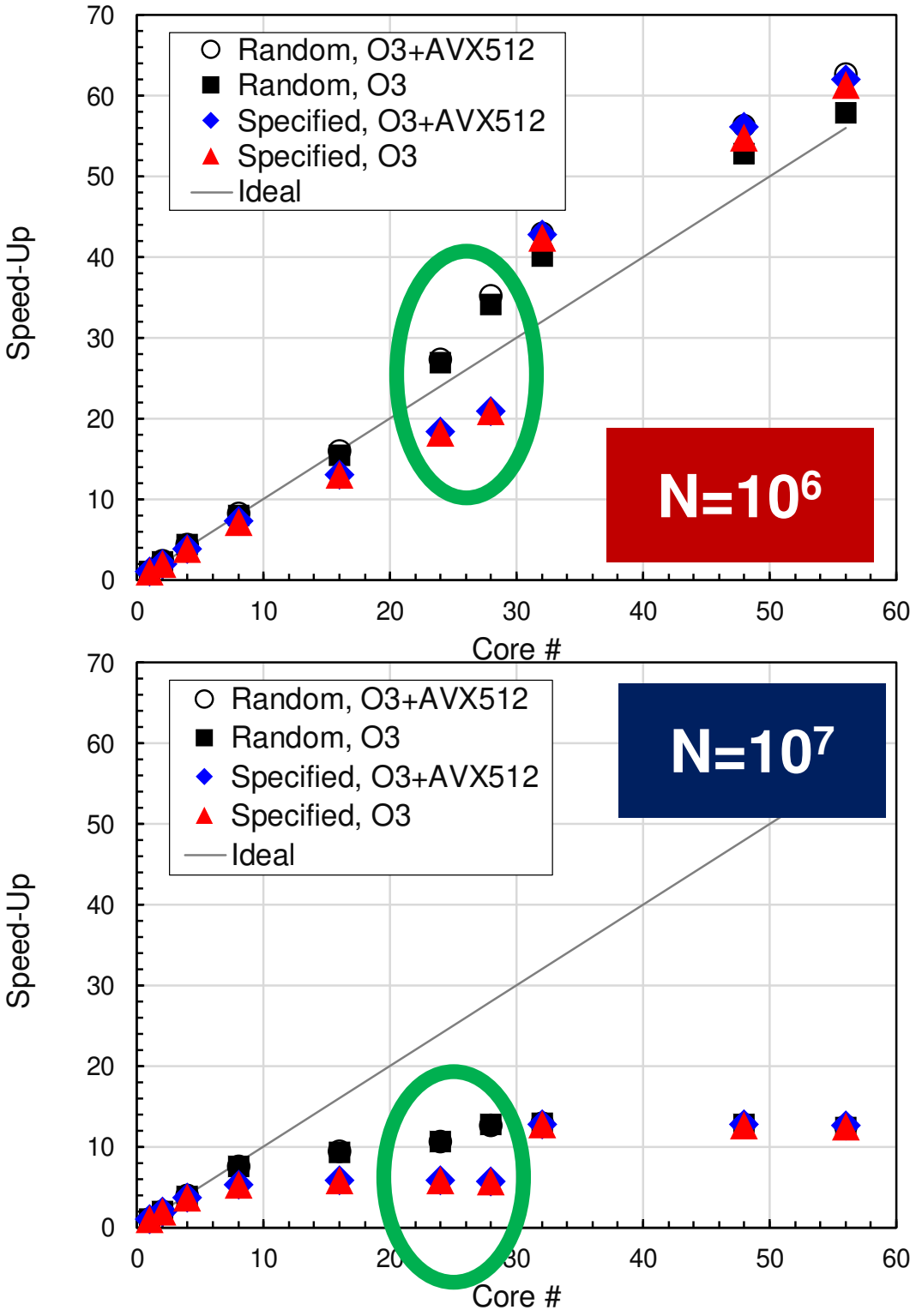




Category	Capacity	X-Way Set Associative	Cache Line
L1$Data	32 KB/core	8-Way	64B
L1$Instruction	32 KB/core	8-Way	64B
L2	1.00 MB/core	16-Way	64B
L3	38.5 MB/socket	11-Way	64B



Up to 56 cores (single node)



- Required Memory
- $N=10^6$: 80MB
  - Very Close to Cache Size
- $N=10^7$: 800MB

- Memory throughput on each socket is constant for 8+ cores (Stream)
- If problem size is small, cache can be well-utilized. Therefore, effect of memory bandwidth is small.

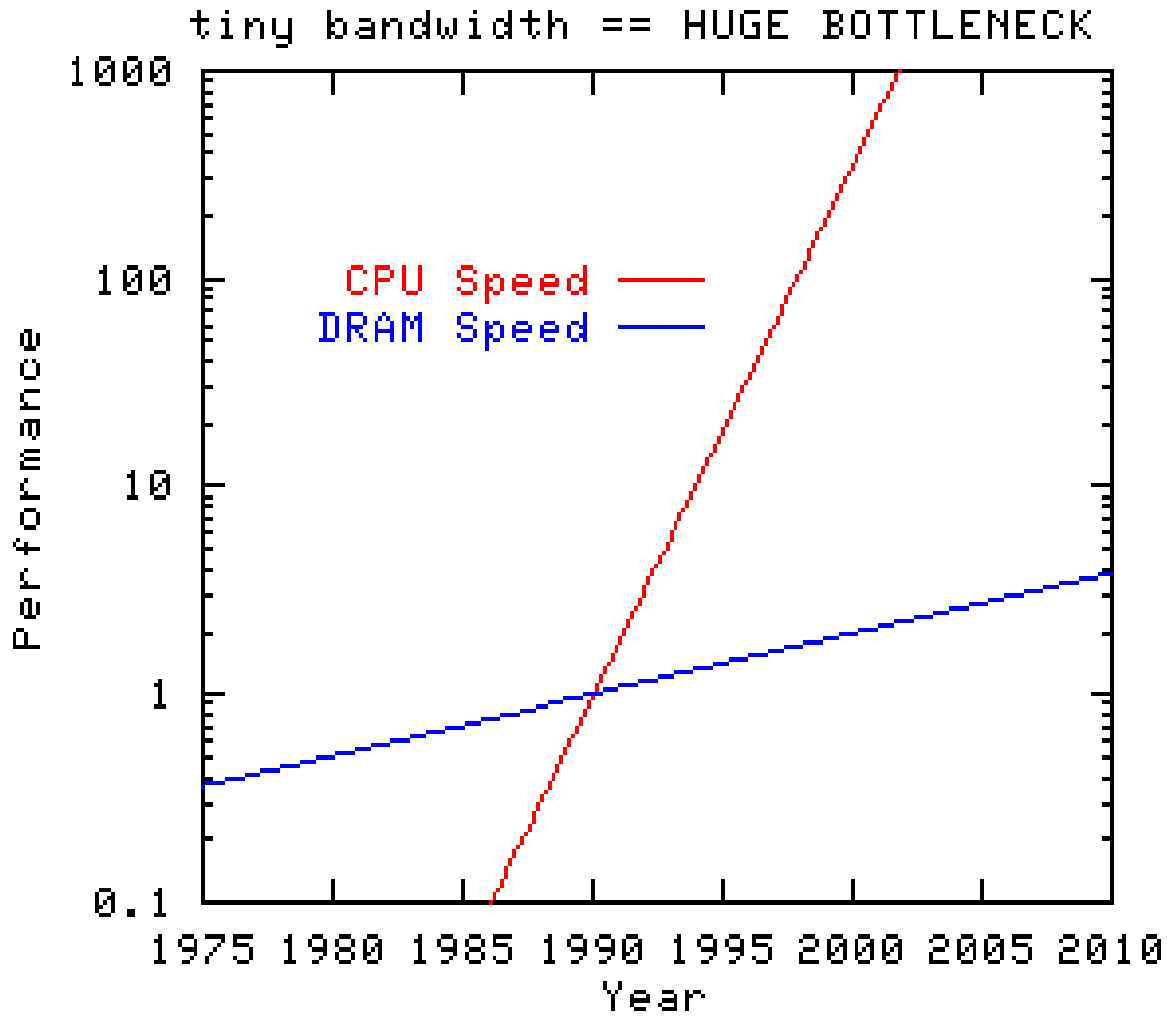
STREAM benchmark

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/

Sparse/Dense Matrices

```
do i= 1, N
  Y(i)= D(i)*X(i)
  do k= index(i-1)+1, index(i)
    Y(i)= Y(i) + AMAT(k)*X(item(k))
  enddo
enddo
```

```
do j= 1, N
  do i= 1, N
    Y(j)= Y(j) + A(i,j)*X(i)
  enddo
enddo
```

- "X" in RHS
  - Dense: continuous on memory, easy to utilize cache
  - Sparse: continuity is not assured (in-direct access), difficult to utilize cache
    - more "memory-bound"

GeoFEM Benchmark

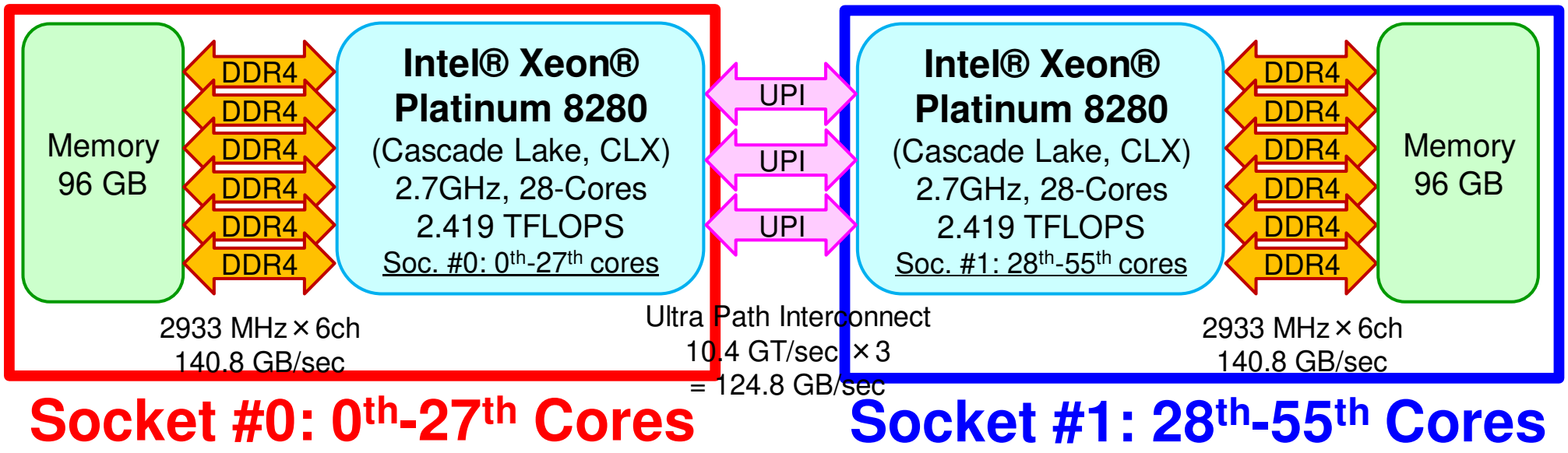
ICCG in FEM for Solid Mechanics

	SR11K/J2	SR16K/M1	T2K	FX10	京
Core #/Node	16	32	16	16	8
Peak Performance (GFLOPS)	147.2	980.5	147.2	236.5	128.0
STREAM Triad (GB/s)	101.0	264.2	20.0	64.7	43.3
B/F	0.686	0.269	0.136	0.274	0.338
GeoFEM (GFLOPS)	19.0	72.7	4.69	16.0	11.0
% to Peak	12.9	7.41	3.18	6.77	8.59
LLC/core (MB)	18.0	4.00	2.00	0.75	0.75

