Introduction to Parallel FEM in Fortran
Parallel Data Structure

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Parallel Computing

- Faster, Larger & More Complicated

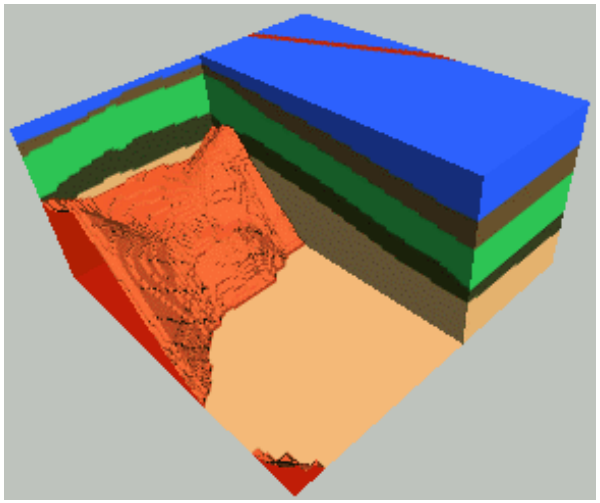
- Scalability
  - Solving N^x scale problem using N^x computational resources during same computation time
    - for large-scale problems: **Weak Scaling**
    - e.g. CG solver: more iterations needed for larger problems
  - Solving a problem using N^x computational resources during 1/N computation time
    - for faster computation: **Strong Scaling**

What is Parallel Computing ? (1/2)

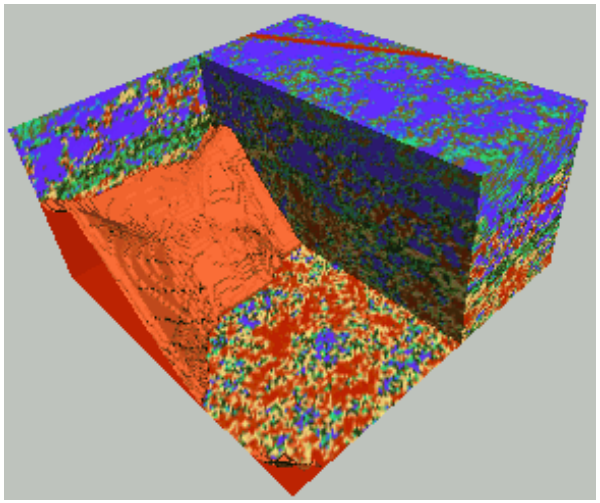
- to solve larger problems faster

Homogeneous/Heterogeneous Porous Media

Lawrence Livermore National Laboratory



Homogeneous

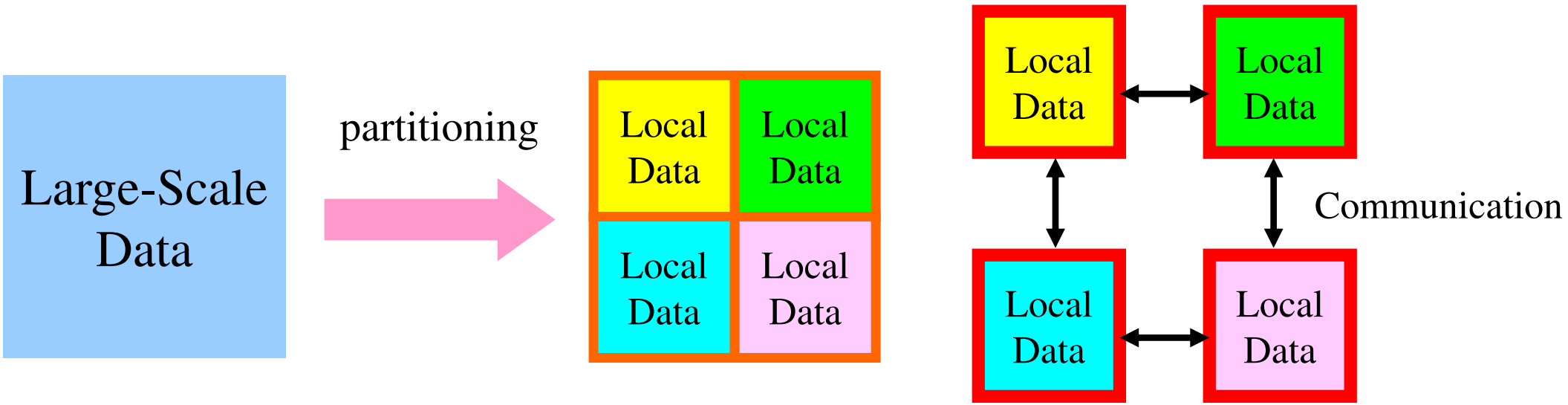


Heterogeneous

very fine meshes are required for simulations of heterogeneous field.

What is Parallel Computing ? (2/2)

- PC with 1GB memory : 1M meshes are the limit for FEM
  - Southwest Japan with 1,000km x 1,000km x 100km in 1km mesh -> 10^8 meshes
- Large Data -> Domain Decomposition -> Local Operation
- Inter-Domain Communication for Global Operation



What is Communication ?

- Parallel Computing -> Local Operations
- Communications are required in Global Operations for Consistency.

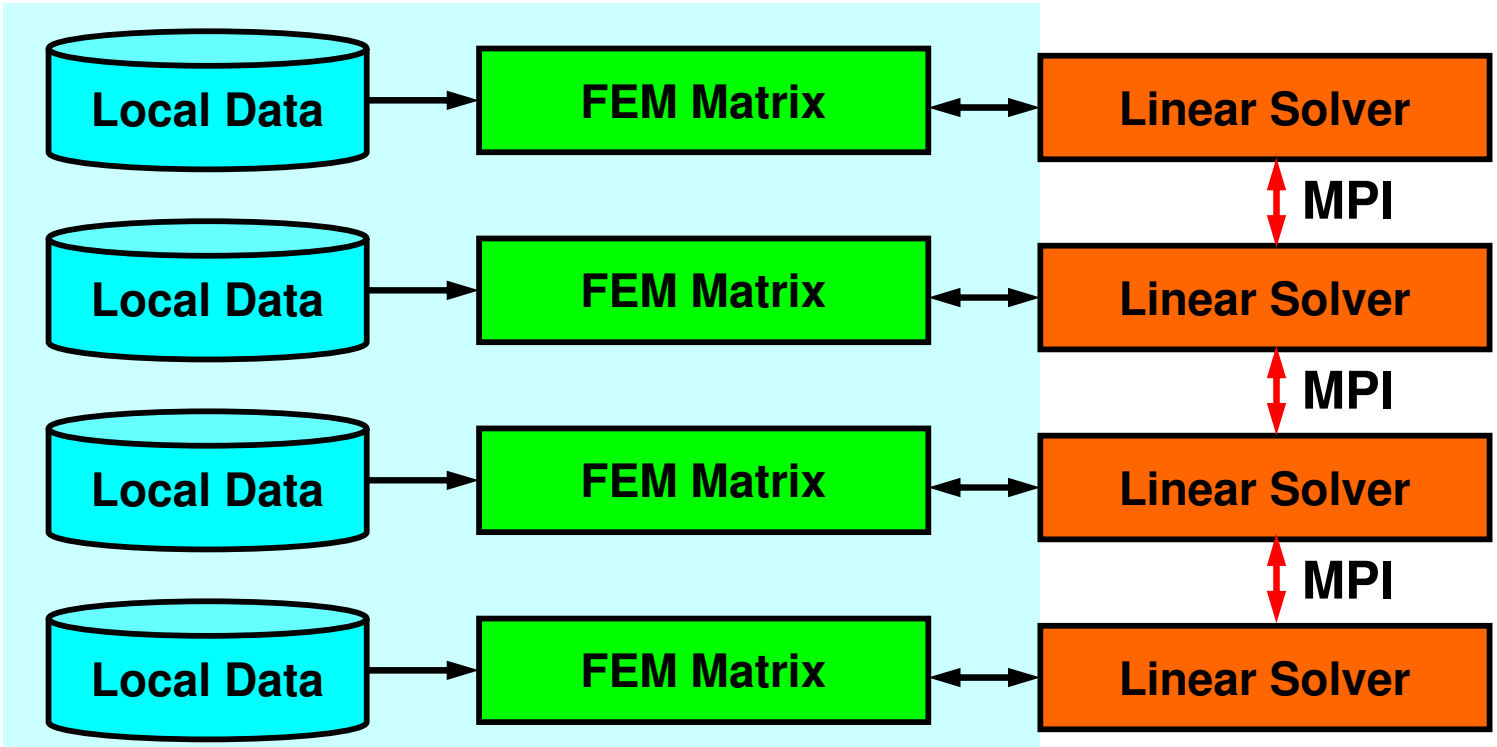
Operations in Parallel FEM

SPMD: Single-Program Multiple-Data

Large Scale Data -> partitioned into Distributed Local Data Sets.

FEM code can assemble coefficient matrix for each local data set : this part could be completely local, same as serial operations

Global Operations & Communications happen only in Linear Solvers dot products, matrix-vector multiply, preconditioning

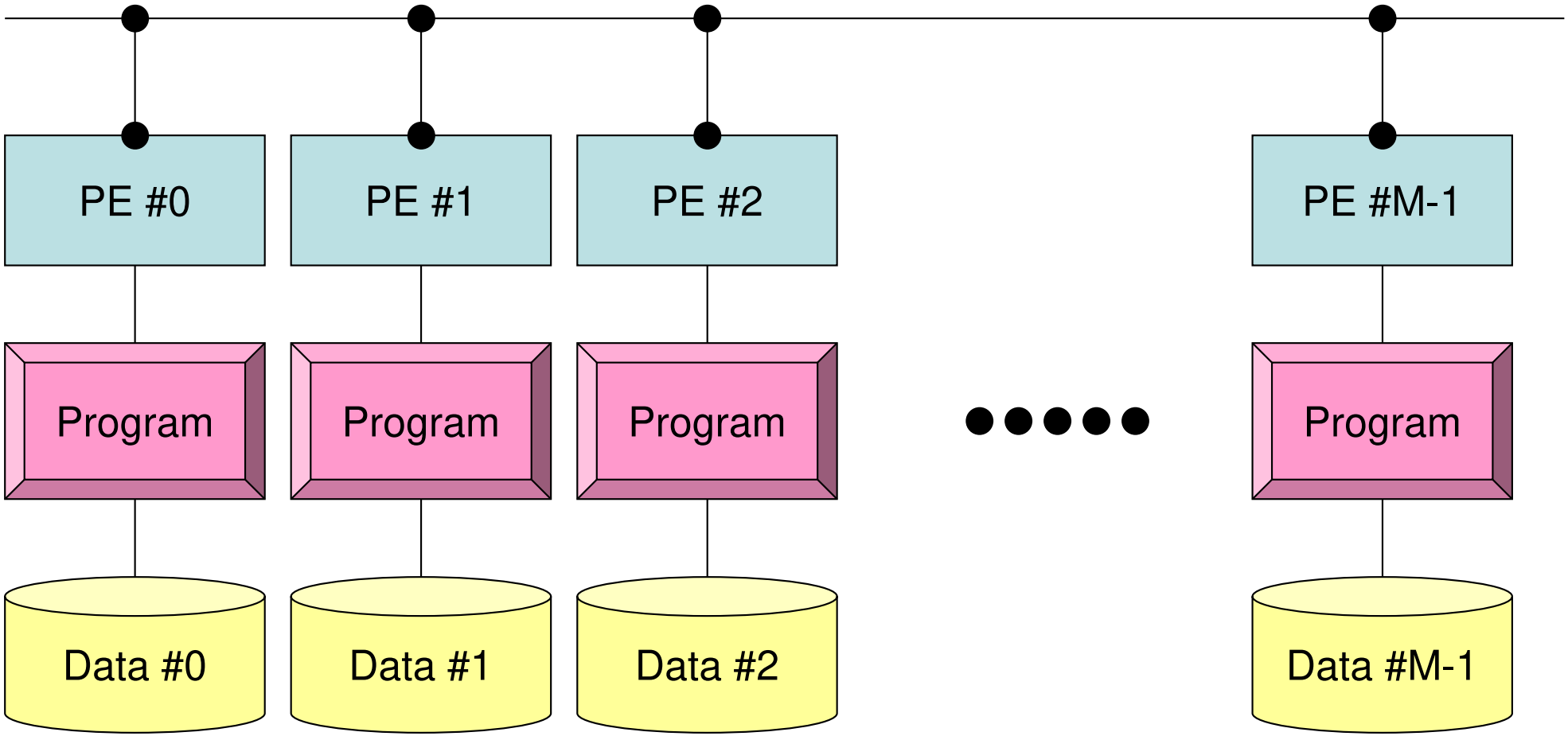


PE: Processing Element
Processor, Domain, Process

SPMD

You understand 90% MPI, if you understand this figure.

```
mpirun -np M <Program>
```



Each process does same operation for different data

Large-scale data is decomposed, and each part is computed by each process

It is ideal that parallel program is not different from serial one except communication.

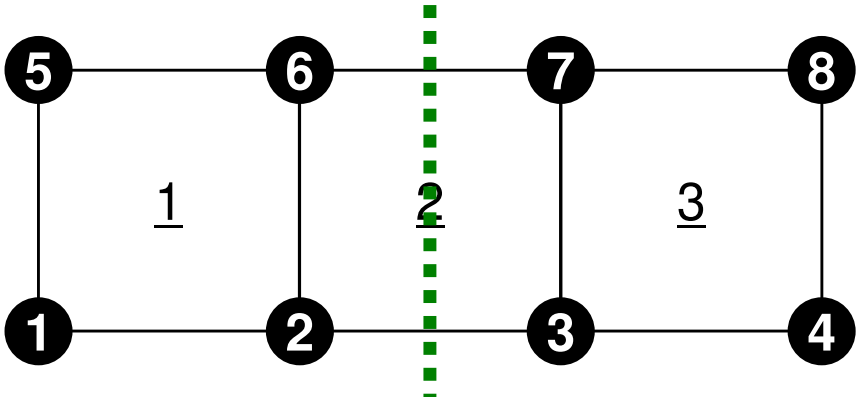
Parallel FEM Procedures

- Design on “Local Data Structure” is important
  - for SPMD-type operations in the previous page

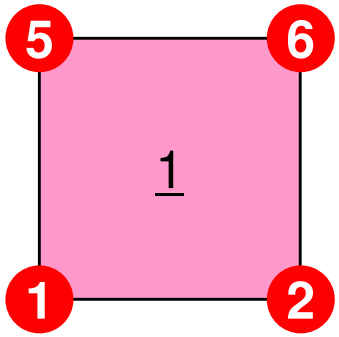
- Matrix Generation
- Preconditioned Iterative Solvers for Linear Equations

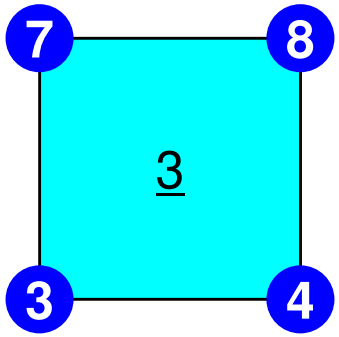
Bi-Linear Square Elements

Values are defined on each node

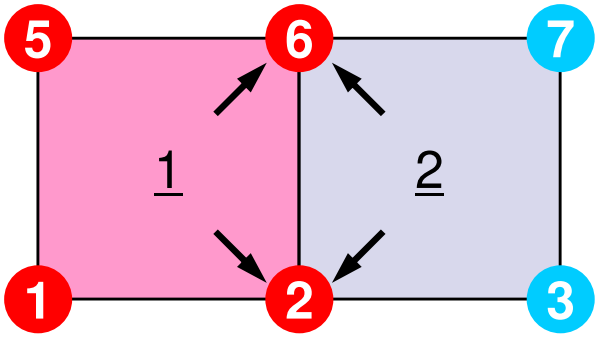


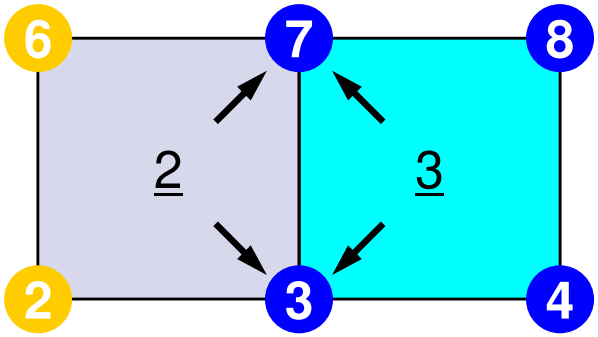
divide into two domains by “node-based” manner, where number of “nodes (vertices)” are balanced.



