

Introduction to Parallel FEM in Fortran Parallel Data Structure

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

Parallel Computing

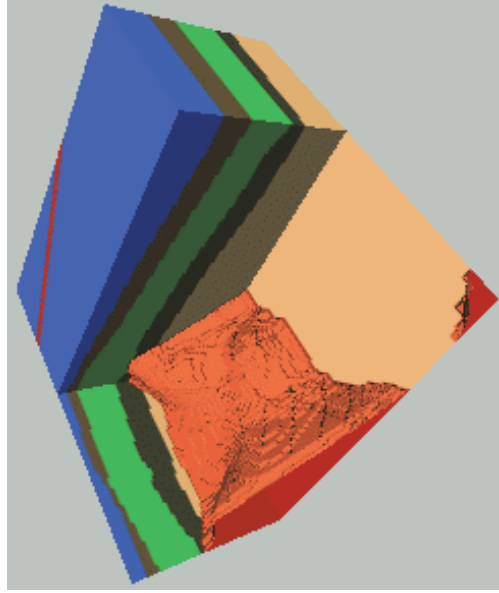
- **Faster, Larger & More Complicated**
- Scalability
 - Solving N^x scale problem using N^x computational resources during same computation time
 - for large-scale problems: Weak Scaling
 - e.g. CG solver: more iterations needed for larger problems
 - Solving a problem using N^x computational resources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

What is Parallel Computing ? (1/2)

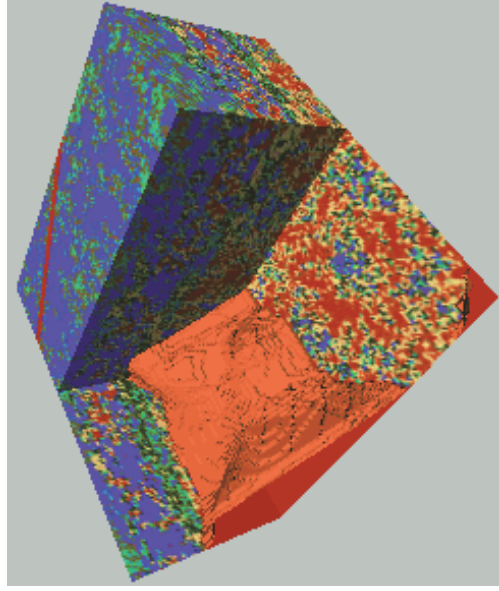
- to solve larger problems faster

Homogeneous/Heterogeneous Porous Media

Lawrence Livermore National Laboratory



Homogeneous

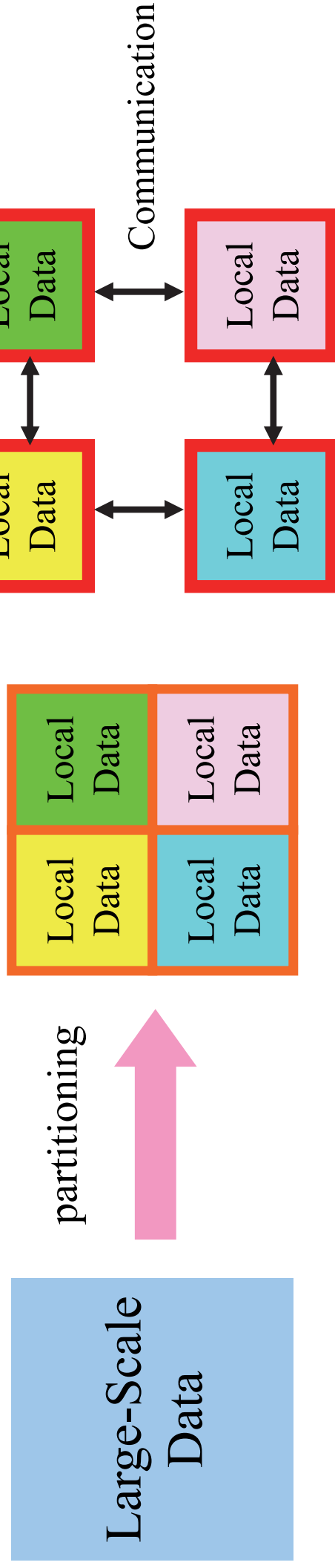


Heterogeneous

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.