Sparse Linear Solver: Memory-Bound

Copy, Compile and Run

```
>$ cd /work/gt73/t73XXX/pFEM
>$ cp /work/gt73/z30088/pFEM/F/stream.tar .
>$ tar xvf stream.tar
>$ cd mpi/stream

>$ mpiifort -align array64byte -O3 -axCORE-AVX512 stream.f -o stream
>$ pjsub XXX.sh
```

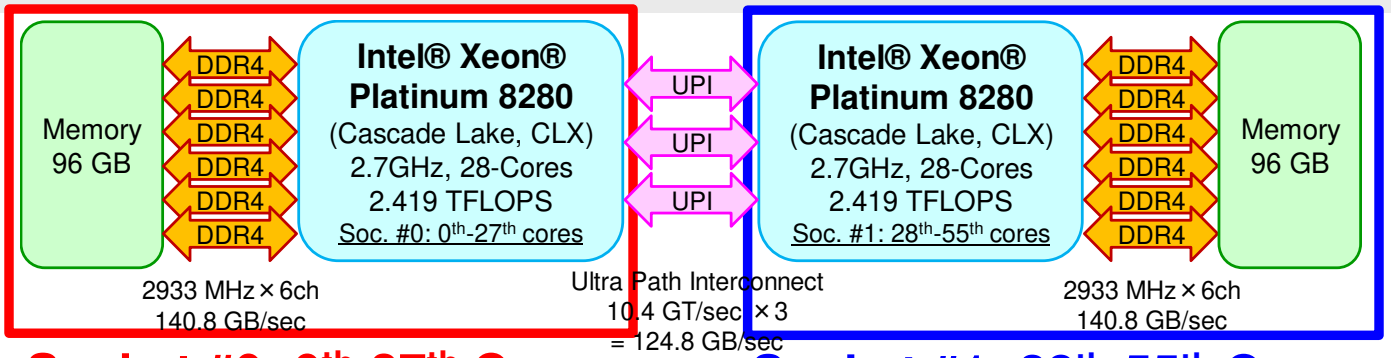


s01.sh: Use 1 core

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=1
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o s01.lst

mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream

export I_MPI_PIN_PROCESSOR_LIST=0
mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream
```

Cores are randomly selected

Core are specified

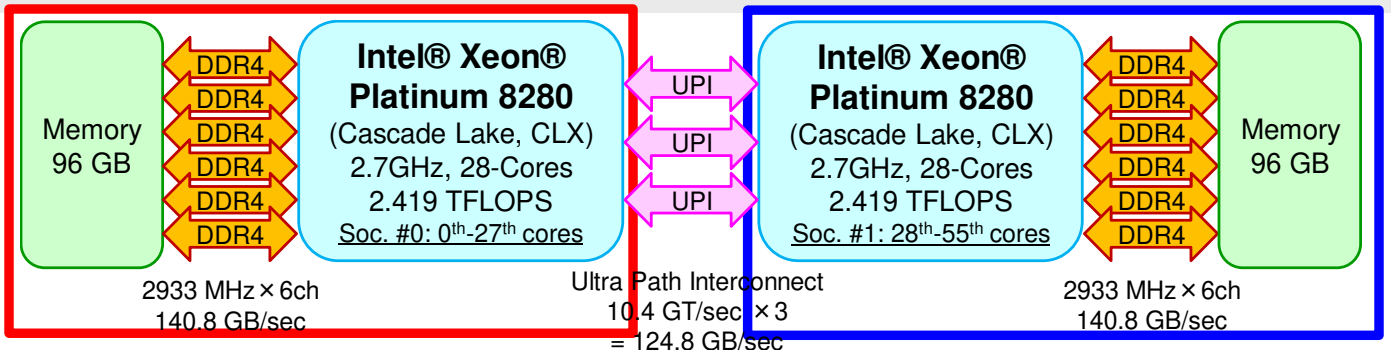


s16.sh: Use 16 cores

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=16
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o s16.lst

mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream

export I_MPI_PIN_PROCESSOR_LIST=0-15
mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream
```

Cores are randomly selected

Core are specified

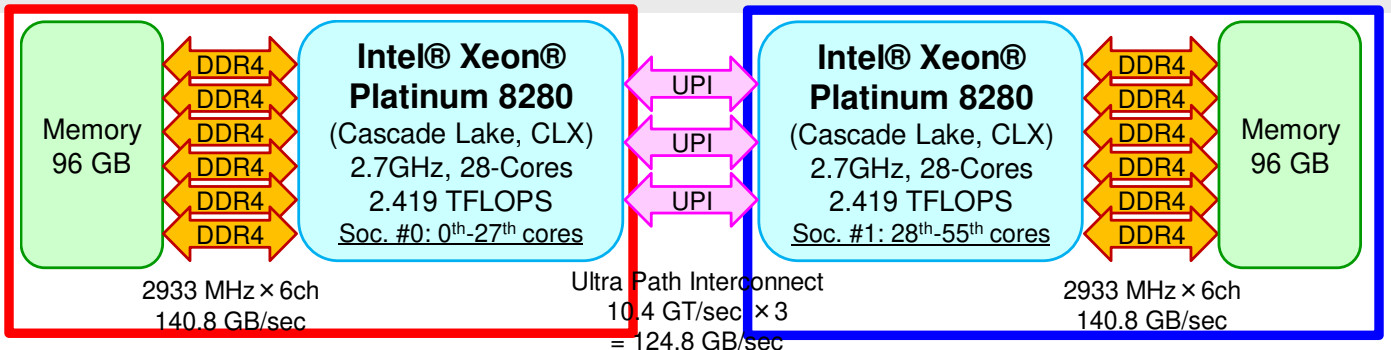


s32.sh: Use 32 cores

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=32
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o s32.lst

mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream

export I_MPI_PIN_PROCESSOR_LIST=0-15,28-43
mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream
```

Cores are randomly selected

Core are specified

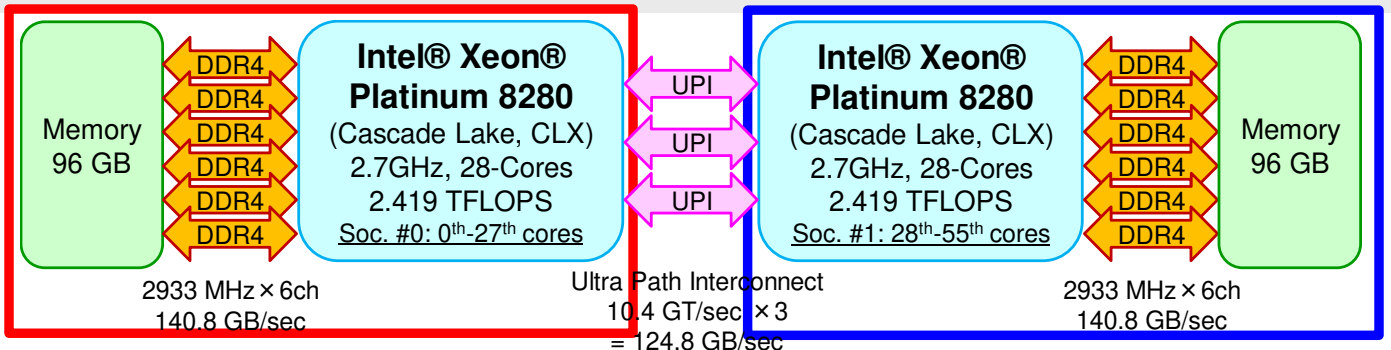


s48.sh: Use 48 cores

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=48
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o s48.lst

mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream

export I_MPI_PIN_PROCESSOR_LIST=0-23,28-51
mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream
```

Cores are randomly selected

Core are specified

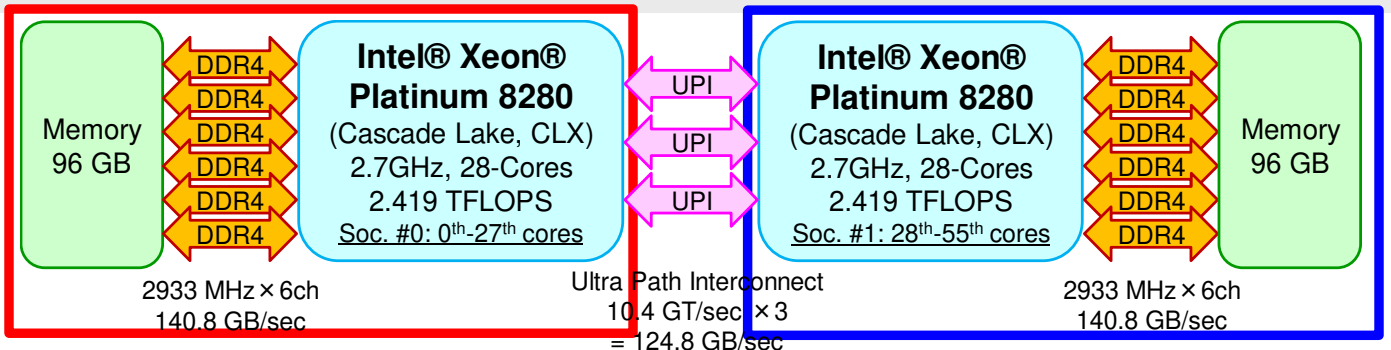


s56.sh: Use 56 cores

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture3
#PJM -L node=1
#PJM --mpi proc=56
#PJM -L elapse=00:15:00
#PJM -g gt73
#PJM -j
#PJM -e err
#PJM -o s56.lst

mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream

export I_MPI_PIN_PROCESSOR_LIST=0-55
mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./stream
mpiexec.hydra -n ${PJM_MPI_PROC} ./stream
```

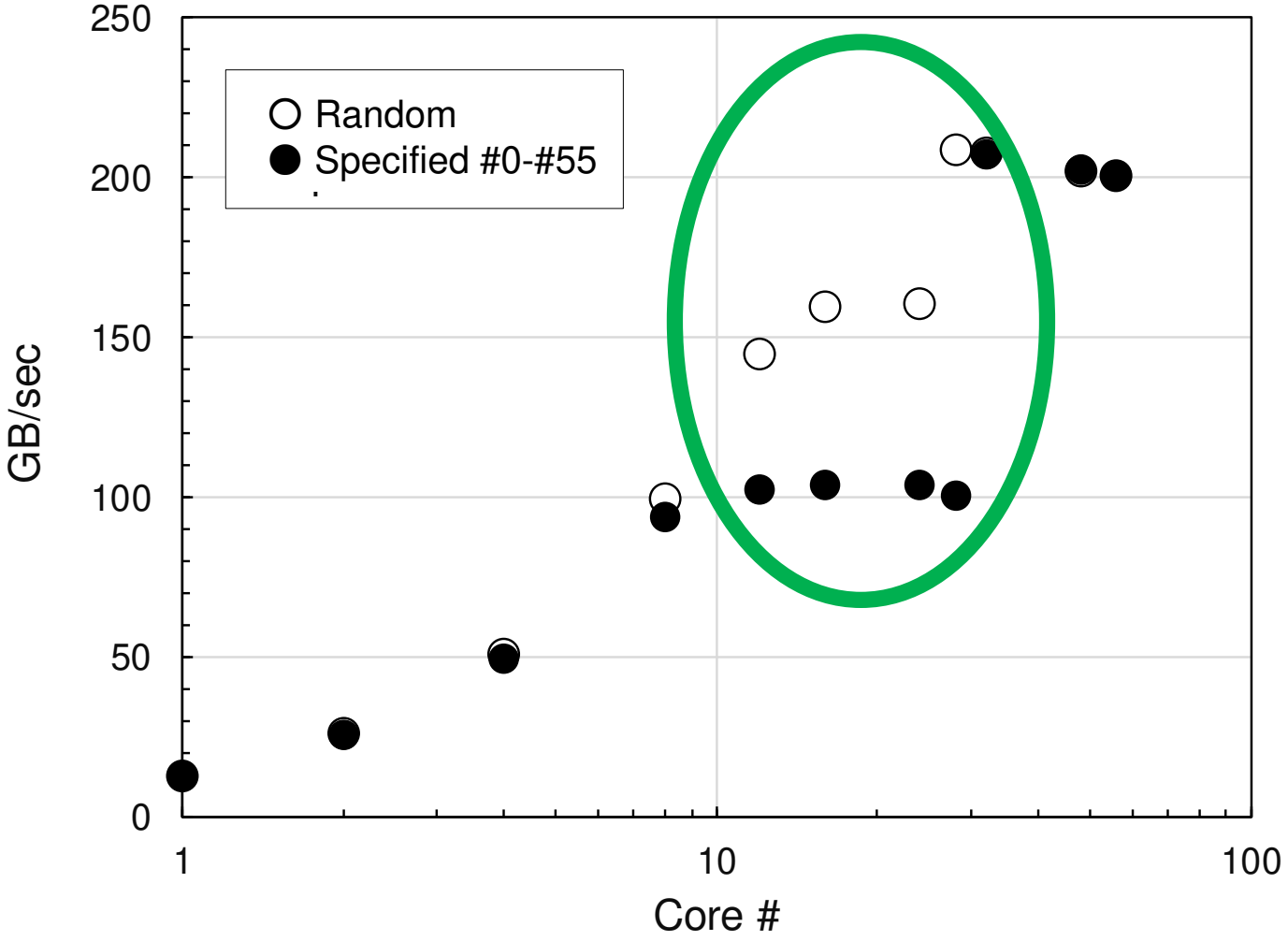
Cores are randomly selected

Core are specified



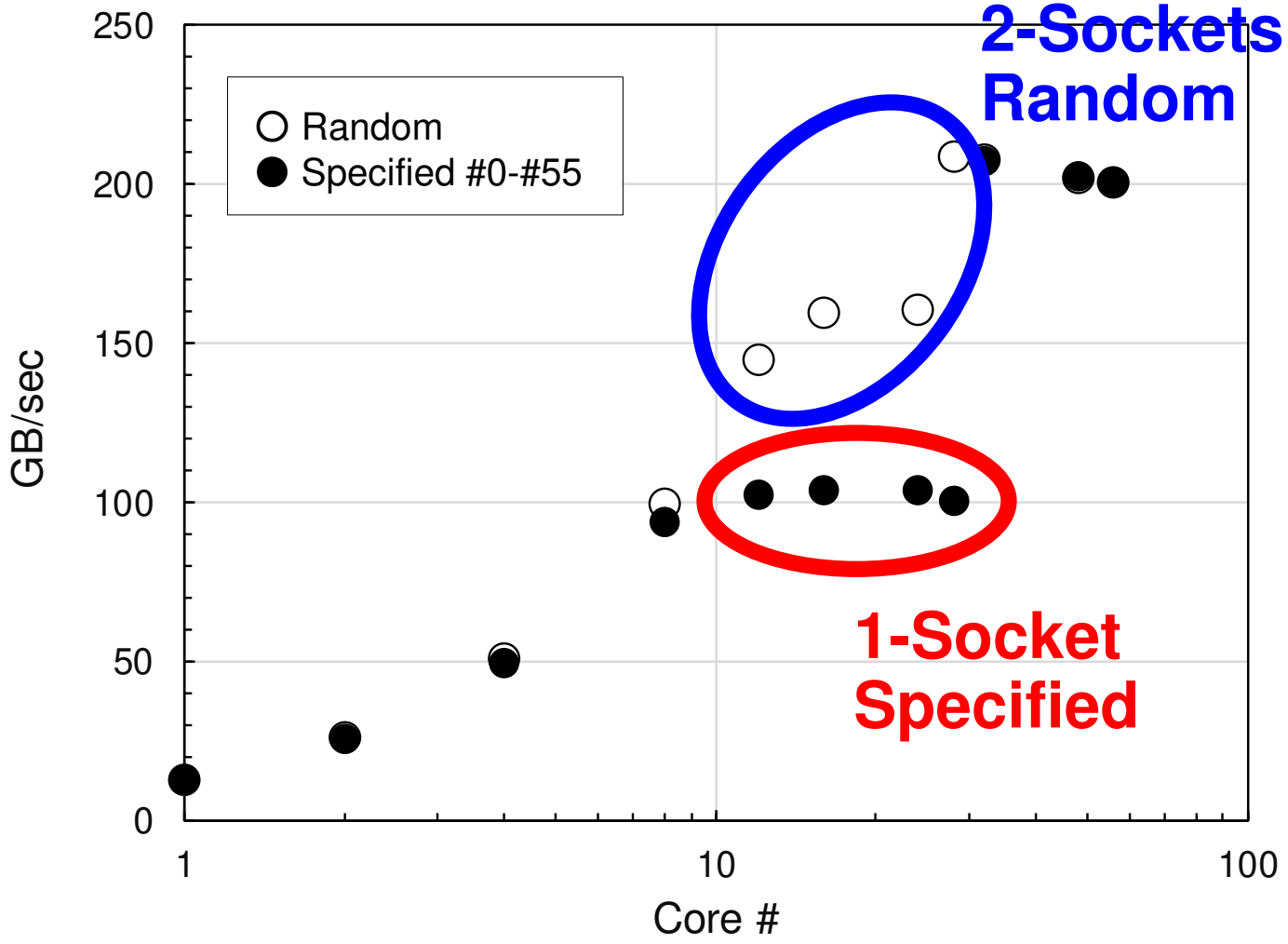
Triad on a Single Node of OBCX Peak is 281.57 GB/sec.

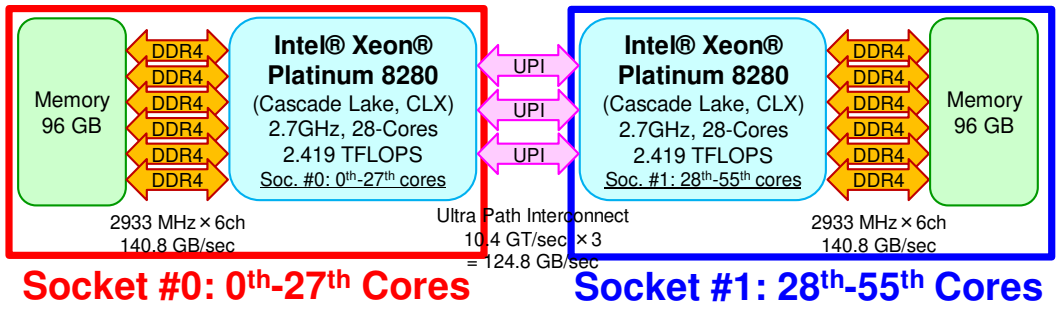
Memory/cache may be more efficiently utilized in “Random” (12-28 cores)



Triad on a Single Node of OBCX Peak is 281.57 GB/sec.

Memory/cache may be more efficiently utilized in “Random” (12-28 cores)





Socket #	Core #	Random	Specified
1	1	1.000	1.000
	2	1.998	1.963
	4	3.912	3.809
	6	5.792	5.682
	8	7.615	7.177
	12	11.089	7.844
	16	12.214	7.968
	24	12.278	7.945
	28	15.962	7.705
2	32	15.901	15.862
	48	15.452	15.497
	56	15.370	15.358

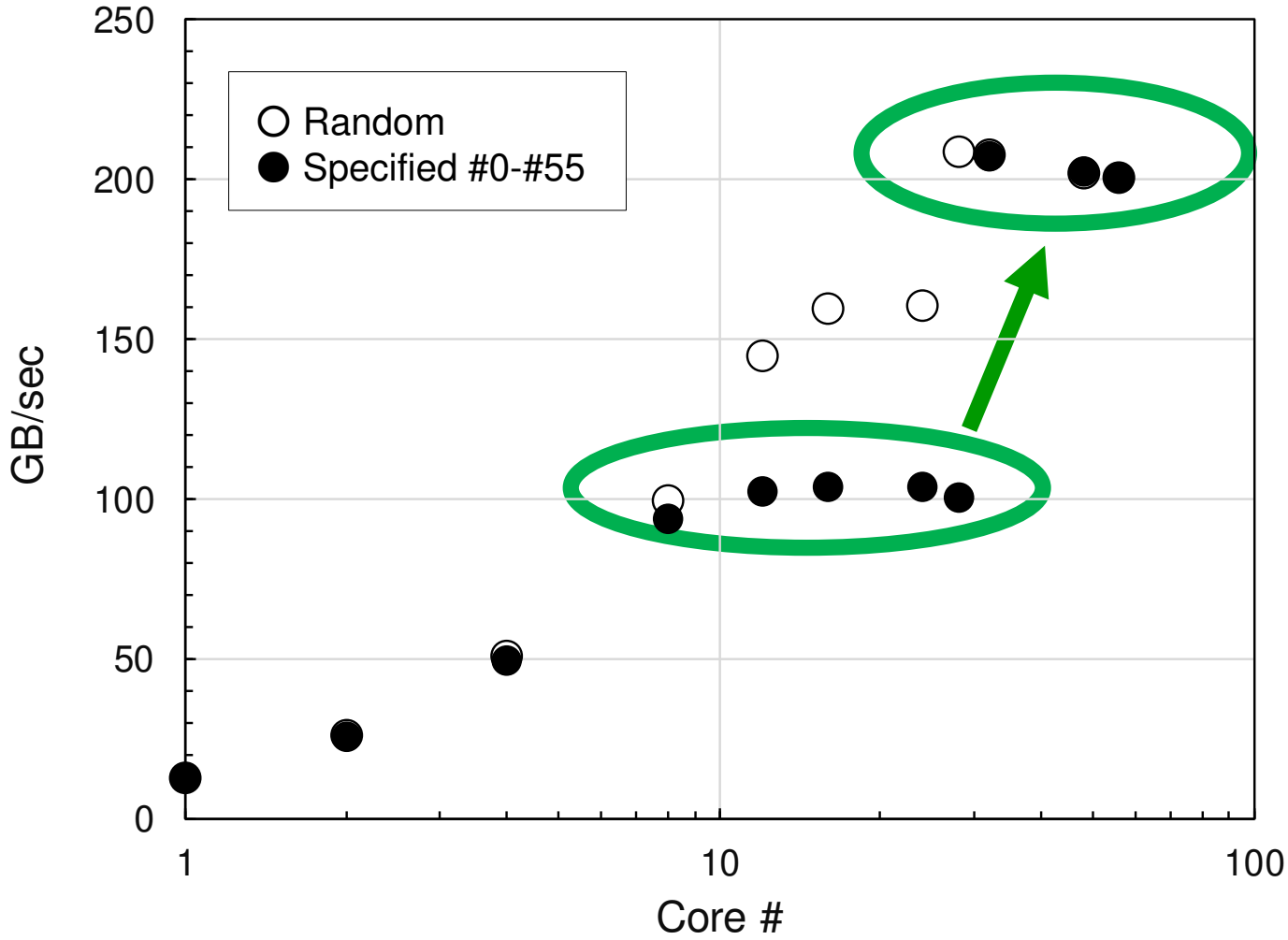
Triad on a Single Node of OBCX

Speed-Up based on Performance with 1 core

- Number of Memory Channels per Socket = 6
  - 6 memory chips can be loaded on each socket
  - Linear speed-up up to 6 cores (processes) on each socket

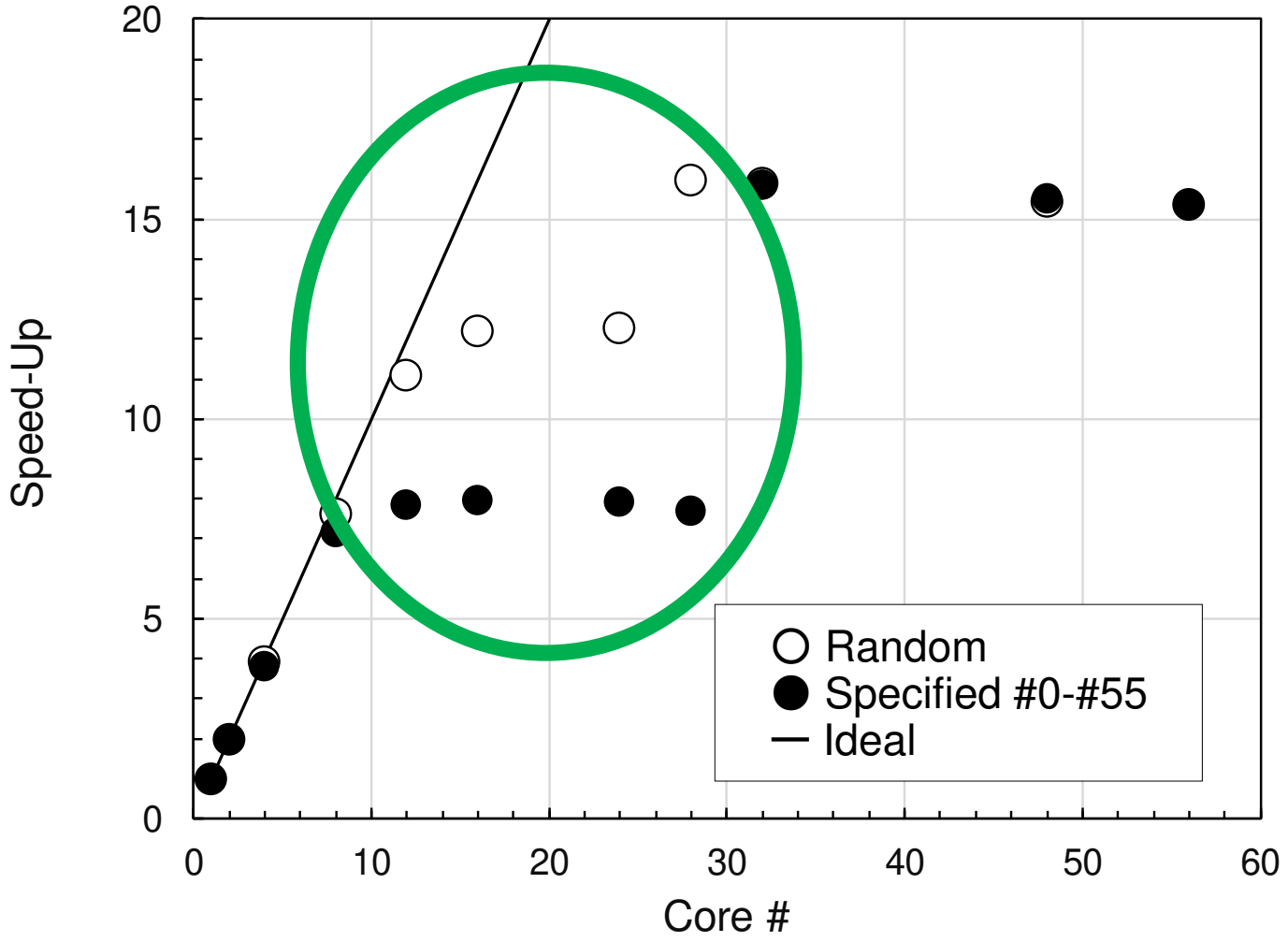
Triad on a Single Node of OBCX Peak is 281.57 GB/sec.