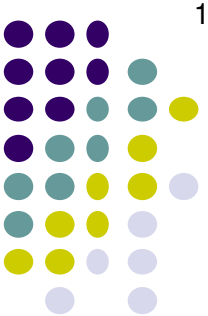


Local information is not enough for matrix assembling.





Information of overlapped elements and connected nodes are required for matrix assembling on boundary nodes.

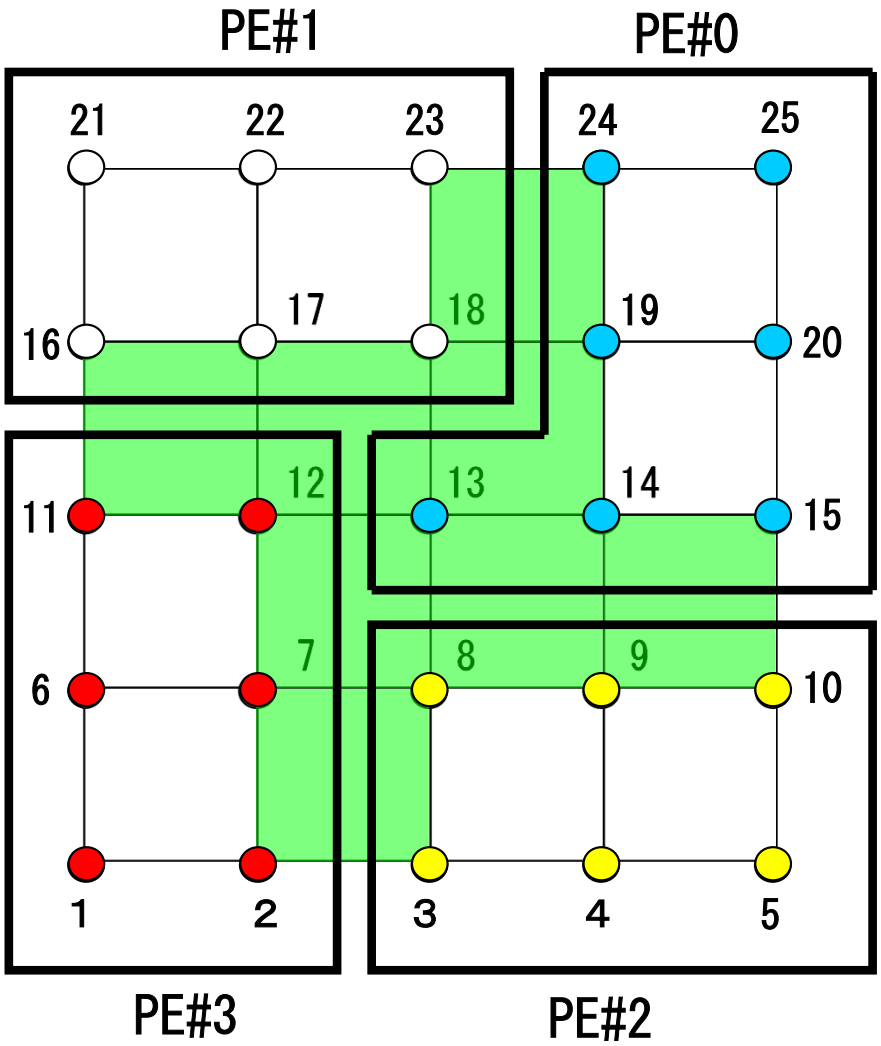


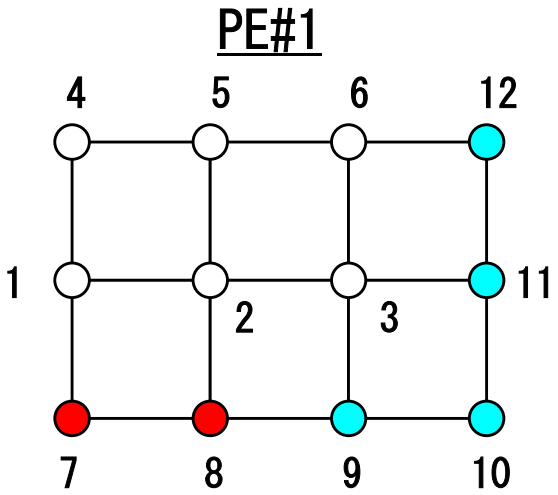
Local Data of Parallel FEM

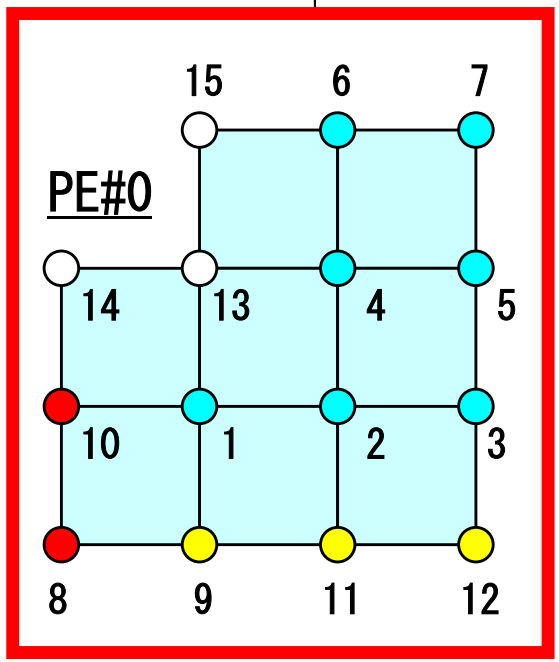
- Node-based partitioning for preconditioned iterative solvers
- Local data includes information for :
  - Nodes originally assigned to the partition/PE
  - Elements which include the nodes (originally assigned to the Partition/PE)
  - All nodes which form the elements but out of the partition
- Nodes are classified into the following 3 categories from the viewpoint of the message passing
  - Internal nodes originally assigned nodes
  - External nodes in the overlapped elements but out of the partition
  - Boundary nodes *external nodes* of other partition (part of internal nodes)
- Communication table between partitions
- NO global information required except partition-to-partition connectivity

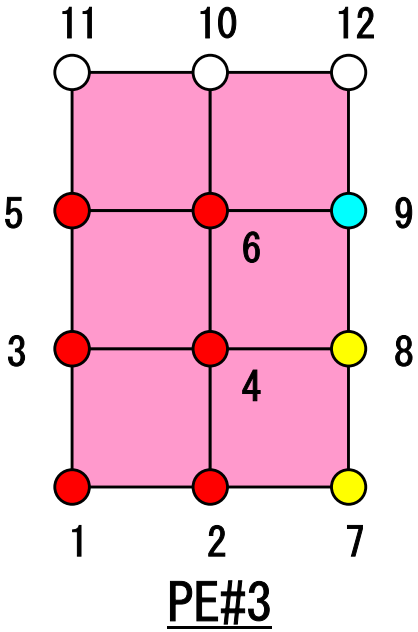
Node-based Partitioning

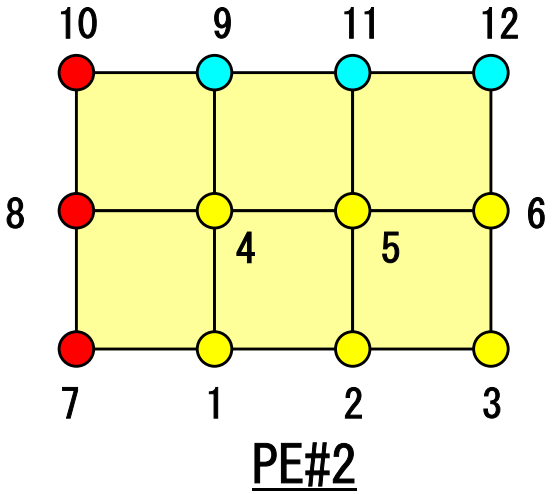
internal nodes - elements - external nodes





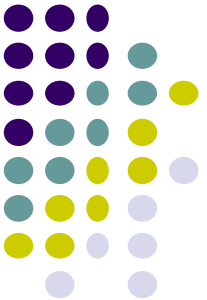






Node-based Partitioning

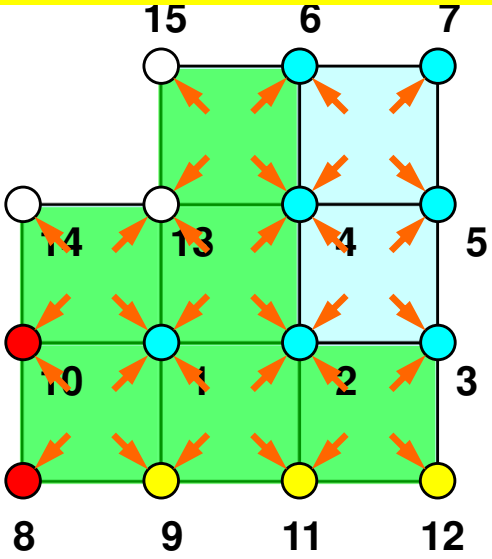
internal nodes - elements - external nodes

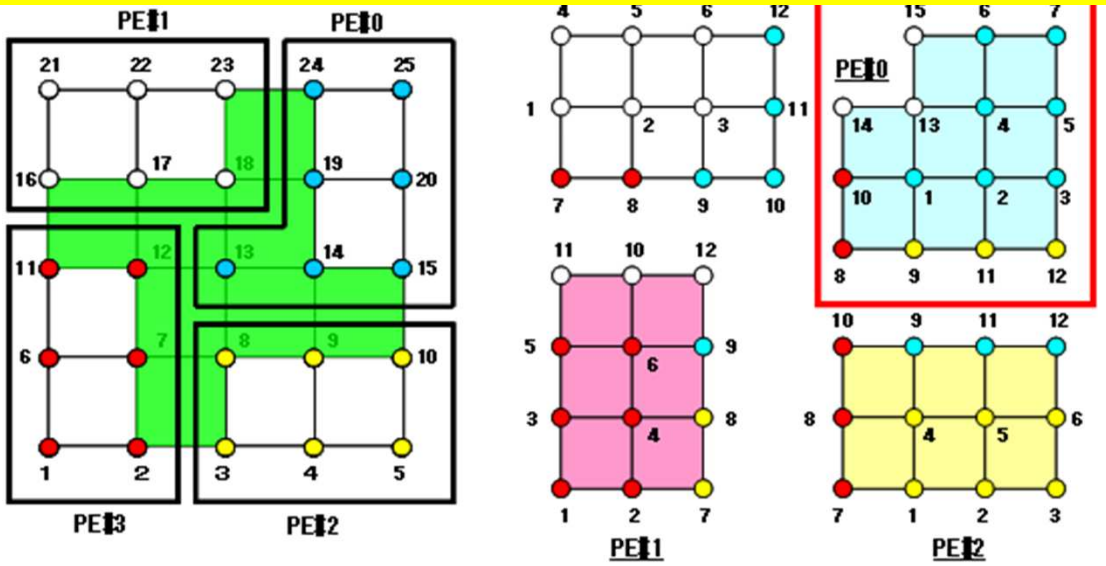


- Partitioned nodes themselves (Internal Nodes) 内点
- Elements which include Internal Nodes 内点を含む要素
- External Nodes included in the Elements 外点

  in overlapped region among partitions.

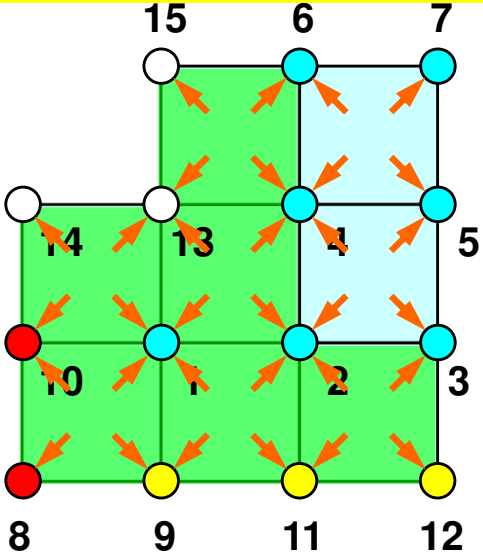
- Info of External Nodes are required for completely local element–based operations on each processor.

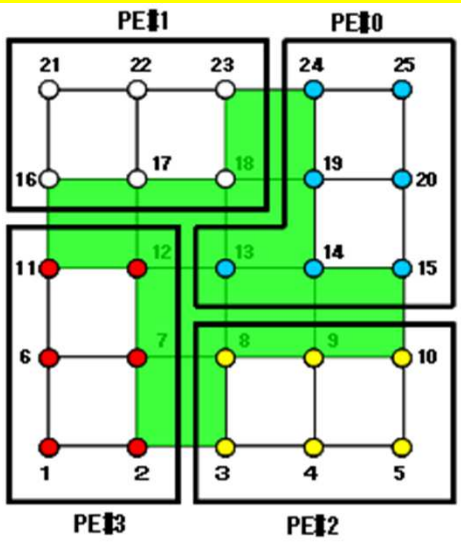


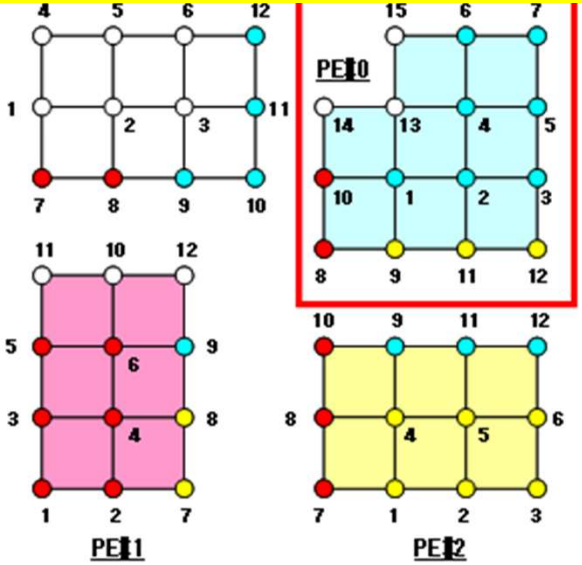


We do not need communication during matrix assemble !!