● : Memory BW is constant with 8-28 cores (saturated), Doubled with 32-56 cores



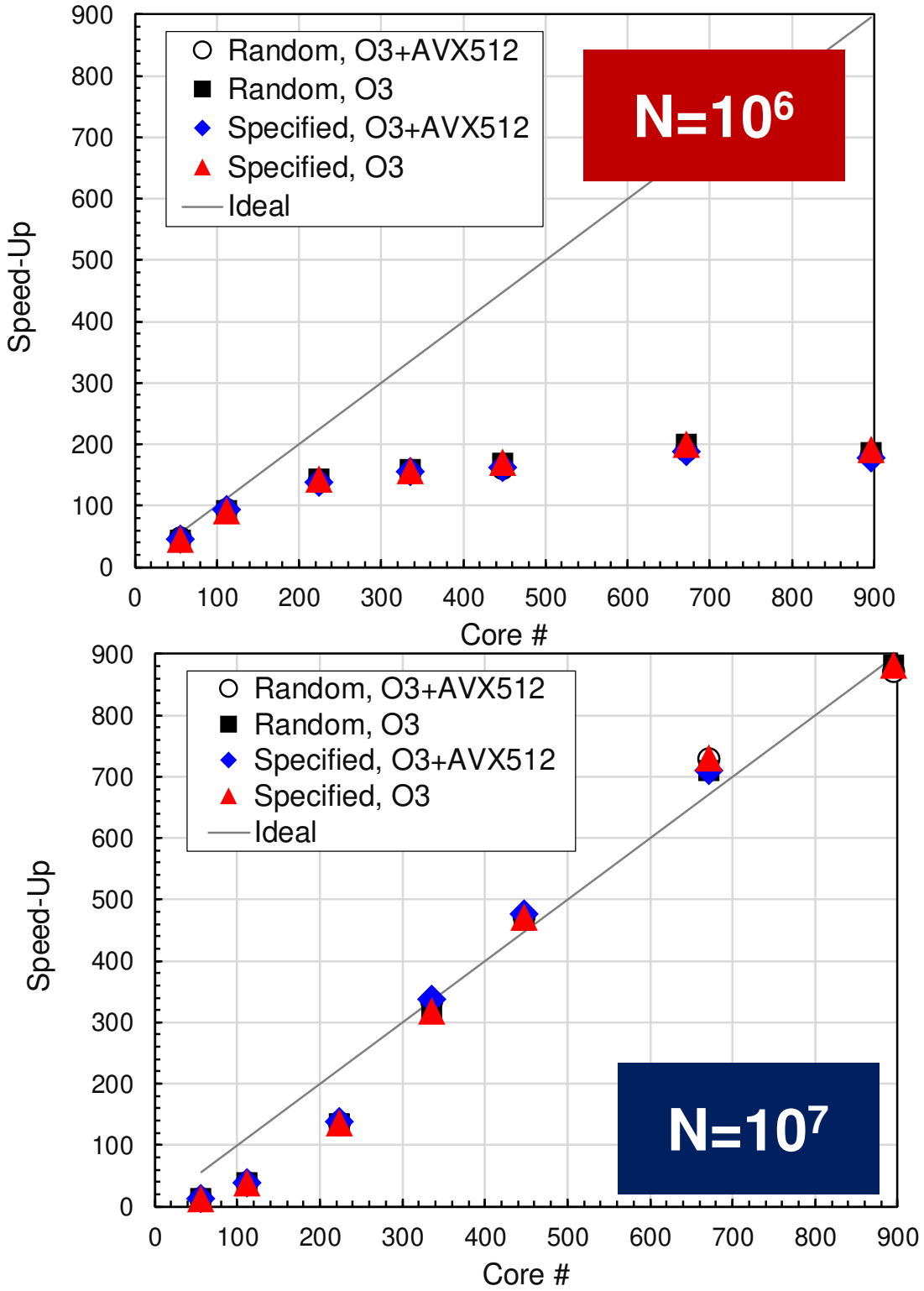
Triad on a Single Node of OBCX Peak is 281.57 GB/sec.

Memory/cache may be more efficiently utilized in “Random” (12-28 cores)



Exercises

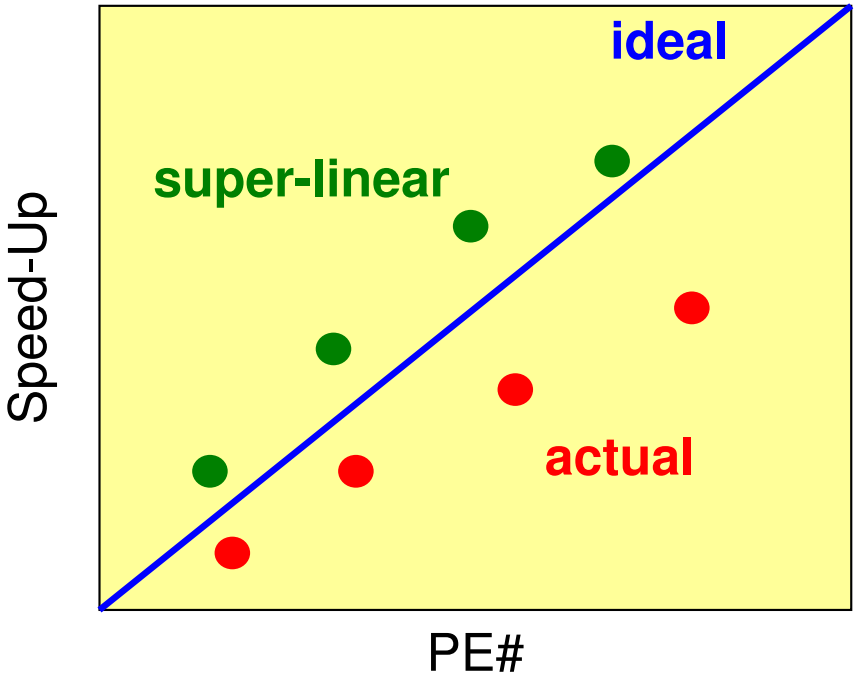
- Running the code
- Try various number of processes (1-56)
- OpenMP-version and Single PE version are available
  - Fortran, C
  - Web-site of STREAM
  - http://www.cs.virginia.edu/stream/



Up to 896 cores (16-nodes)

- Performance at a Single Core= 1.00
- 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 672 cores (12 nodes).

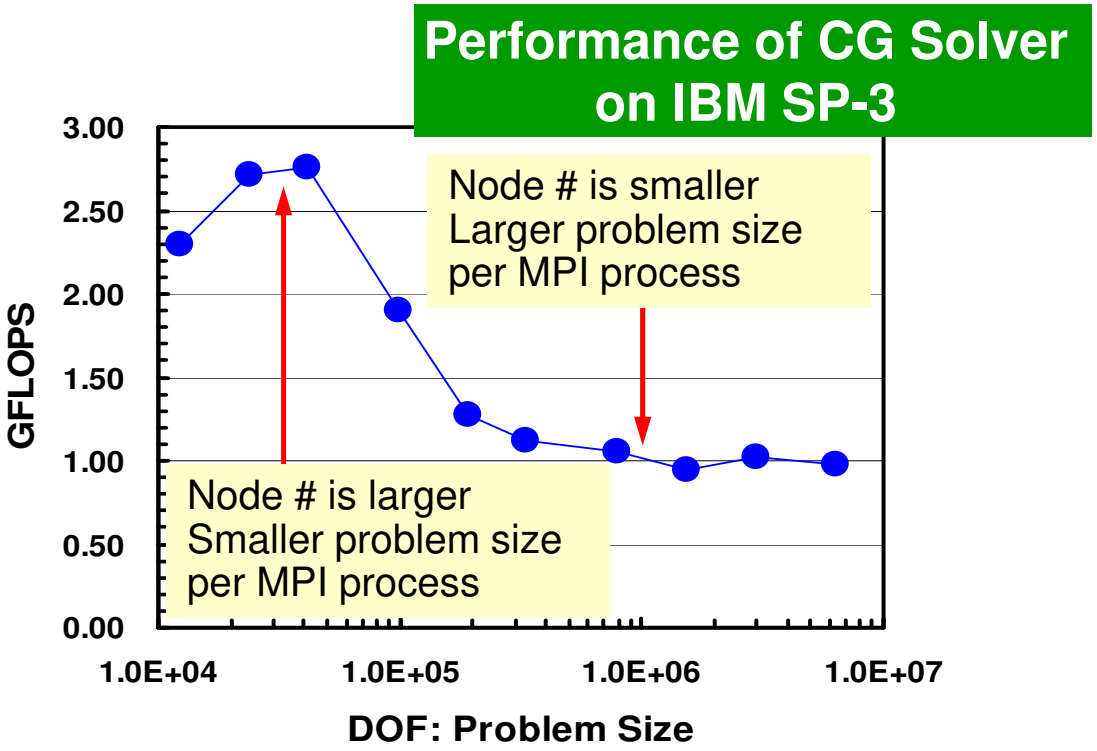
Super-Linear in Strong Scaling

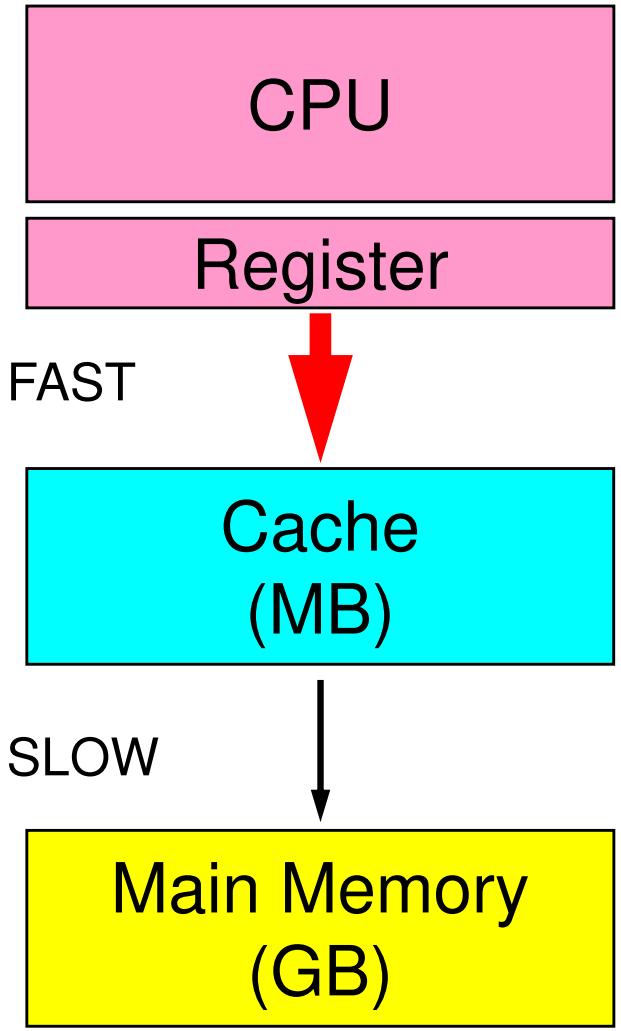


- In strong scaling case where entire problem size is fixed, performance is generally lower than the ideal one due to communication overhead.
- But sometimes, actual performance may be better than the ideal one. This is called “super-linear”

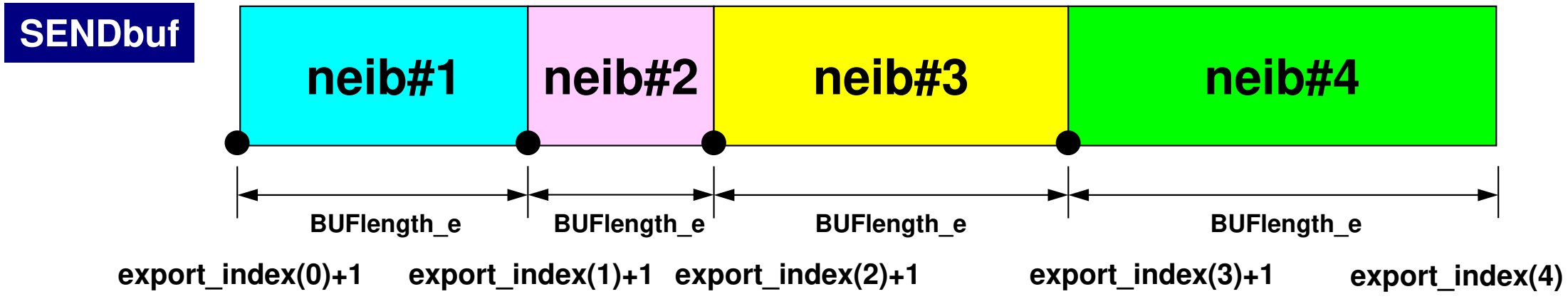
Why does “Super-Linear” happen ?

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





Memory Copy is expensive (1/2)



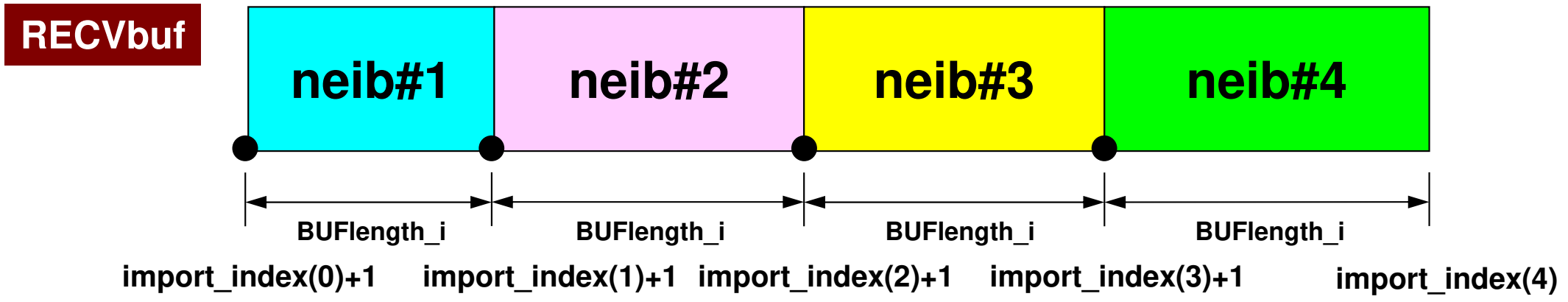

```
 do neib= 1, NEIBPETOT
   do k= export_index(neib-1)+1, export_index(neib)
     kk= export_item(k)
     SENDbuf(k)= VAL(kk)
   enddo
 enddo

 do neib= 1, NEIBPETOT
   iS_e= export_index(neib-1) + 1
   iE_e= export_index(neib  )
   BUFlength_e= iE_e + 1 - iS_e

   call MPI_ISEND                                                    &
&          (SENDbuf(iS_e), BUFlength_e, MPI_INTEGER, NEIBPE(neib), 0,&
&           MPI_COMM_WORLD, request_send(neib), ierr)
 enddo

 call MPI_WAITALL (NEIBPETOT, request_send, stat_send, ierr)
```

Copied to sending buffers

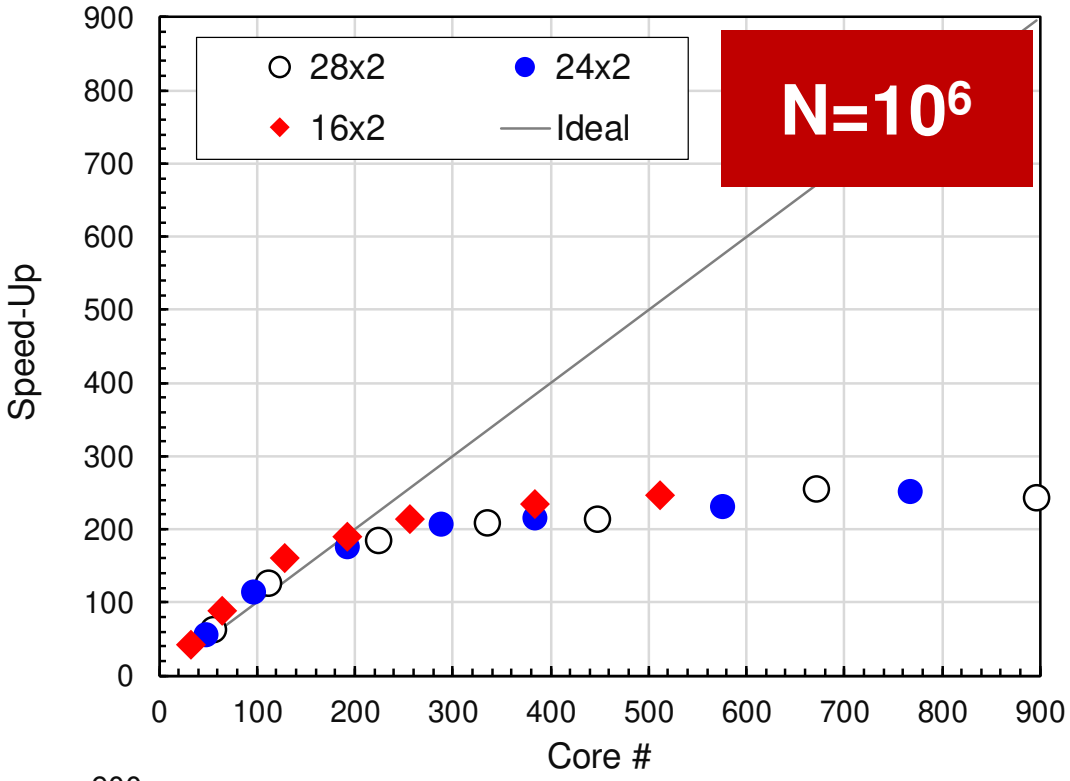
Memory Copy is expensive (2/2)

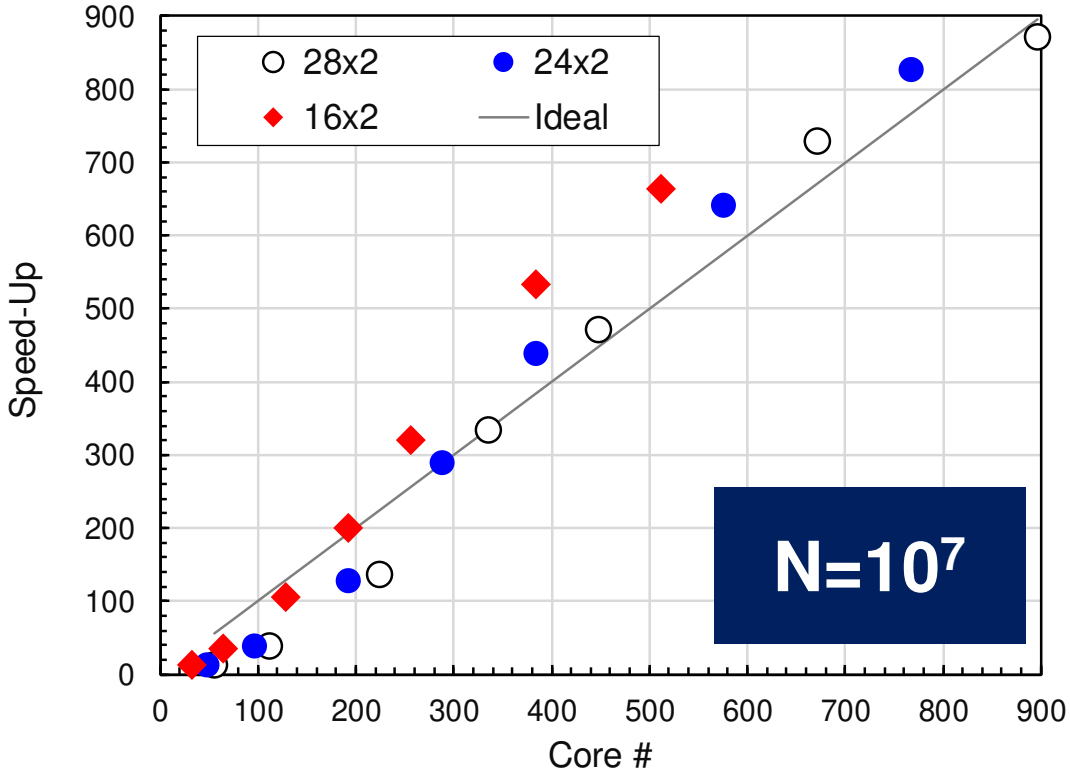
```
 do neib= 1, NEIBPETOT
   iS_i= import_index(neib-1) + 1
   iE_i= import_index(neib  )
   BUFlength_i= iE_i + 1 - iS_i

   call MPI_IRECV                                                  &
&          (RECVbuf(iS_i), BUFlength_i, MPI_INTEGER, NEIBPE(neib), 0,&
&           MPI_COMM_WORLD, request_recv(neib), ierr)
  enddo

  call MPI_WAITALL (NEIBPETOT, request_recv, stat_recv, ierr)