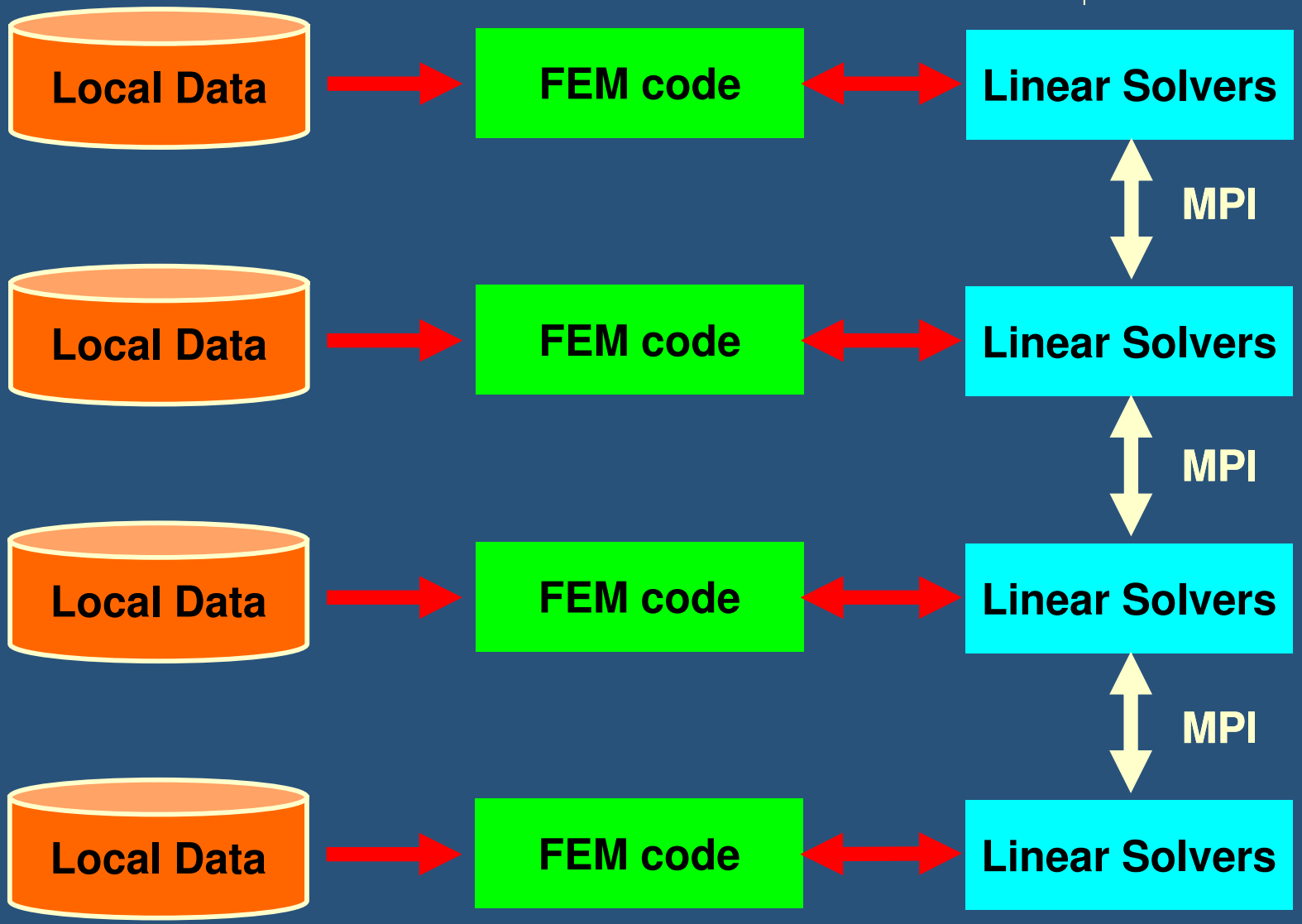
- Partitioned nodes themselves (Internal Nodes)
- Elements which include Internal Nodes
- External Nodes included in the Elements
  in overlapped region among partitions.
- Info of External Nodes are required for completely local element–based operations on each processor.







Parallel Computing in FEM
SPMD: Single-Program Multiple-Data



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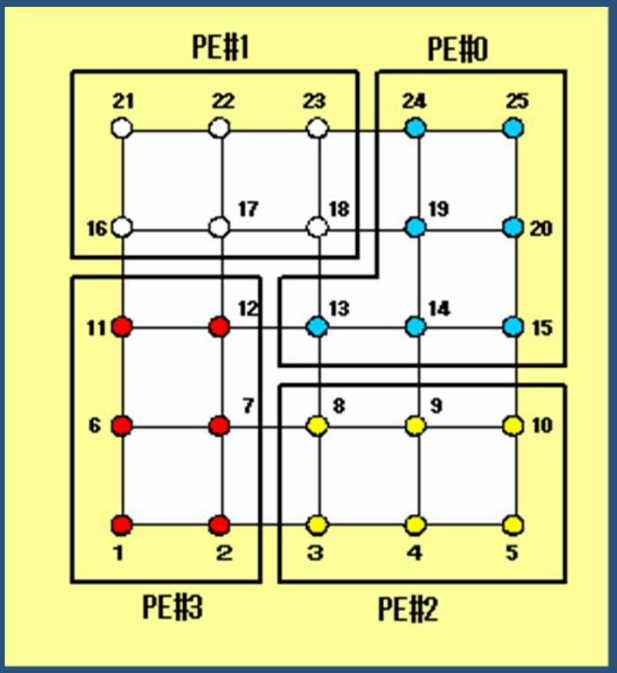

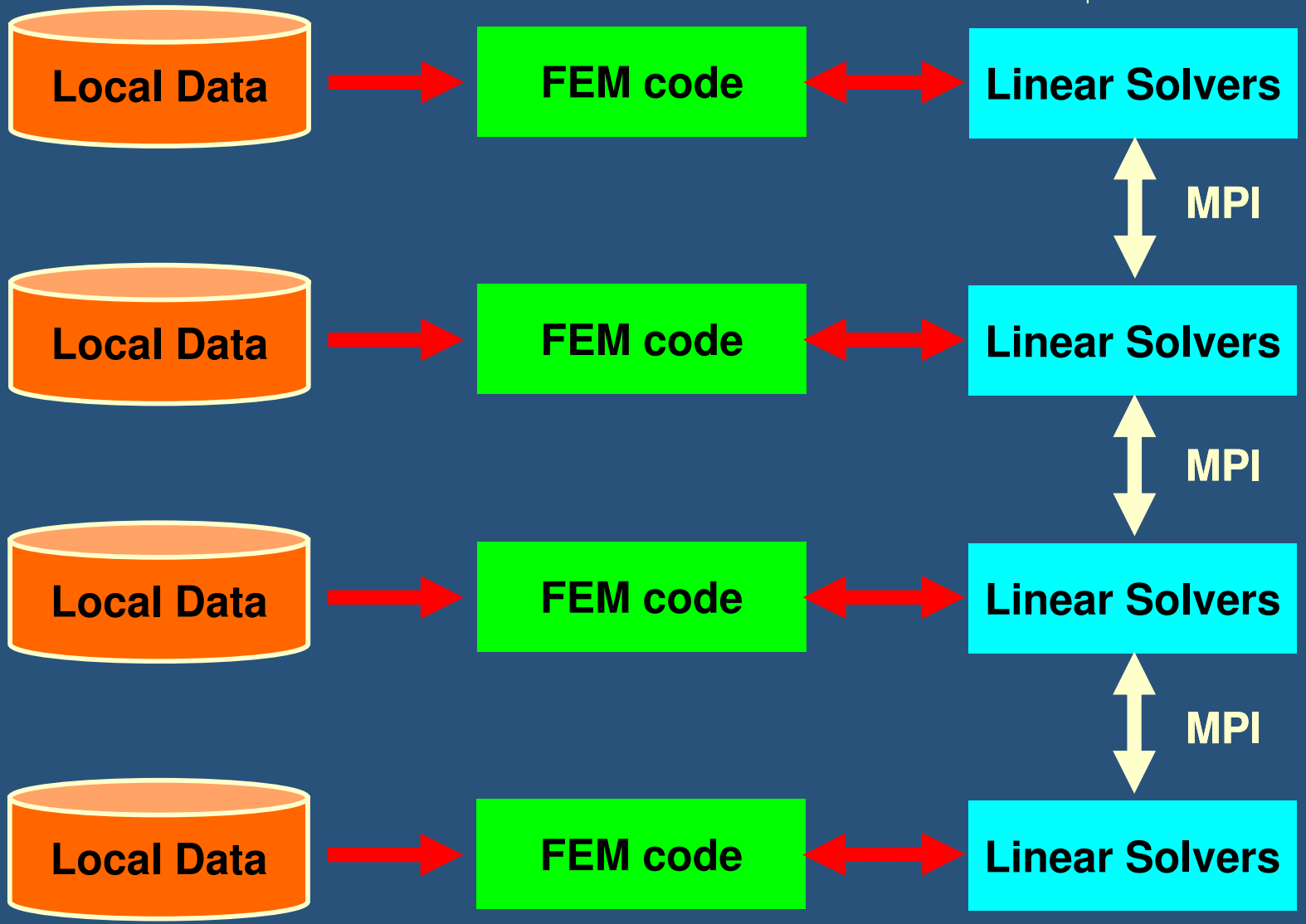

Parallel Computing in FEM

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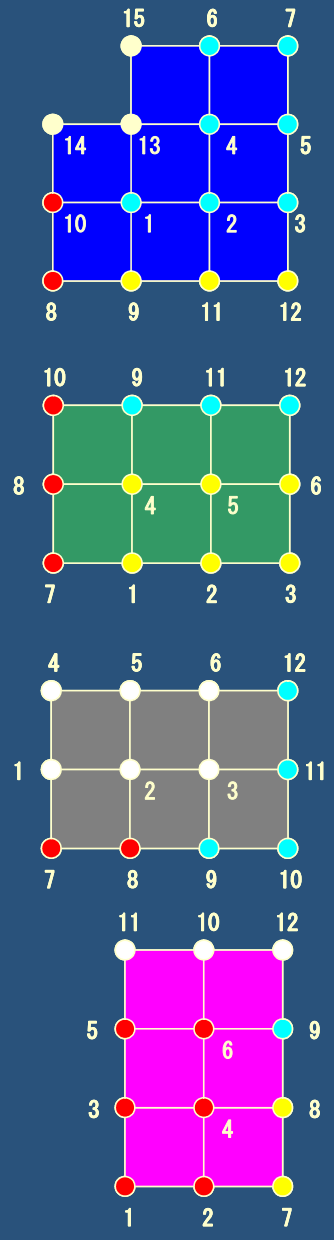

Local Data → FEM code ↔ Linear Solvers

MPI

Local Data → FEM code ↔ Linear Solvers

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Parallel Computing in FEM

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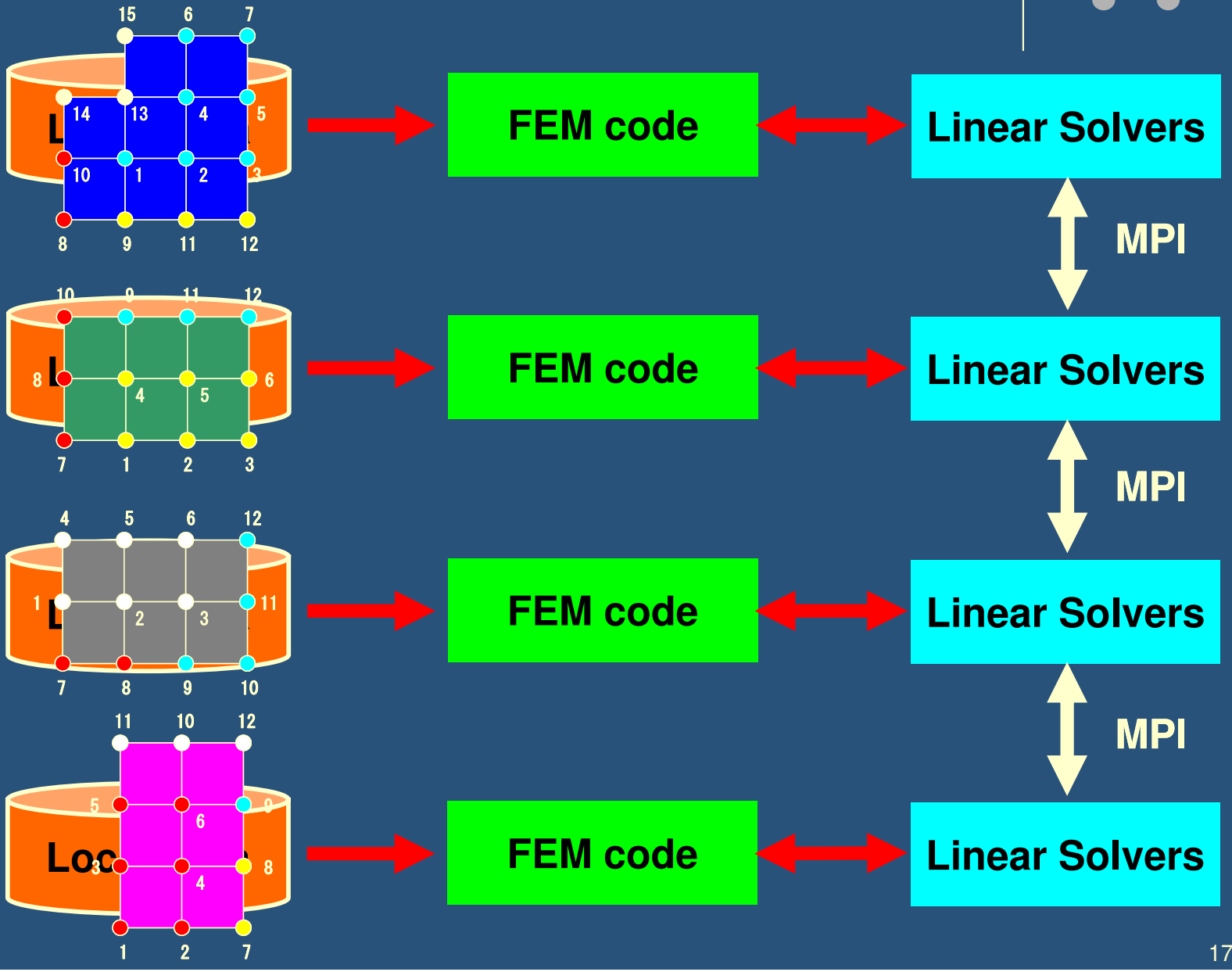

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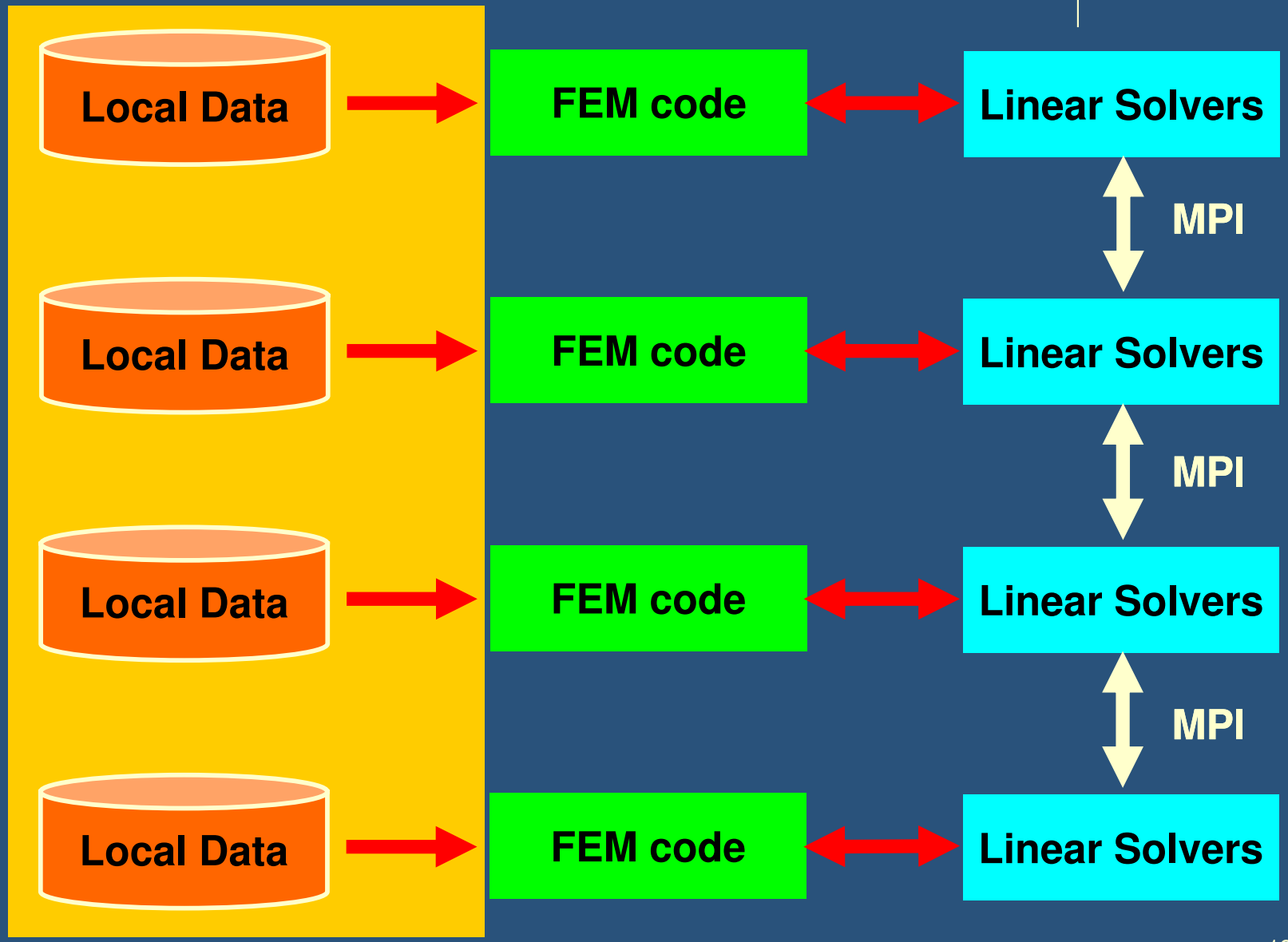
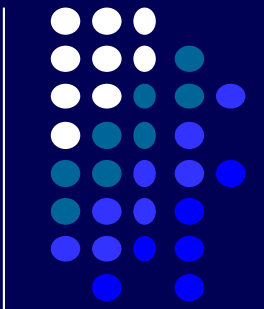
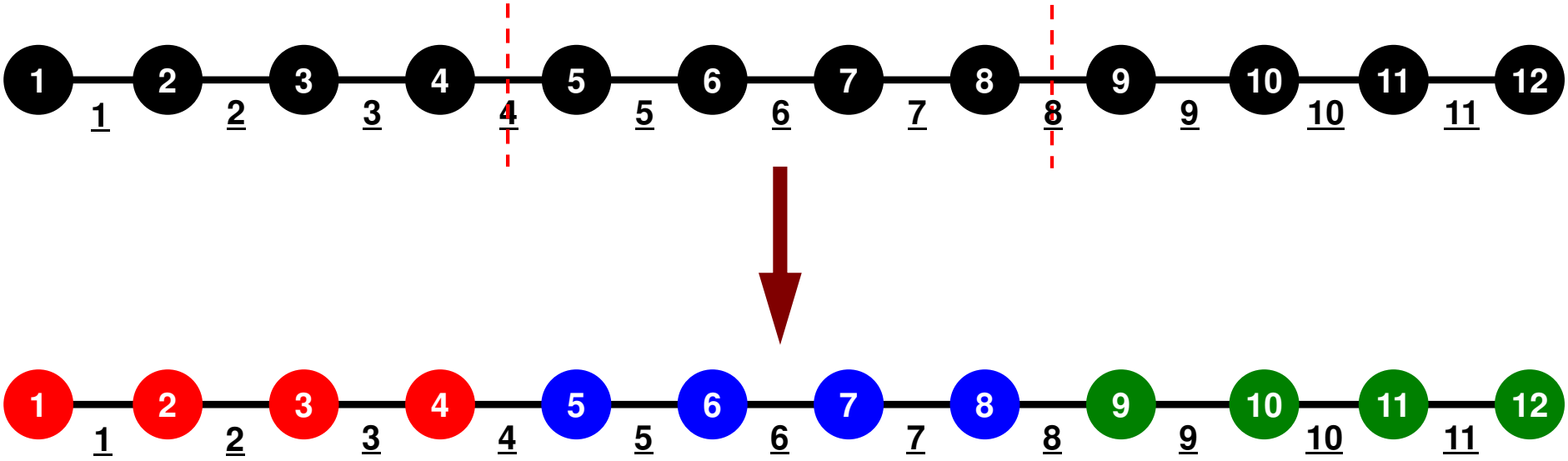


What is Communications ?



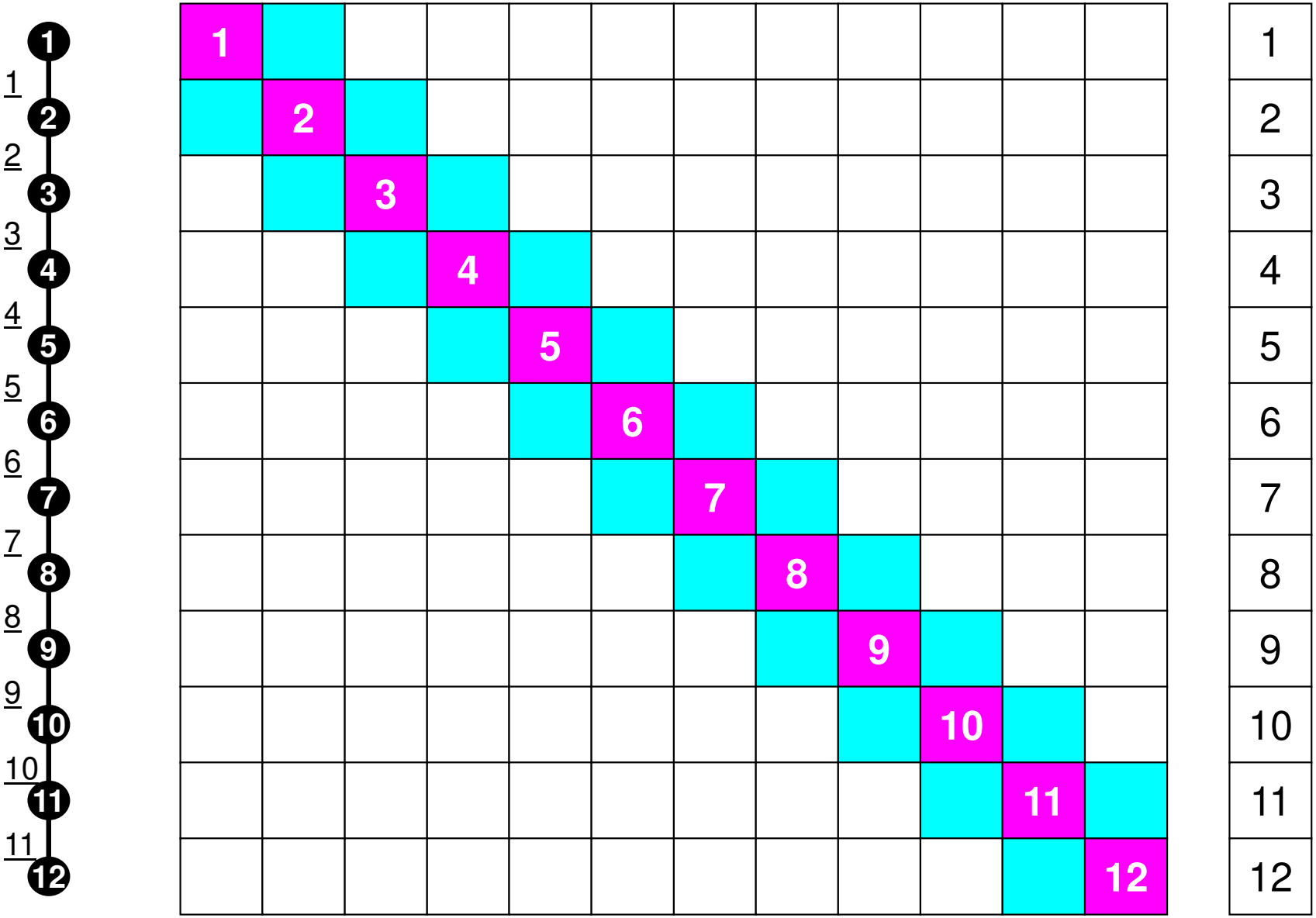
- to get information of “external nodes” from external partitions (local data)
- “Communication tables” contain the information