  do neib= 1, NEIBPETOT
     do k= import_index(neib-1)+1, import_index(neib)
       kk= import_item(k)
       VAL(kk)= RECVbuf(k)
     enddo
  enddo
```

Copied from receiving buffer

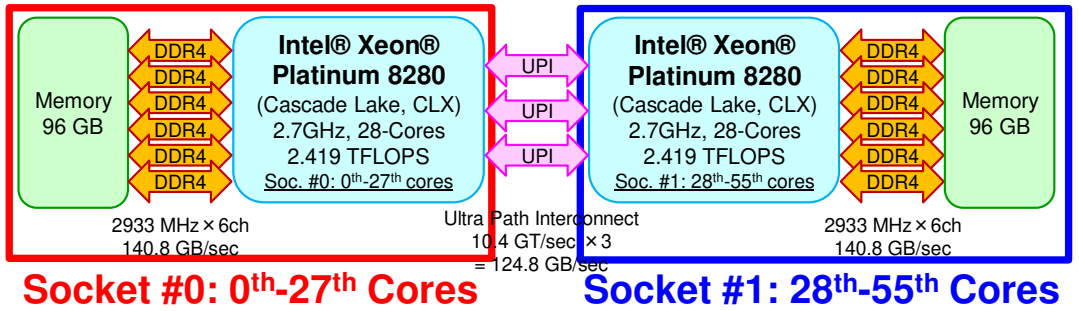


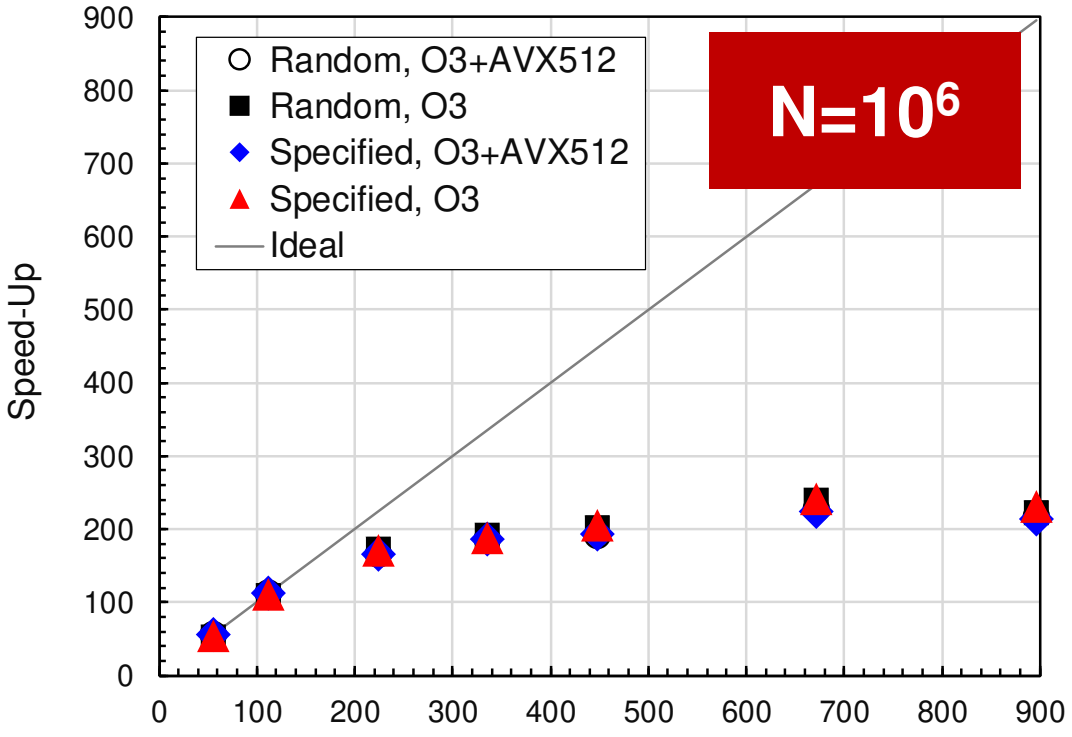
Up to 16-nodes
Random, O3+AVX512

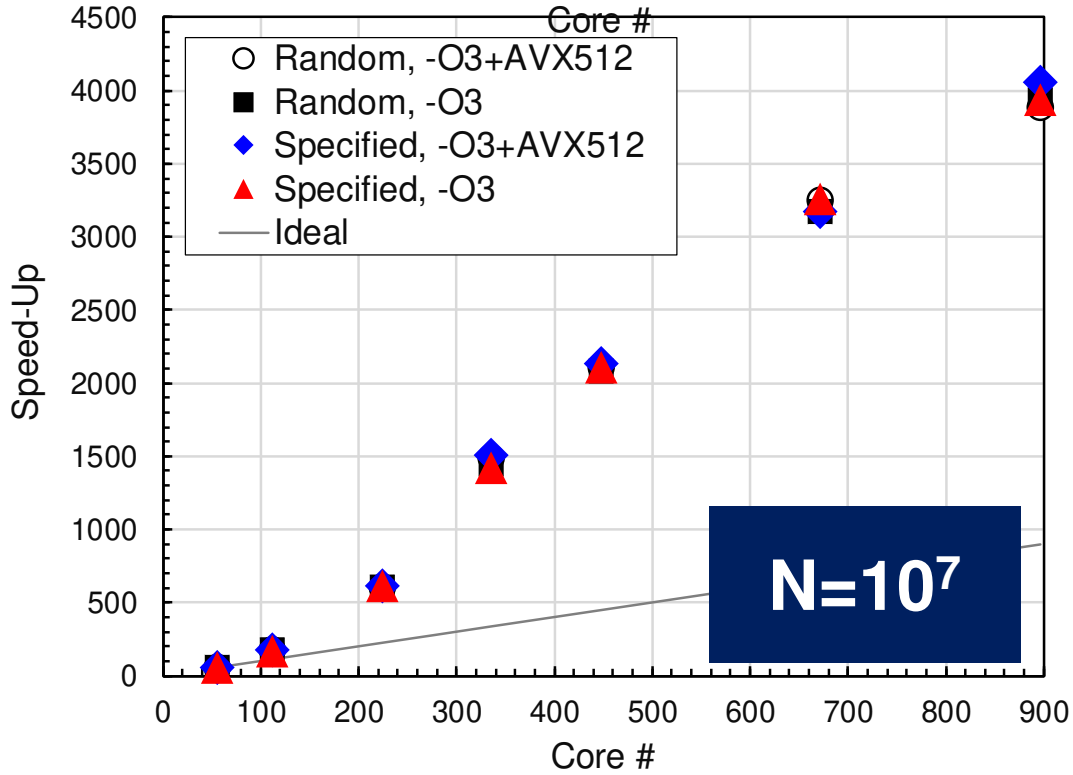




- MPI Processes per Node
  - 16x2, 24x2, 28x2
- N=10^6
  - No diff. if core# is larger
- N=10^7
  - At same core#, 16x2 is the best: Memory is more efficiently utilized



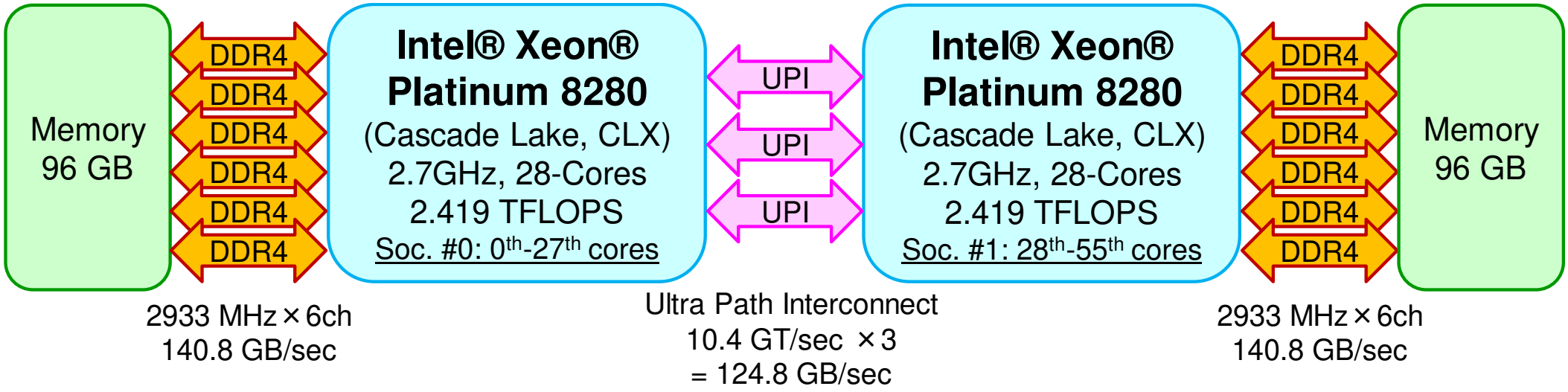




Up to 896 cores (16-nodes)

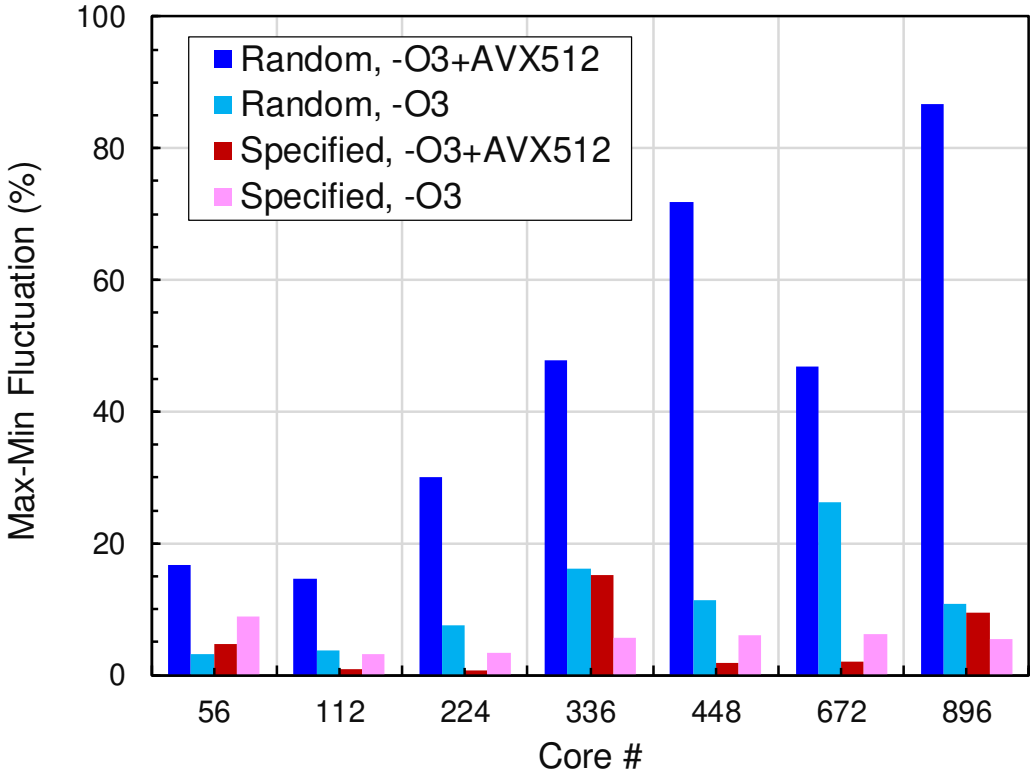
- Performance at 56 cores (= single node) = 56.0
- It is reasonable to evaluate strong scalability for multiple nodes based on the performance by a node with 56 cores
- L2 cache: 1MB/core
- L3: 38.5MB/socket (shared)
- $N=10^6$
  - Significant Comm. Overhead
- $N=10^7$
  - Very Superlinear

Category	Capacity	X-Way Set Associative	Cache Line
L1$Data	32 KB/core	8-Way	64B
L1$Instruction	32 KB/core	8-Way	64B