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

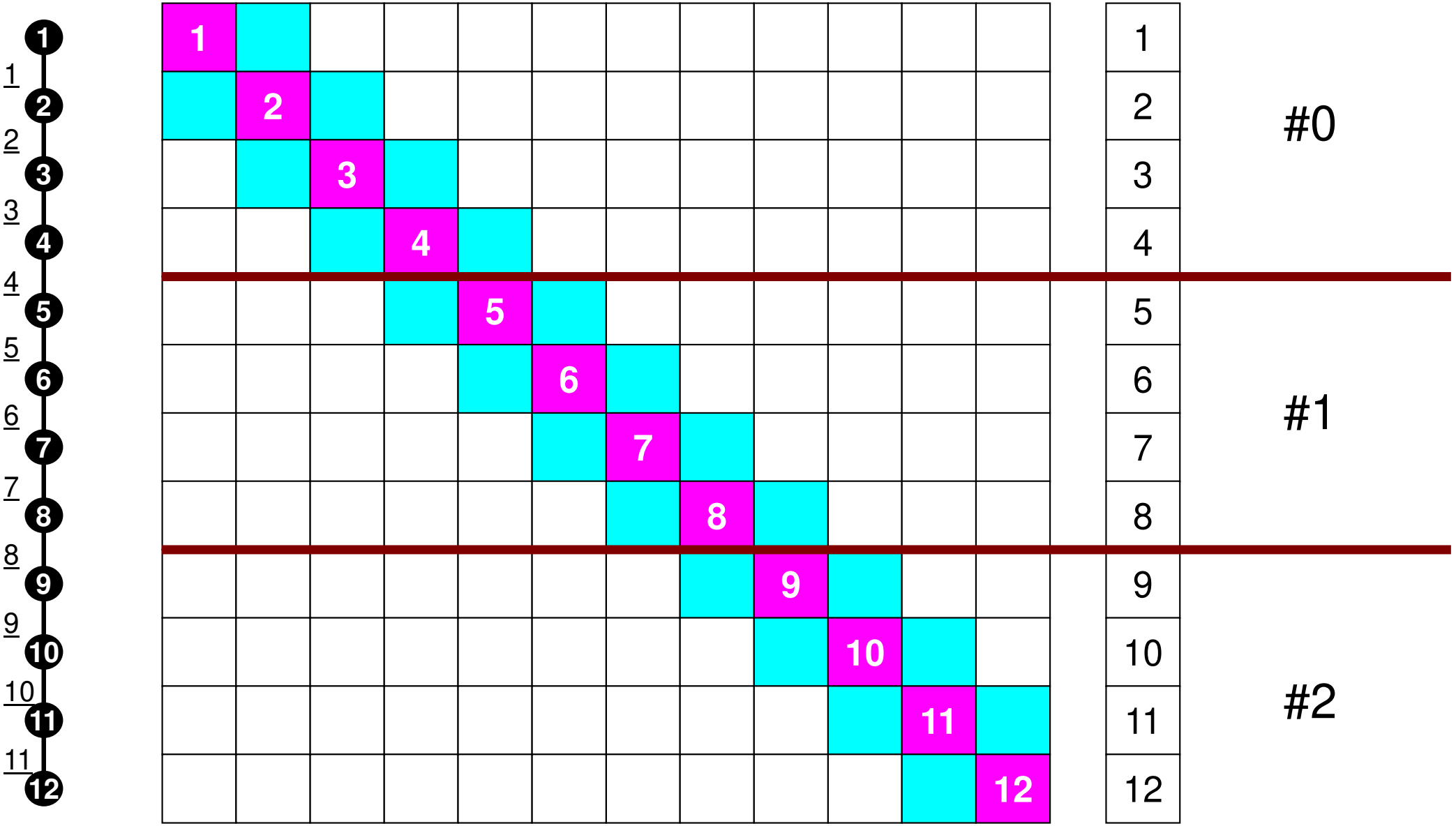


1D FEM: 12 nodes/11 elem's/3 domains

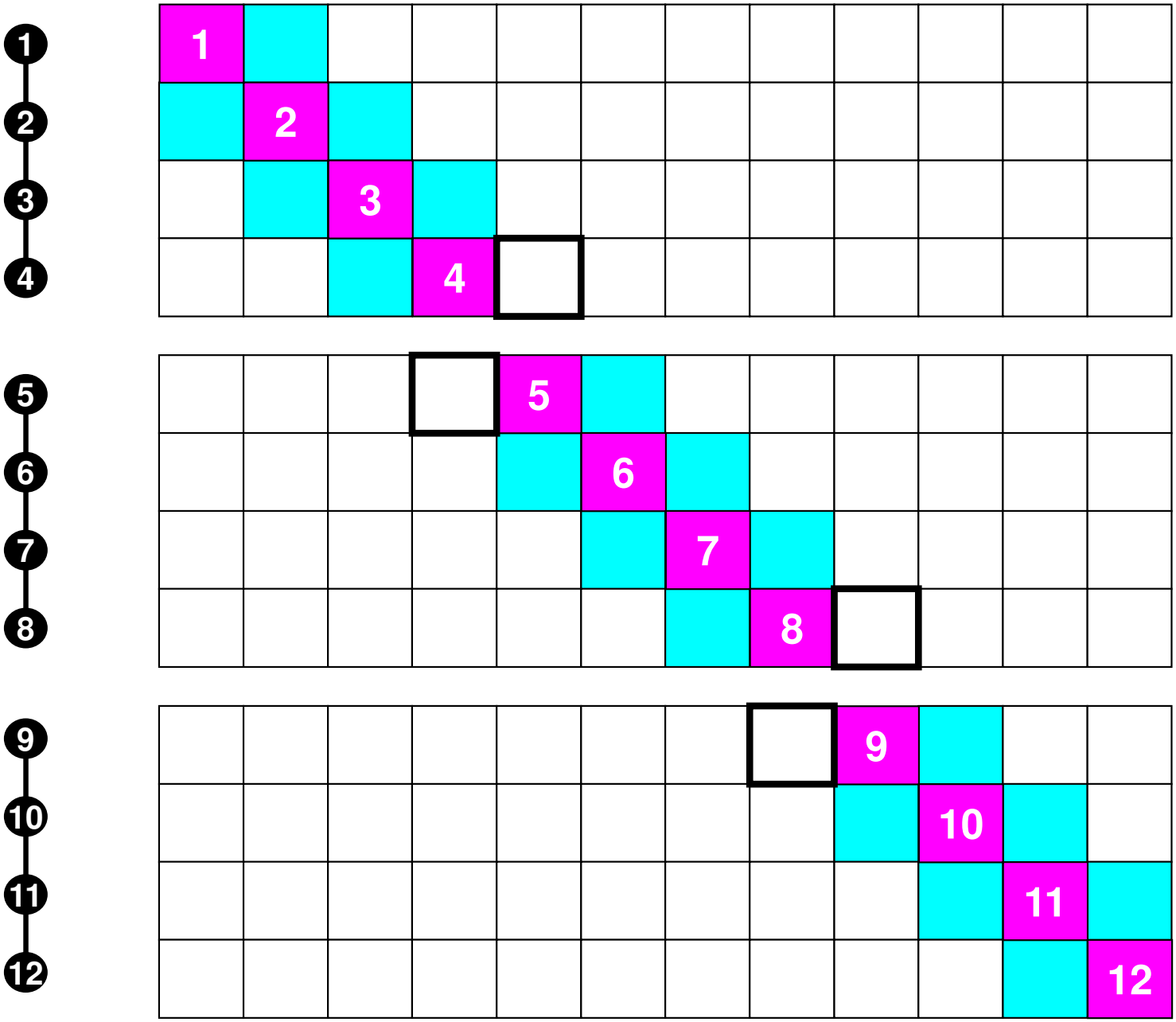
三重対角行列：Tri-Diagonal Matrix



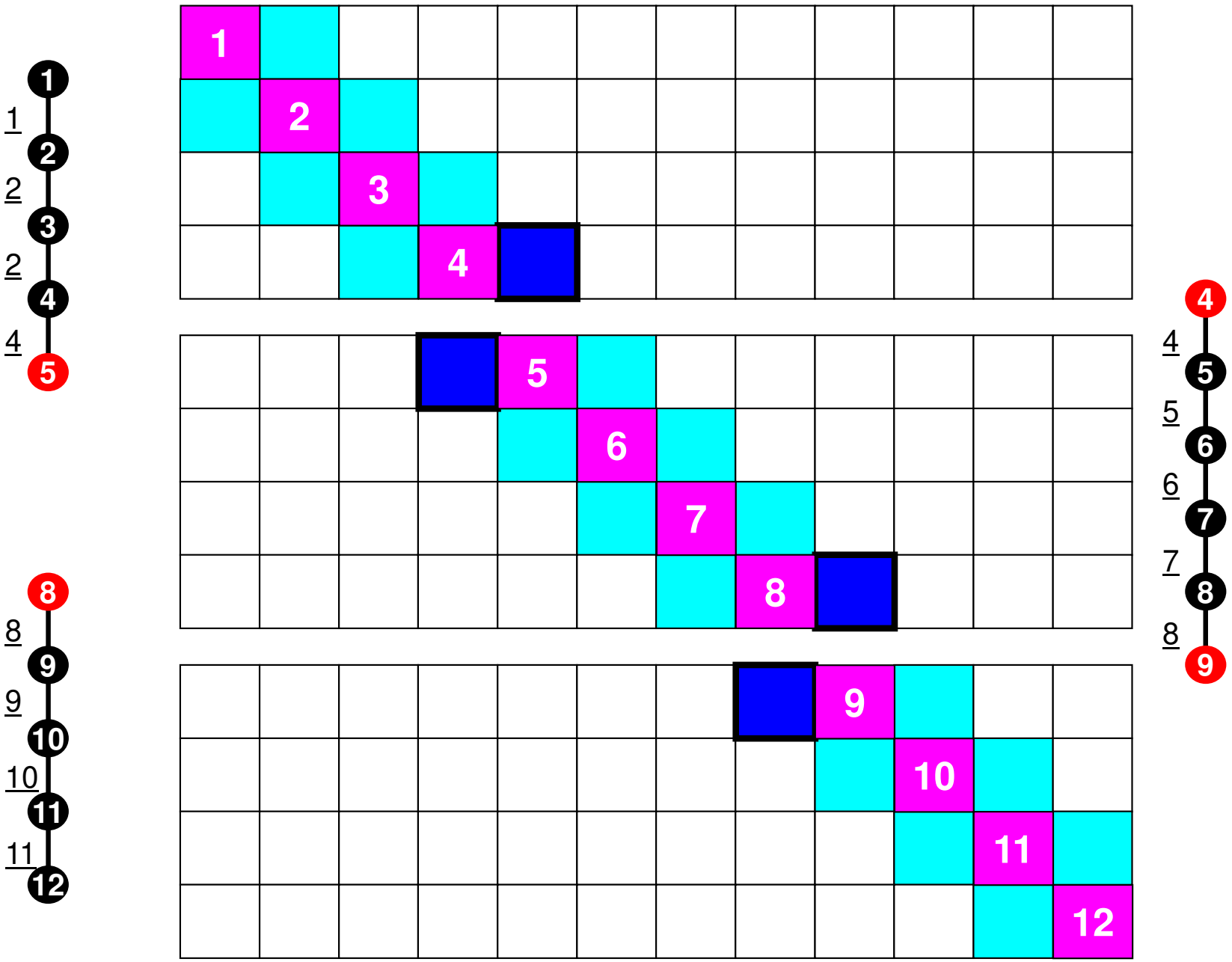
“Internal Nodes” should be balanced



Matrices are incomplete !



Connected Elements + External Nodes



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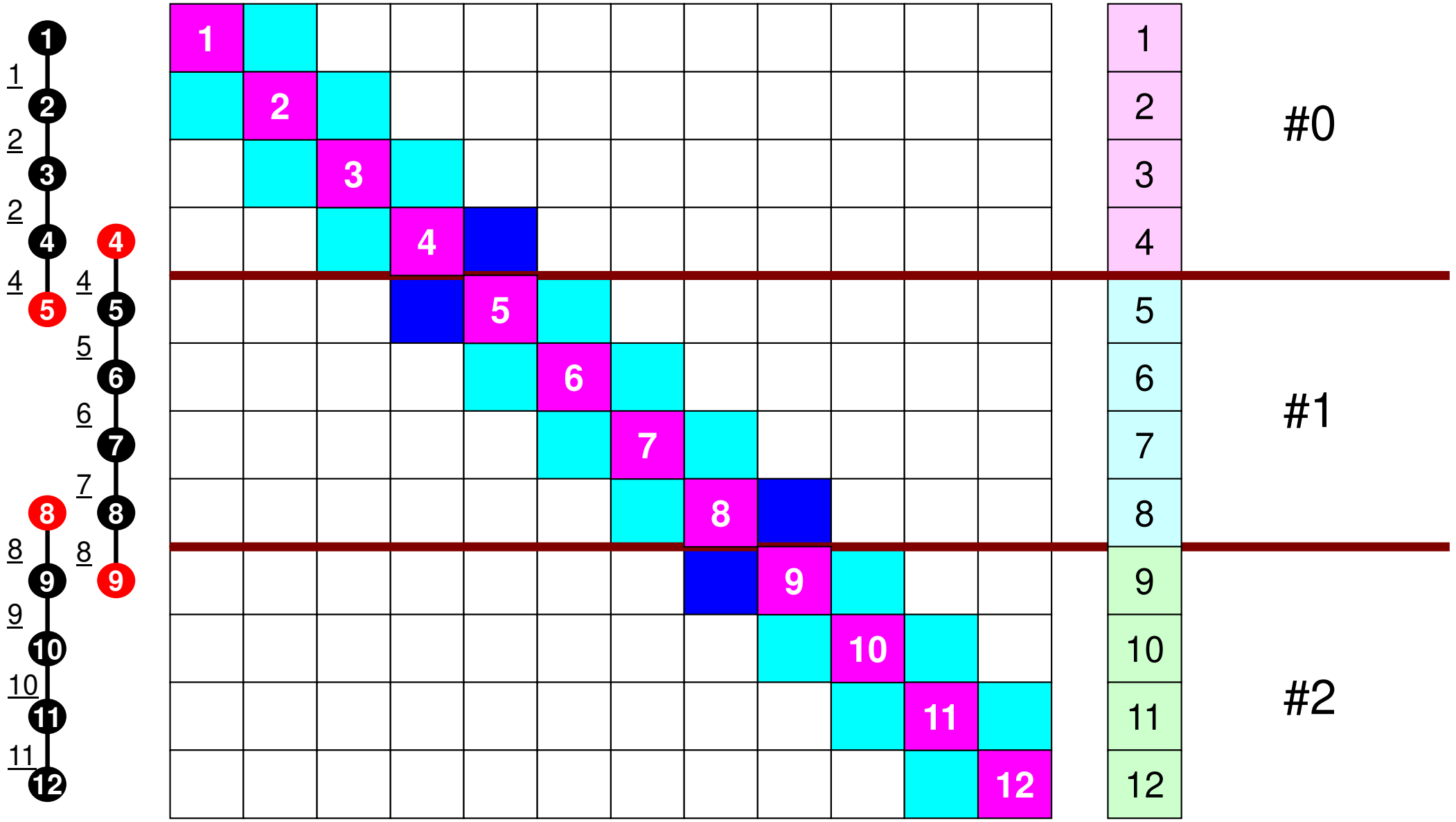

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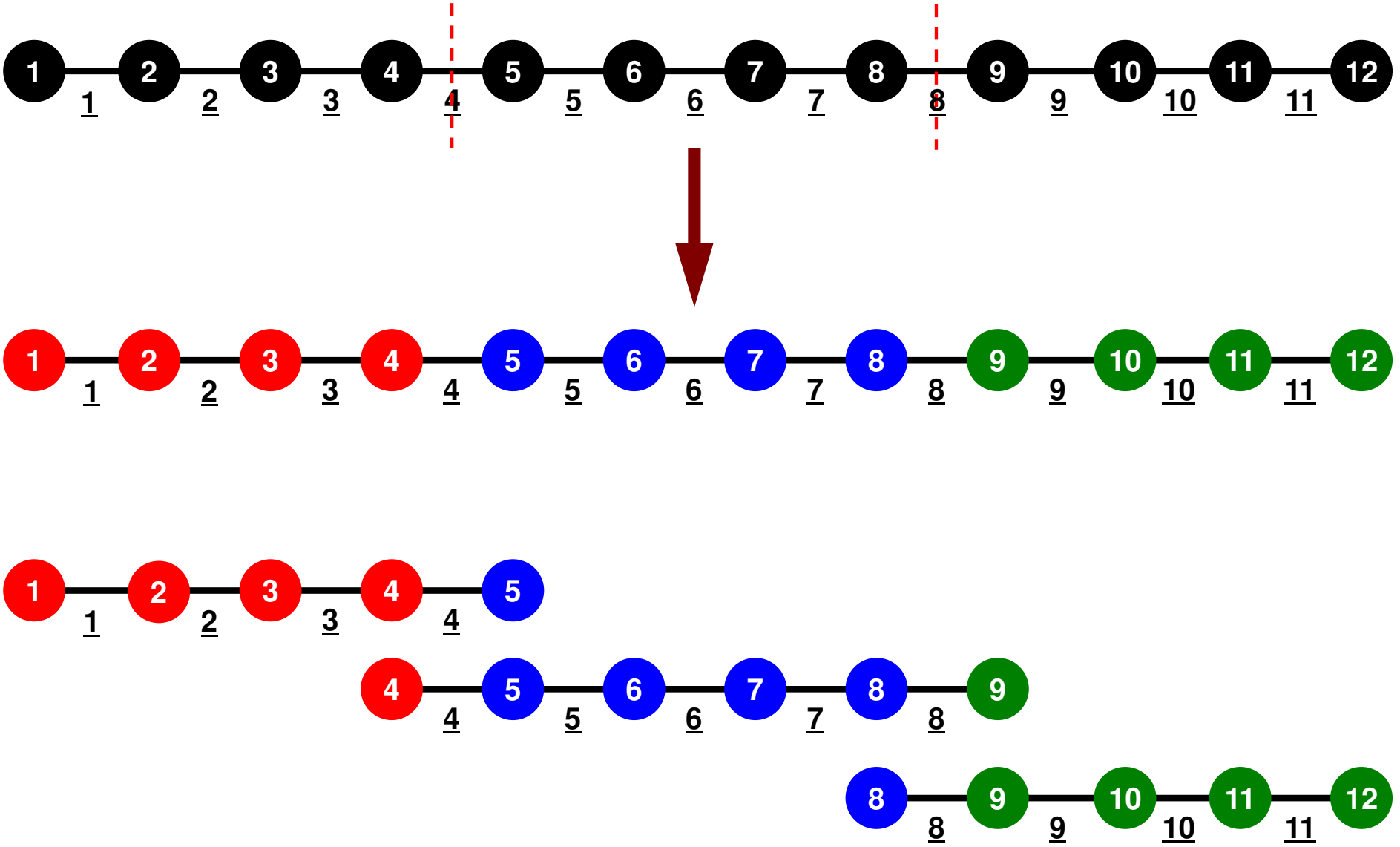
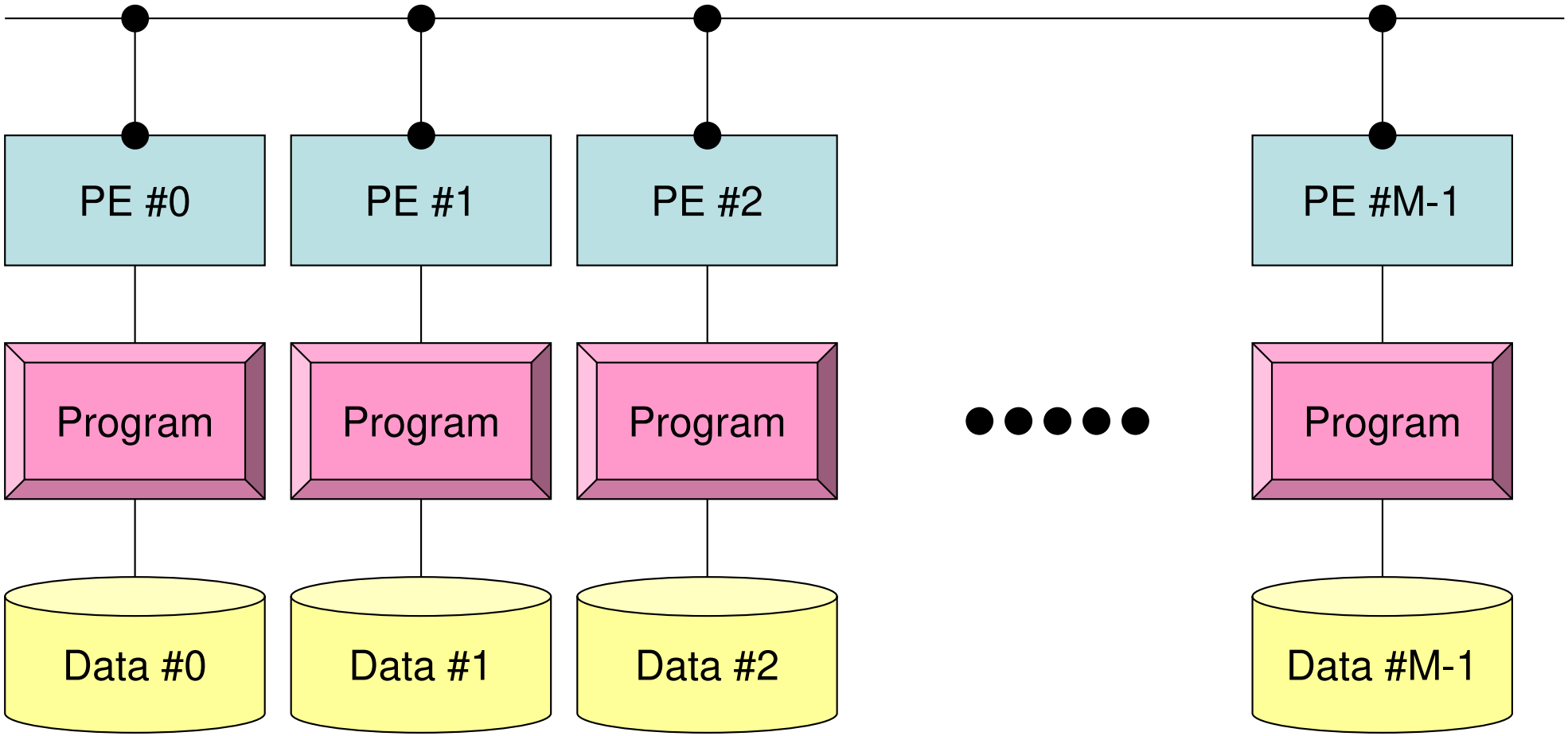


PE: Processing Element
Processor, Domain, Process

SPMD

You understand 90% MPI, if you understand this figure.

```
mpirun -np M <Program>
```



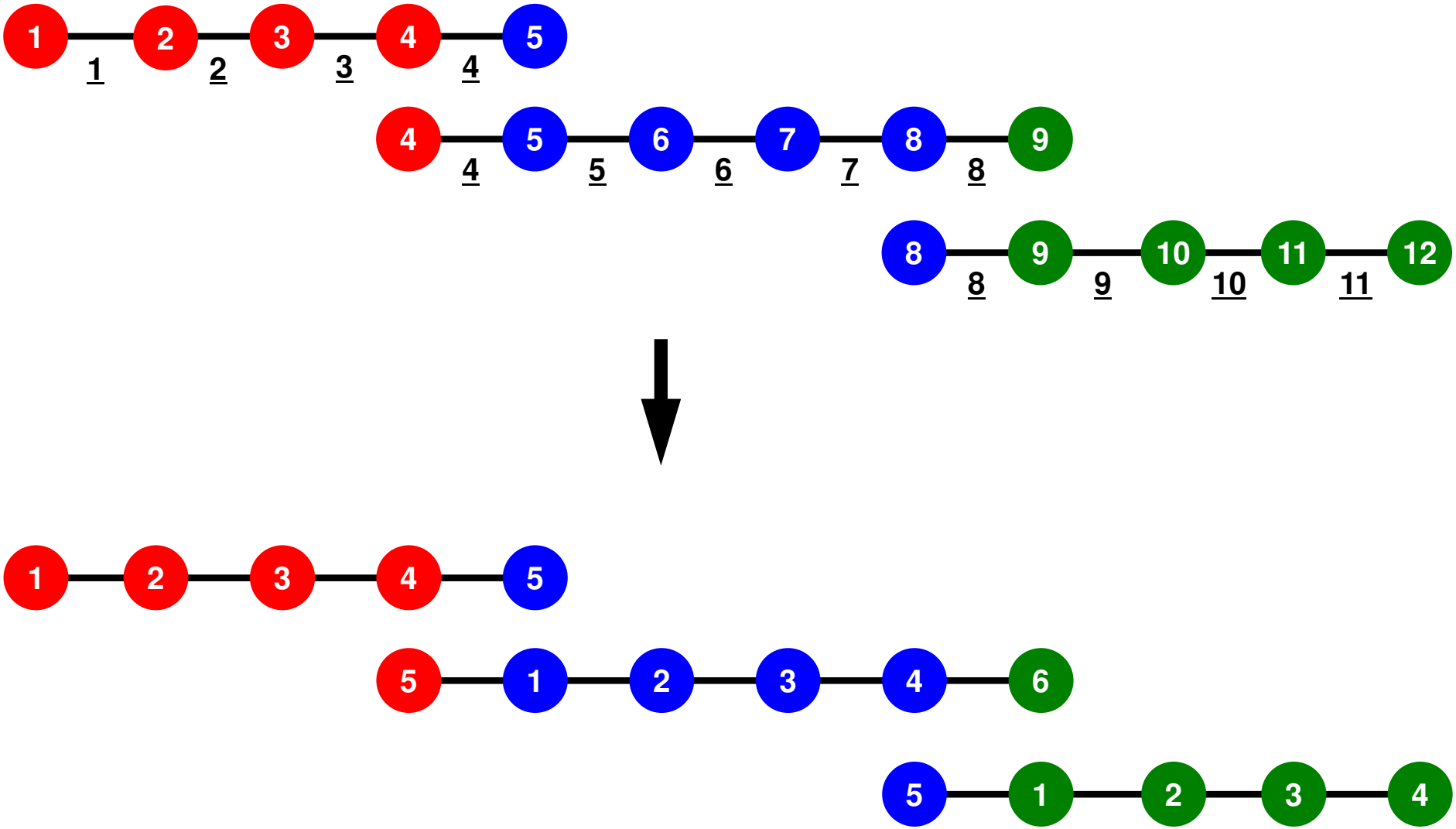
Each process does same operation for different data

Large-scale data is decomposed, and each part is computed by each process

It is ideal that parallel program is not different from serial one except communication.