L2	1.00 MB/core	16-Way	64B
L3	38.5 MB/socket	11-Way	64B

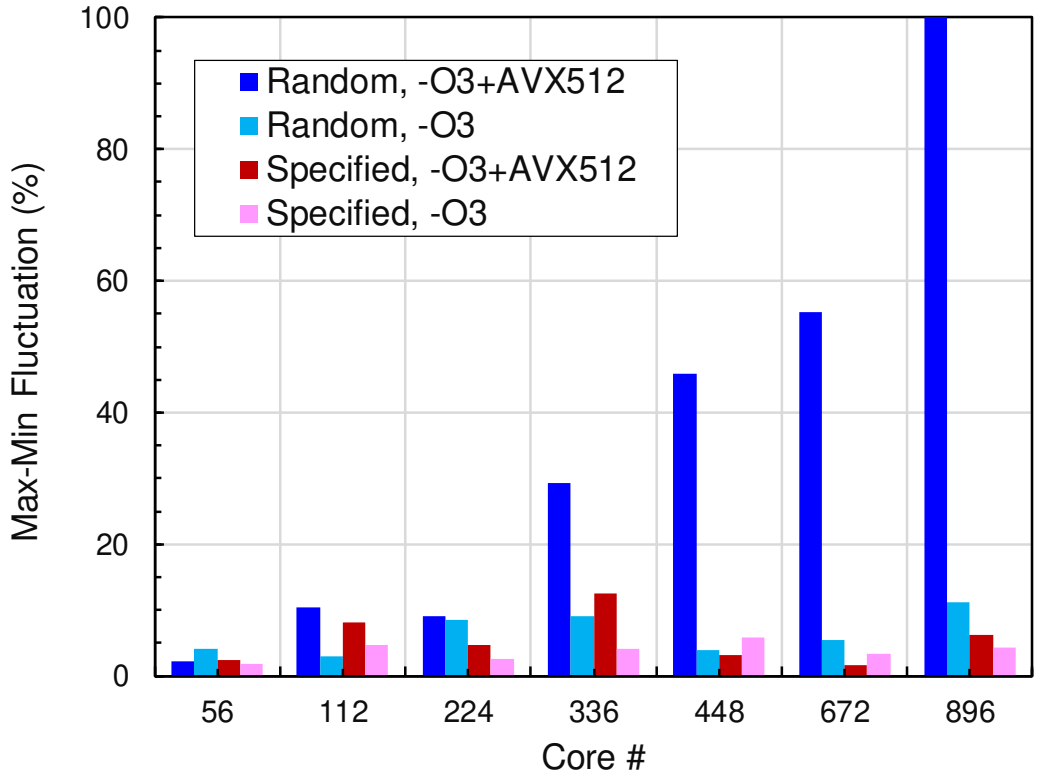


Fluctuation of Computation Time for 5 measurements

N=10^6



N=10^7

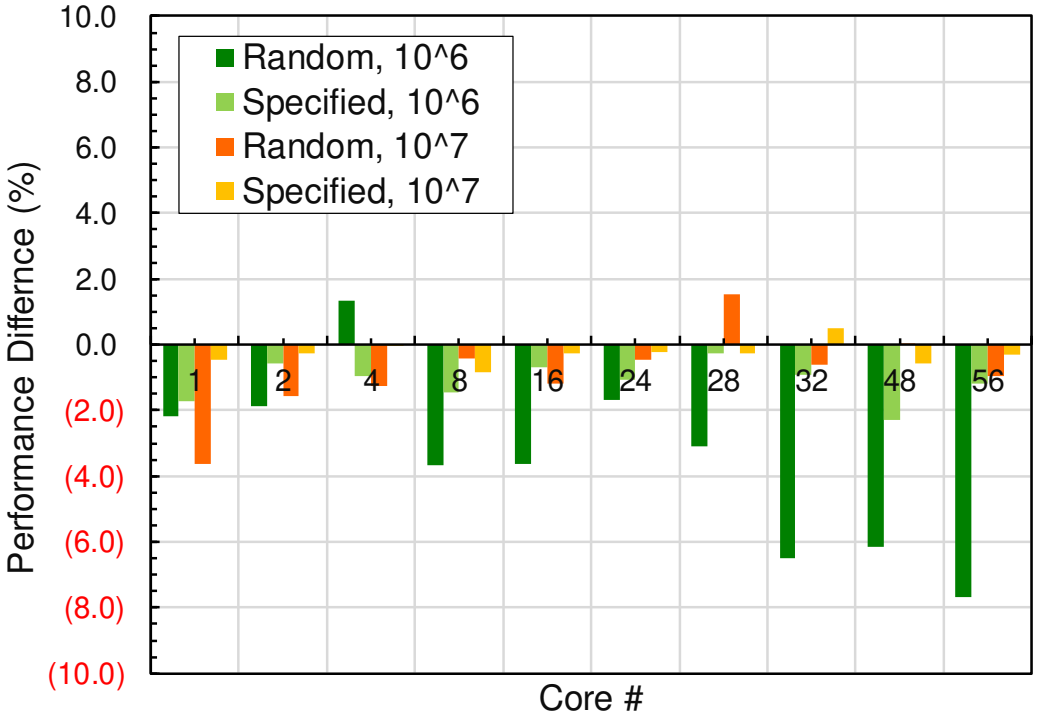


“-O3+AVX512” and “-O3” Best Case of 5 Measurements

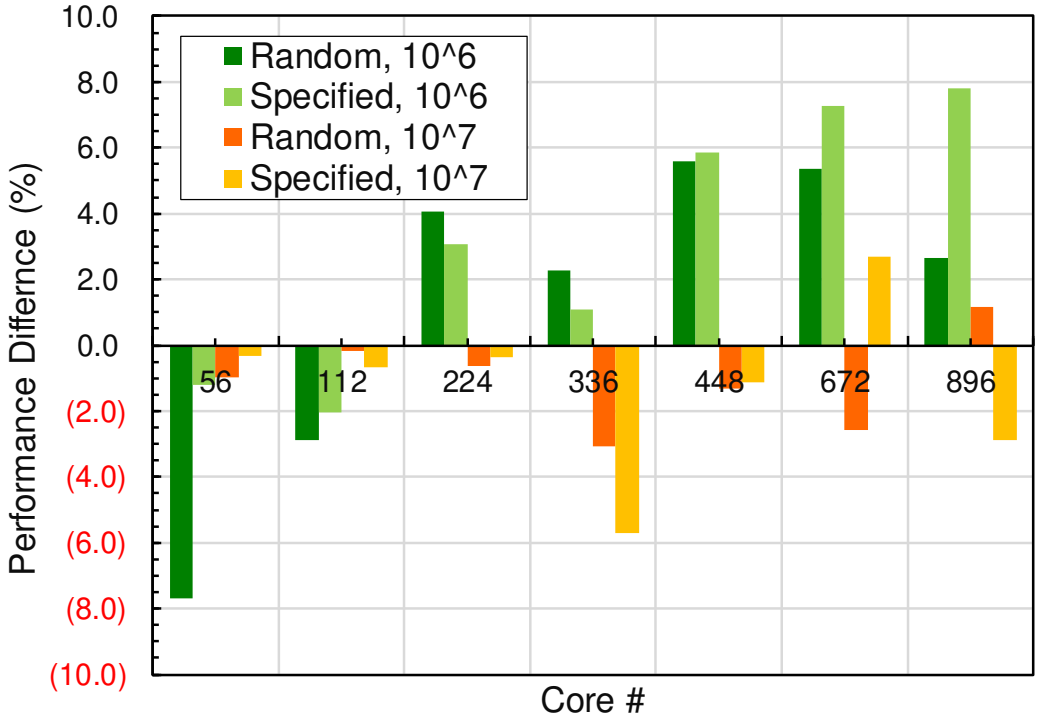
+: -O3 is better, -: -O3 is worse

“-O3” is rather faster in 10^6 cases with many cores

up to 1 node, 56cores



up to 16 nodes, 896 cores



Summary: Parallel FEM

- Proper design of data structure of distributed local meshes.

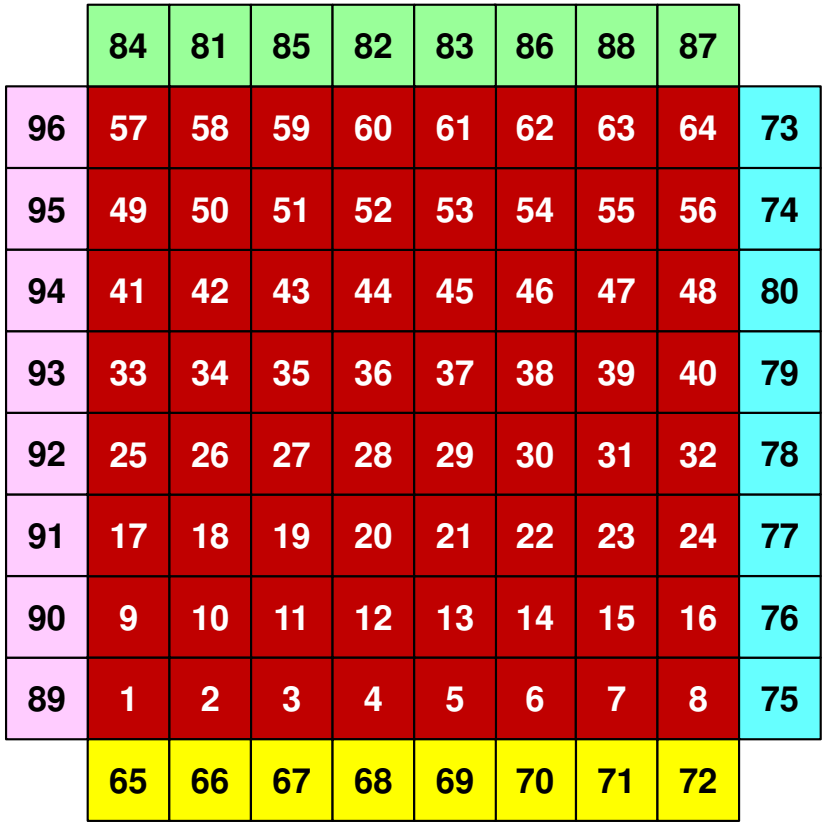
- Open Technical Issues
  - Parallel Mesh Generation, Parallel Visualization
  - Parallel Preconditioner for Ill-Conditioned Problems
  - Large-Scale I/O

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

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



[A]{p}= {q} (Original): 1d.c

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

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

[A]{p}= {q} (Mod.): No Copy for RECV: 1d2.c

```
StatSend = malloc(sizeof(MPI_Status) * 2 * NeibPETot);
RequestSend = malloc(sizeof(MPI_Request) * 2 * NeibPETot);

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(&P[ir+N], len_r, MPI_DOUBLE, NeibPE[neib],
            0, MPI_COMM_WORLD, &RequestSend[neib+NeibPETot]);
}

MPI_Waitall(2*NeibPETot, RequestSend, StatSend);
```

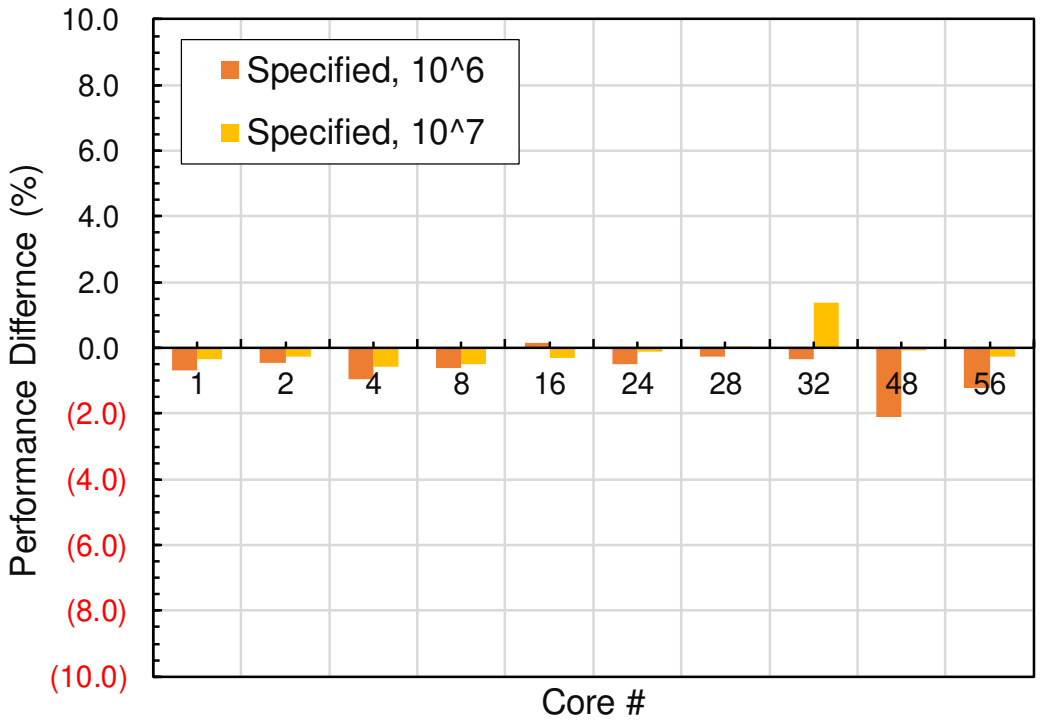
“Original” and “Modified” Best Case of 5 Measurements

+: “Modified” is better, -: “Modified” is worse

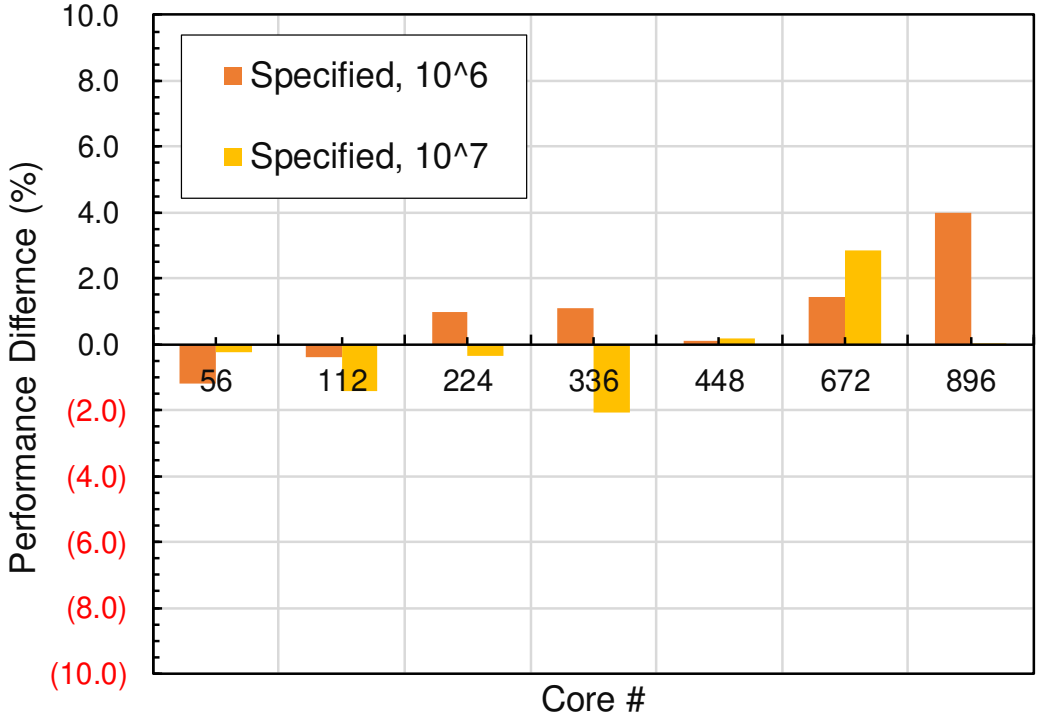
“Modified” is faster in 10^6 cases with many cores

But differences are small

up to 1 node, 56cores



up to 16 nodes, 896 cores



Further Investigations

- Compare with/without NUMA control

```
mpiexec.hydra -n ${PJM_MPI_PROC} numactl -l ./a.out
mpiexec.hydra -n ${PJM_MPI_PROC} ./a.out
```

- MPI_Send/MPI_Recv can be used for 1D case
  - Only limited number of neighbors

- Explain why number of iterations does not change, as number of MPI processes changes.