Local Numbering for SPMD

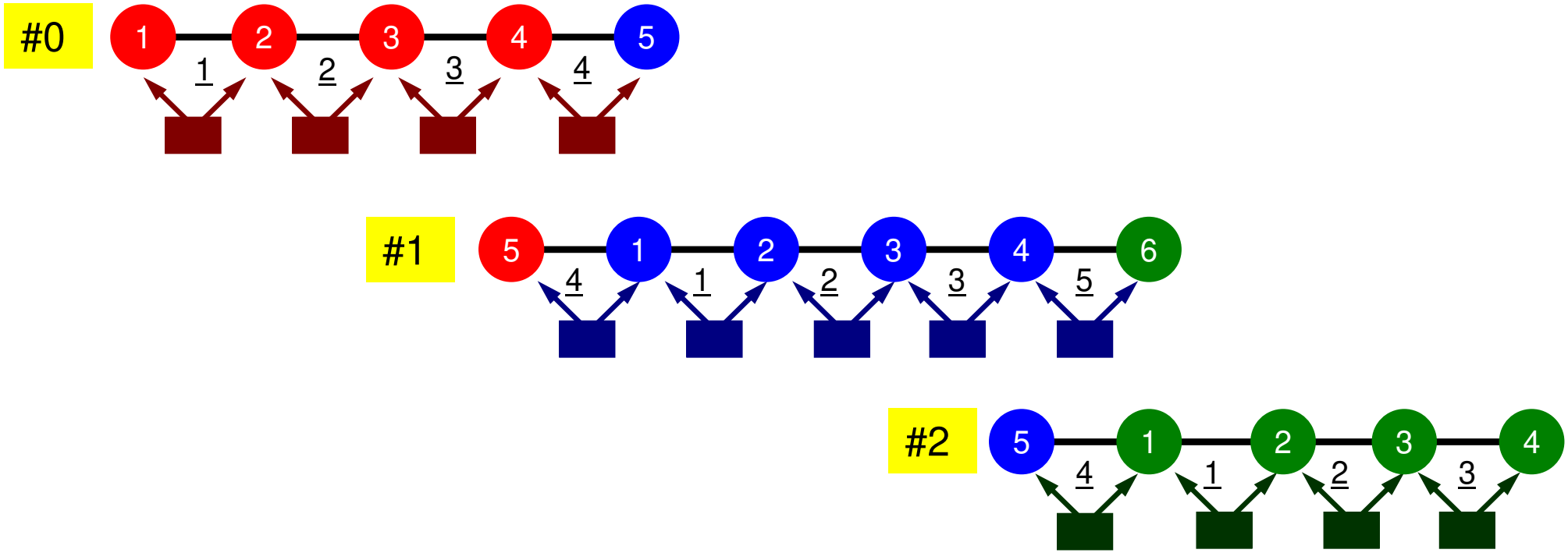
Numbering of internal nodes is 1-N (0-N-1), same operations in serial program can be applied. Numbering of external nodes: N+1, N+2 (N,N+1)



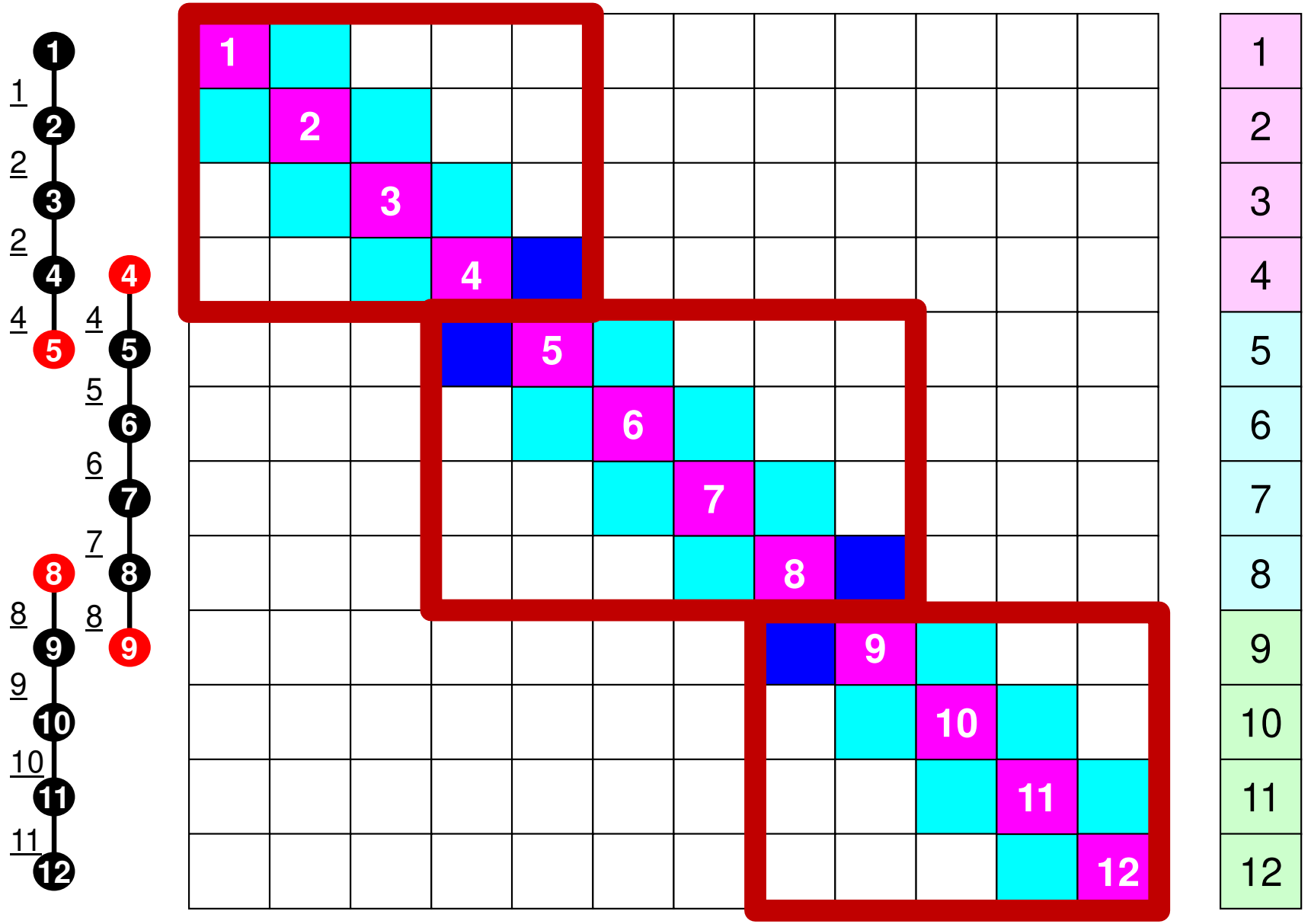
1D FEM: 12 nodes/11 elem's/3 domains

Integration on each element, element matrix -> global matrix

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



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



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

Preconditioned CG Solver

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

- Preconditioning
  - Diagonal Scaling/Point Jacobi
- Parallel operations are required in
  - Dot Products
  - Mat-Vec. Multiplication
    - SpMV: Sparse Mat-Vec. Mult.

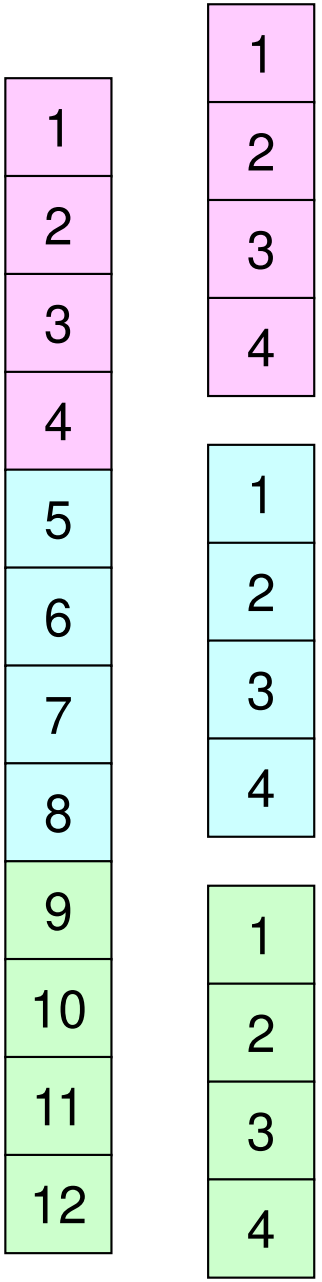
$$[M]=\begin{bmatrix} D_1 & 0 & \dots & 0 & 0 \\ 0 & D_2 & & 0 & 0 \\ \dots & & \dots & & \dots \\ 0 & 0 & & D_{N-1} & 0 \\ 0 & 0 & \dots & 0 & D_N \end{bmatrix}$$

Preconditioning, DAXPY

Local Operations by Only Internal Points: Parallel Processing is possible

```
!C
!C-- {z}= [Minv]{r}

      do i= 1, N
        W(i,Z)= W(i,DD) * W(i,R)
      enddo
```

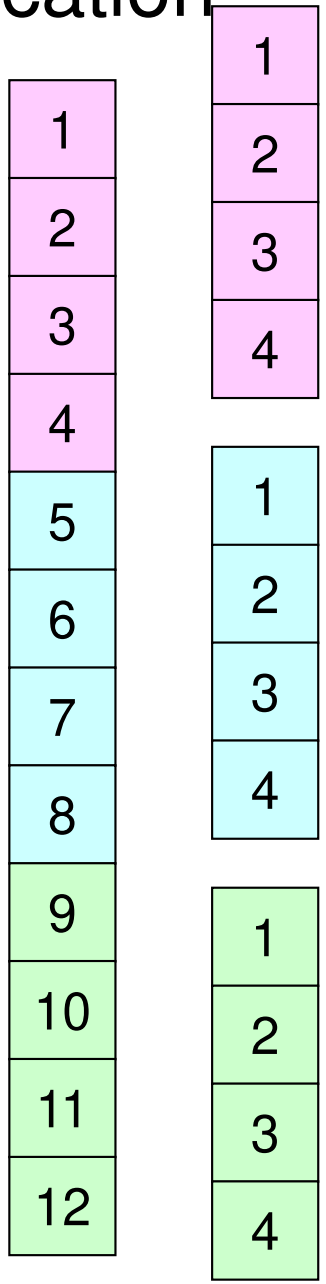
```
!C
!C-- {x}= {x} + ALPHA*{p}        DAXPY: double a{x} plus {y}
!C   {r}= {r} - ALPHA*{q}

      do i= 1, N
        PHI(i)= PHI(i) + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
```



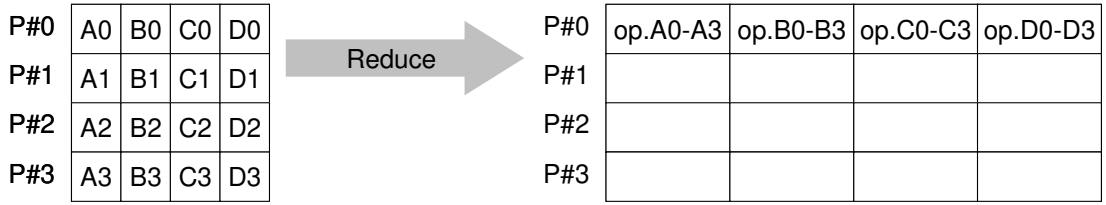
Dot Products

Global Summation needed: Communication ?

```
!C
!C-- ALPHA= RHO / {p}{q}

      C1= 0.d0
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      ALPHA= RHO / C1
```



MPI_REDUCE



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

- **`call MPI_REDUCE`**
  `(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)`
  - **`sendbuf`** choice I starting address of send buffer
  - **`recvbuf`** choice O starting address receive buffer
    type is defined by "**`datatype`**"
  - **`count`** I I number of elements in send/receive buffer
  - **`datatype`** I 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`** I 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`** I I rank of root process
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

Fortran

Preconditioned CG Solver

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

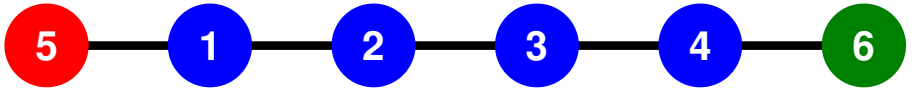
- Preconditioning
  - Diagonal Scaling/Point Jacobi
- Parallel operations are required in
  - Dot Products
  - Mat-Vec. Multiplication
    - SpMV: Sparse Mat-Vec. Mult.

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

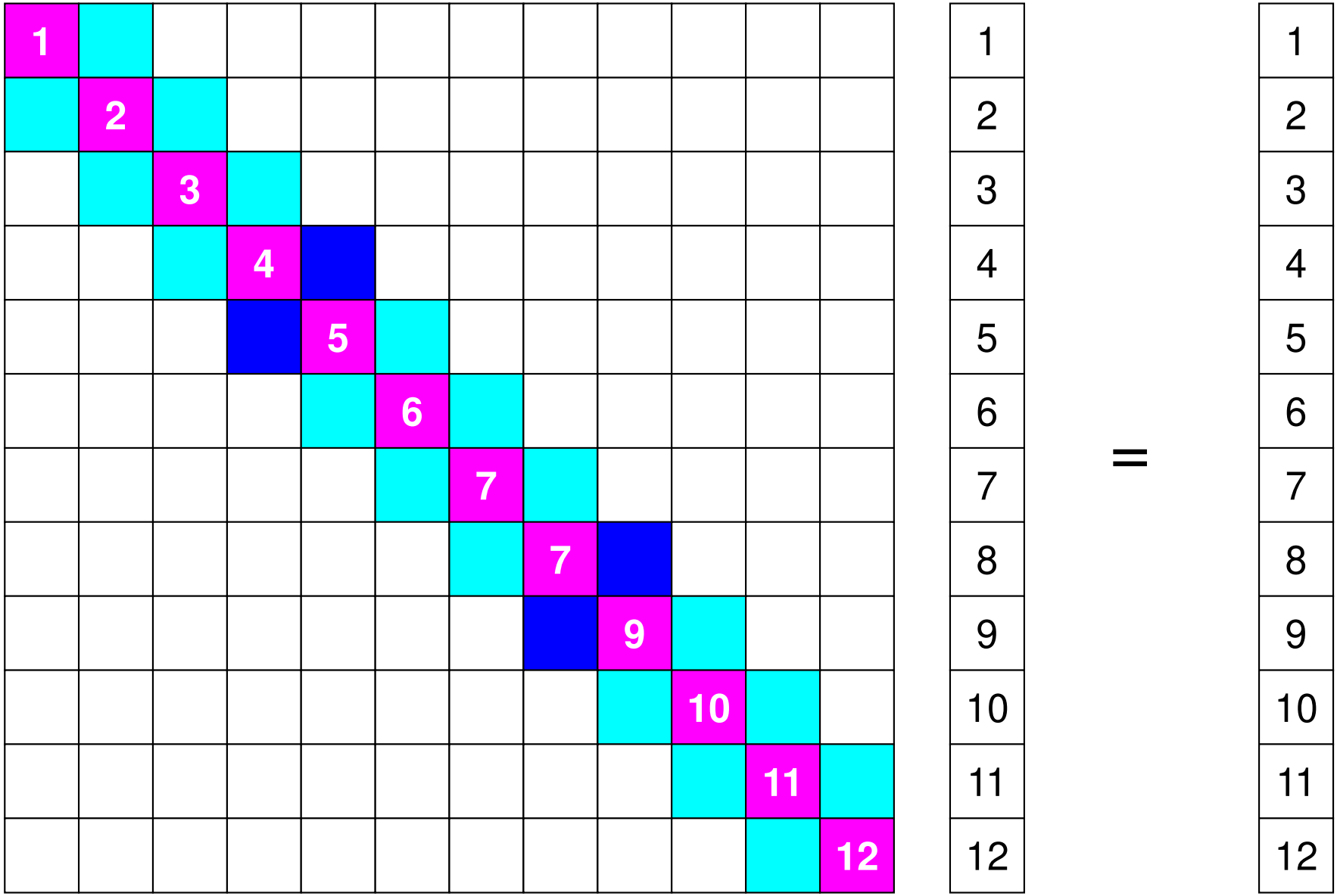
Matrix-Vector Products

Values at External Points: P-to-P Communication

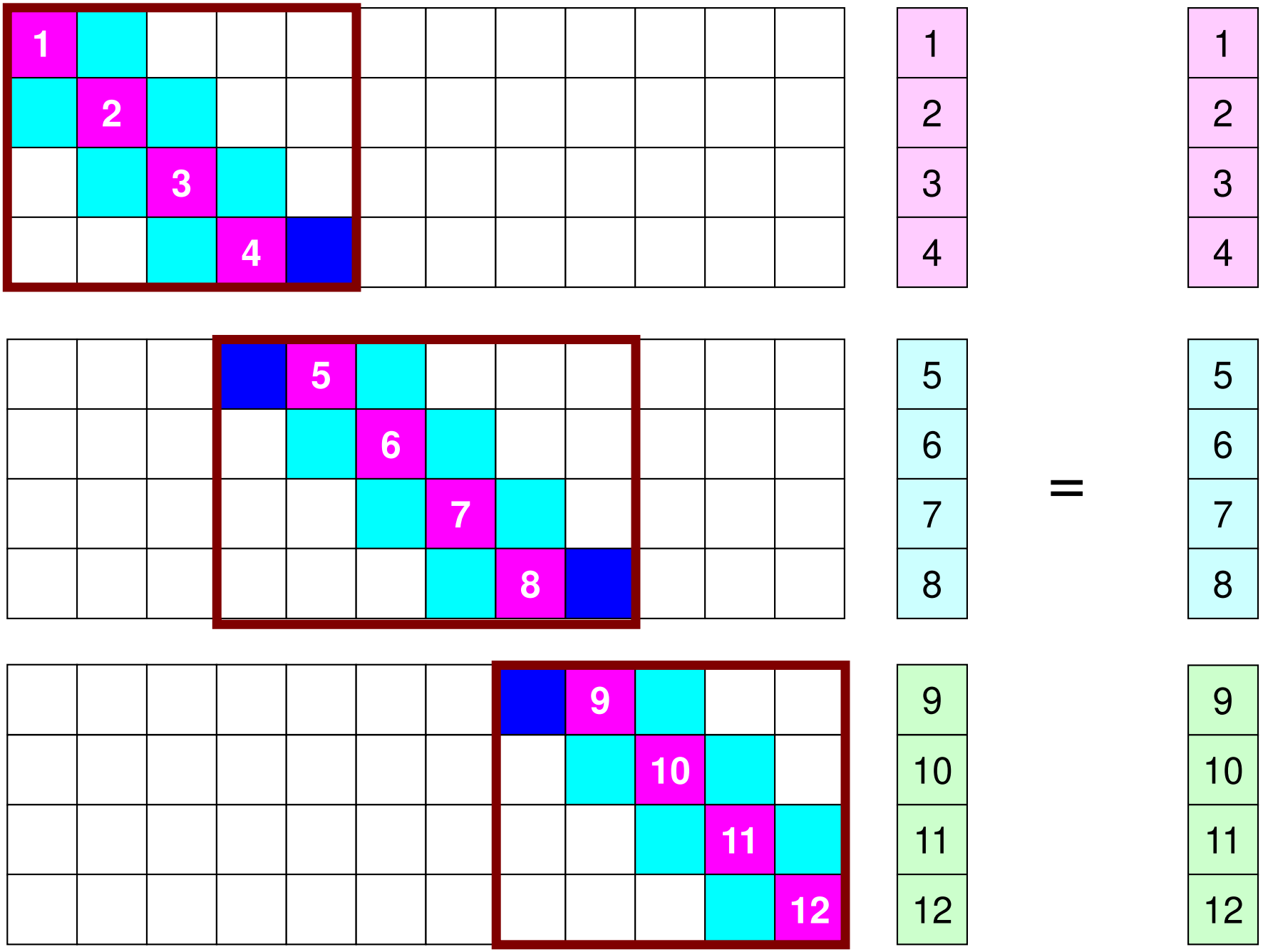
```
!C
!C-- {q}= [A]{p}

      do i= 1, N
        W(i,Q) = DIAG(i)*W(i,P)
        do j= INDEX(i-1)+1, INDEX(i)
          W(i,Q) = W(i,Q) + AMAT(j)*W(ITEM(j),P)
        enddo
      enddo
```



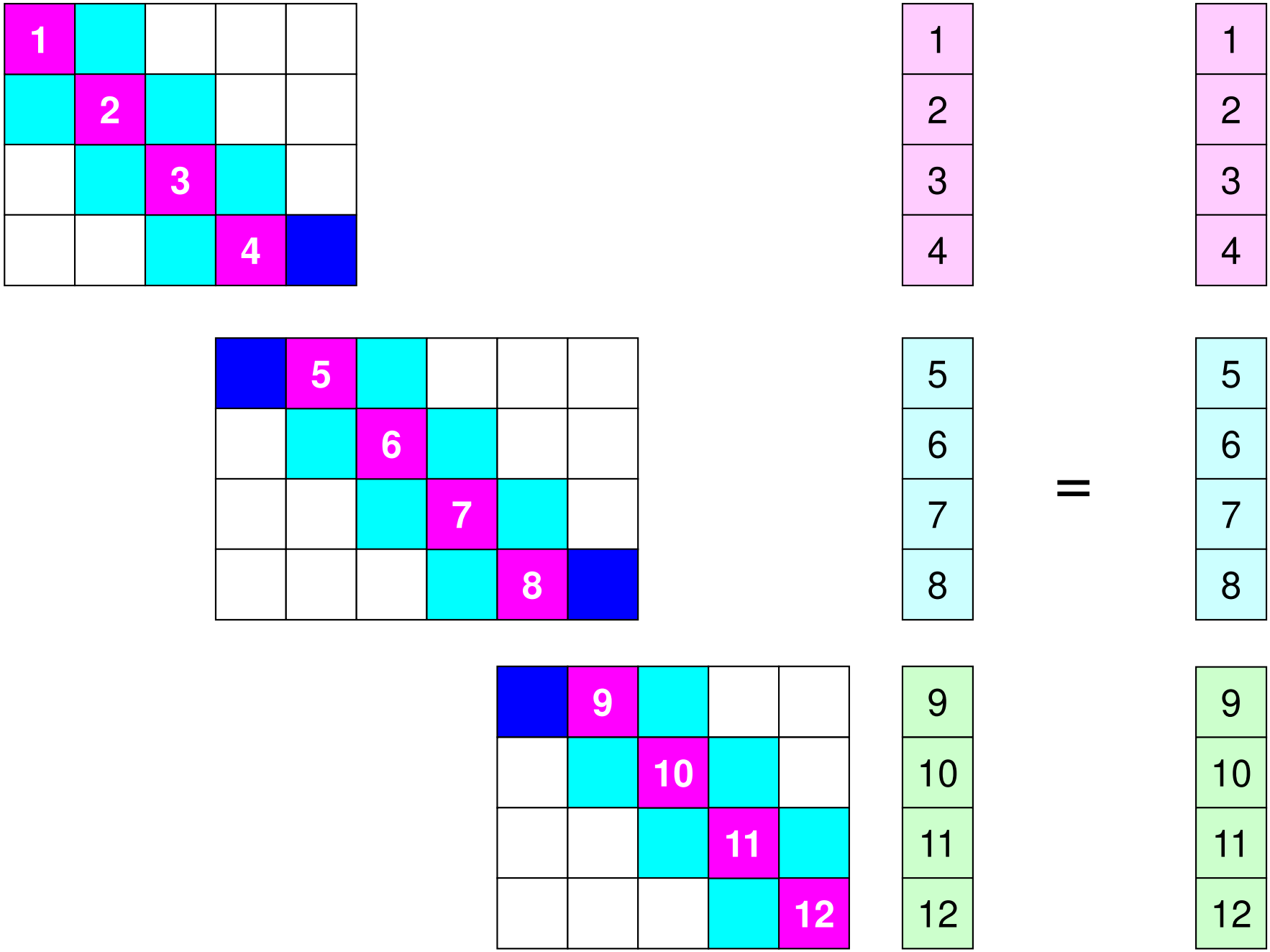
Mat-Vec Products: Local Op. Possible



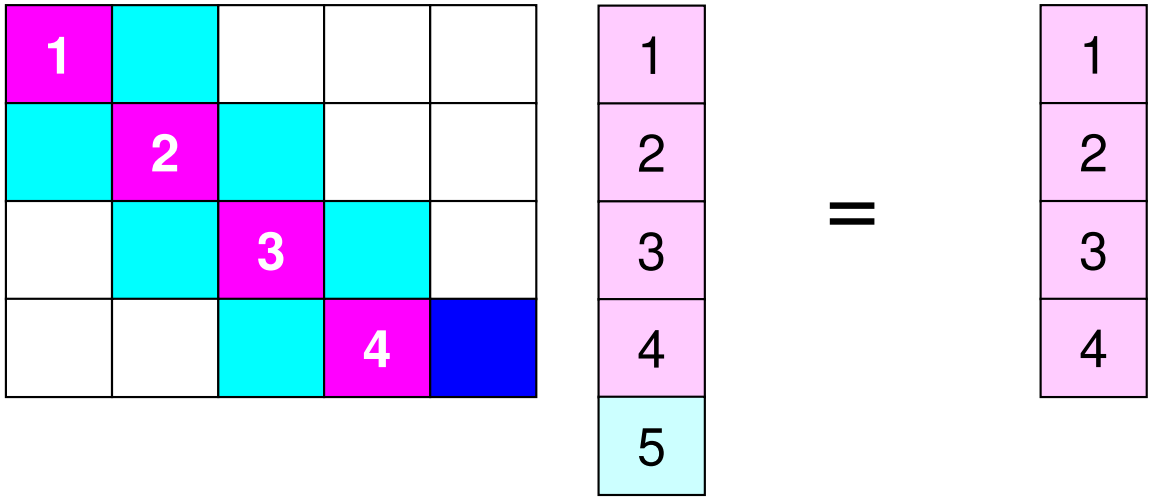
Mat-Vec Products: Local Op. Possible



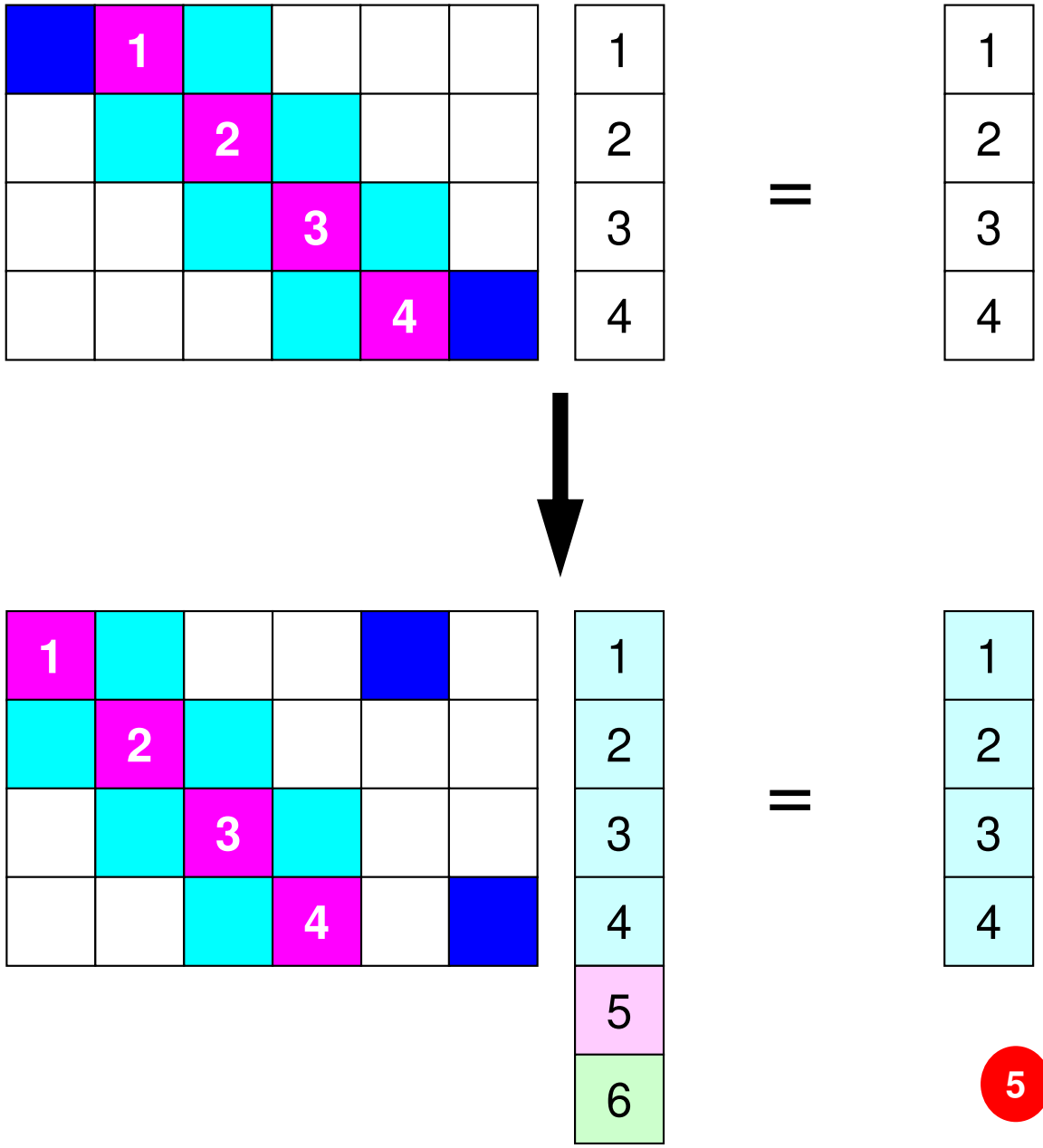
Mat-Vec Products: Local Op. Possible



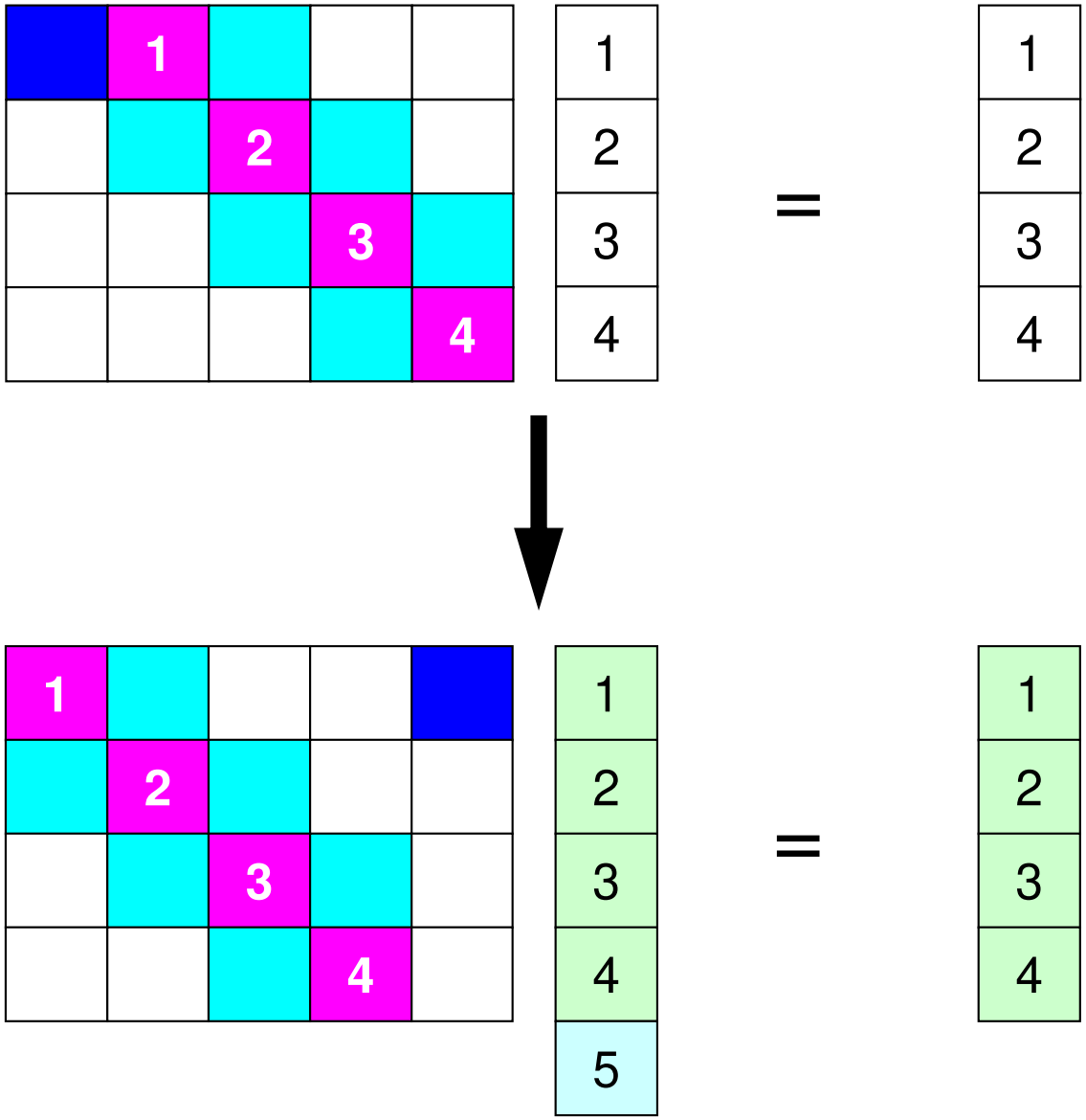
Mat-Vec Products: Local Op. #0



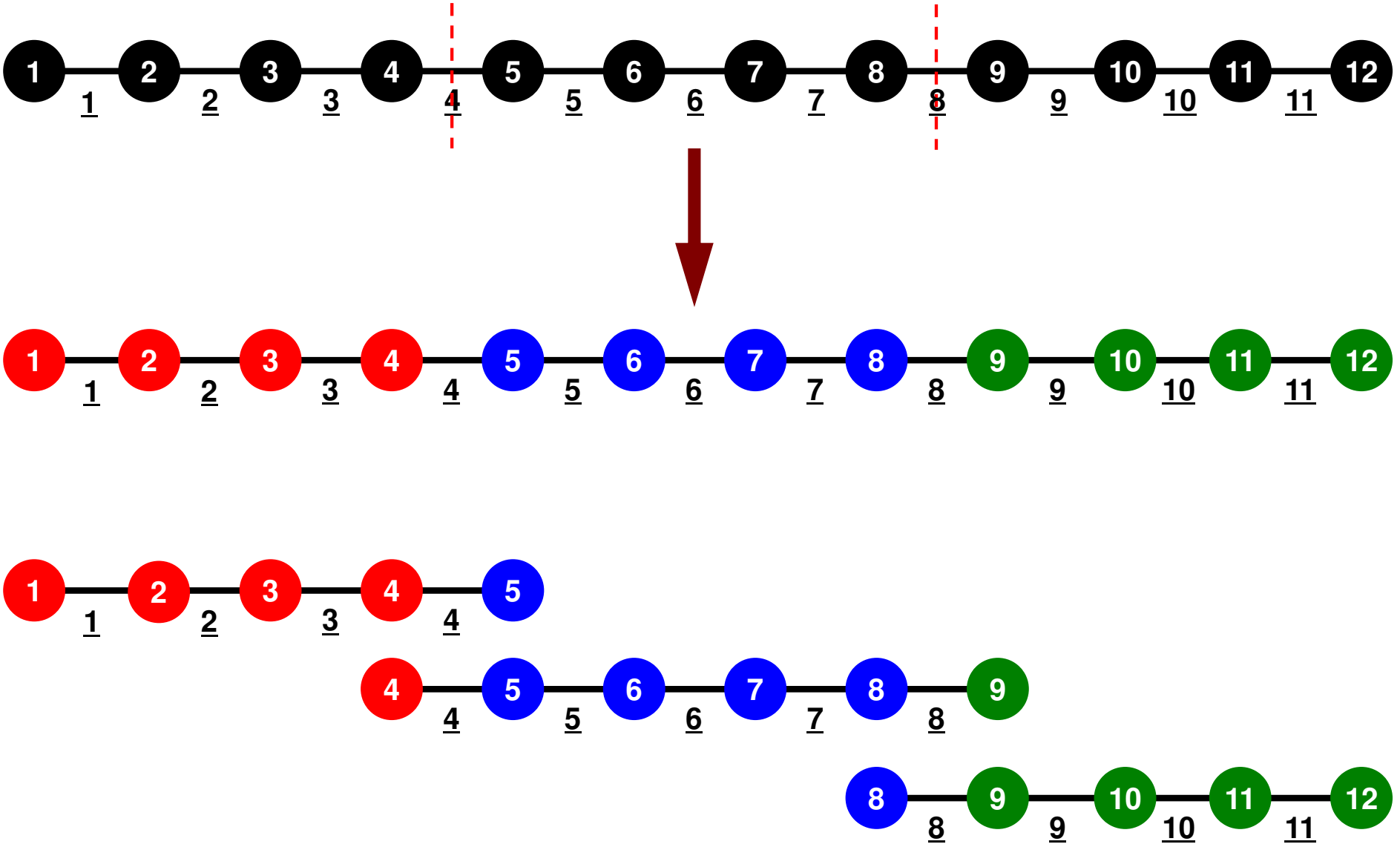
Mat-Vec Products: Local Op. #1



Mat-Vec Products: Local Op. #2

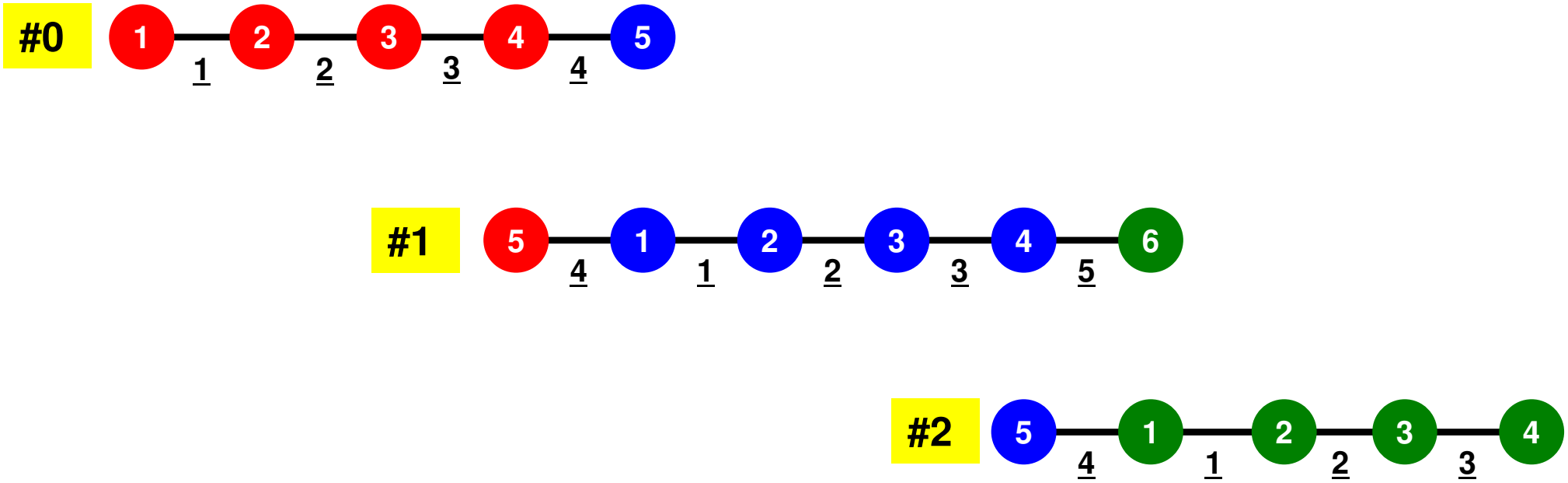


1D FEM: 12 nodes/11 elem's/3 domains



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

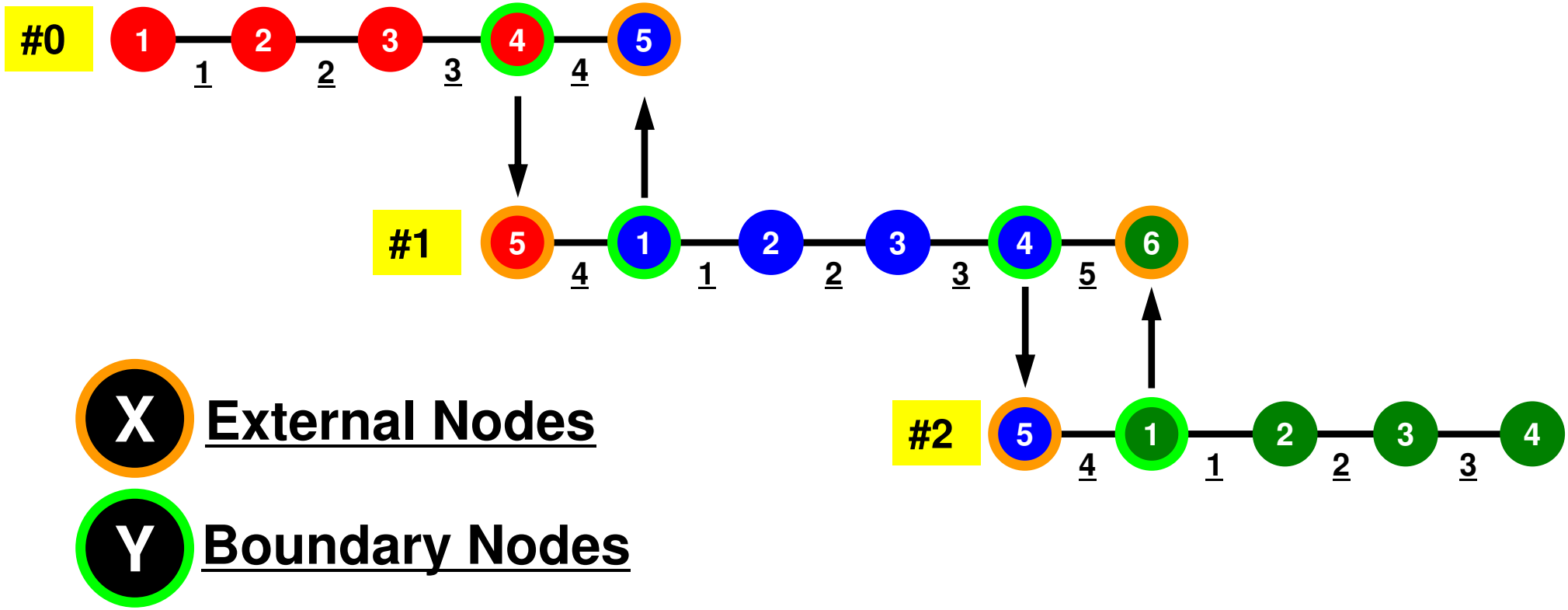
Local ID: Starting from 1 for node and elem at each domain



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

Internal/External/Boundary Nodes

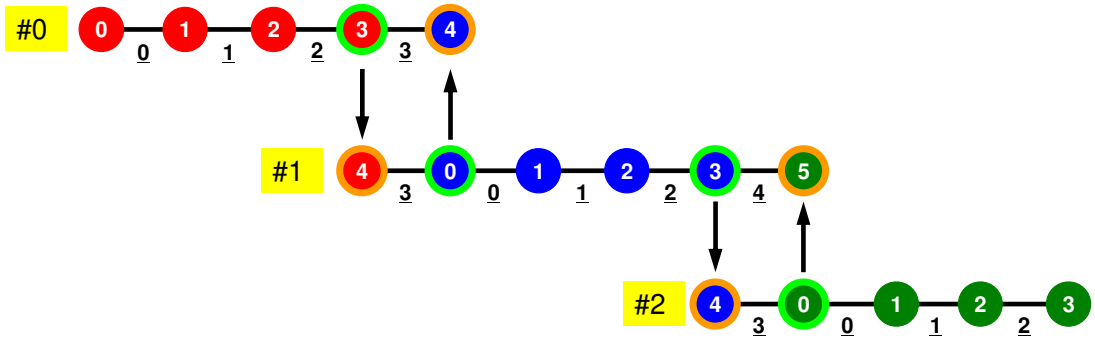
Boundary Nodes: Part of Internal Nodes, and External Nodes of Other Domains



What is Peer-to-Peer Communication ?

- Collective Communication
  - MPI_Reduce, MPI_Scatter/Gather etc.
  - Communications with all processes in the communicator
  - Application Area
    - BEM, Spectral Method, MD: global interactions are considered
    - Dot products, MAX/MIN: Global Summation & Comparison

- Peer-toPeer/Point-to-Point
  - MPI_Send, MPI_Recv
  - Communication with limited processes
    - Neighbors
  - Application Area
    - FEM, FDM: Localized Method



MPI_ISEND

Fortran

- 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**.

- **call MPI_ISEND (sendbuf,count,datatype,dest,tag,comm,request, ierr)**
  - **sendbuf** choice I starting address of sending buffer
  - **count** I I number of elements sent to each process
  - **datatype** I I data type of elements of sending buffer
  - **dest** I I rank of destination
  - **tag** I 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** I I communicator
  - **request** I O communication request array used in `MPI_Waitall`
  - **ierr** I O completion code

Fortran

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`**.

- **`call MPI_IRECV`**
  `(recvbuf,count,datatype,dest,tag,comm,request, ierr)`
  - **`recvbuf`** choice I starting address of receiving buffer
  - **`count`** I I number of elements in receiving buffer
  - **`datatype`** I I data type of elements of receiving buffer
  - **`source`** I I rank of source
  - **`tag`** I 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`** I I communicator
  - **`request`** I O communication request used in `MPI_Waitall`
  - **`ierr`** I O completion code

MPI_WAITALL

Fortran

- **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.

- **call MPI_WAITALL (count,request,status,ierr)**
  - **count** I I number of processes to be synchronized
  - **request** I I/O comm. request used in `MPI_Waitall` (array size: `count`)
  - **status** I O array of status objects
    `MPI_STATUS_SIZE: defined in 'mpif.h', 'mpi.h'`
  - **ierr** I O completion code