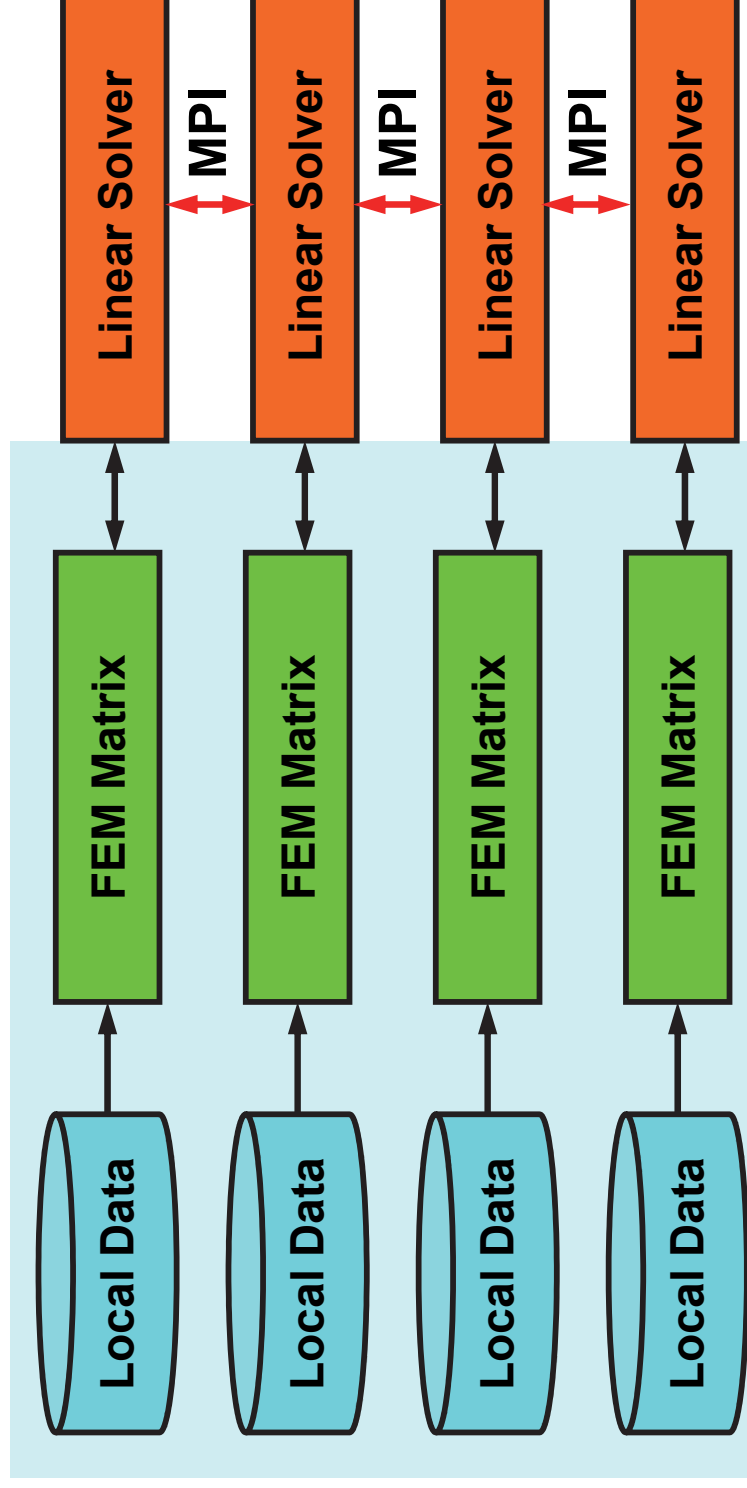
Operations in Parallel FEM

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

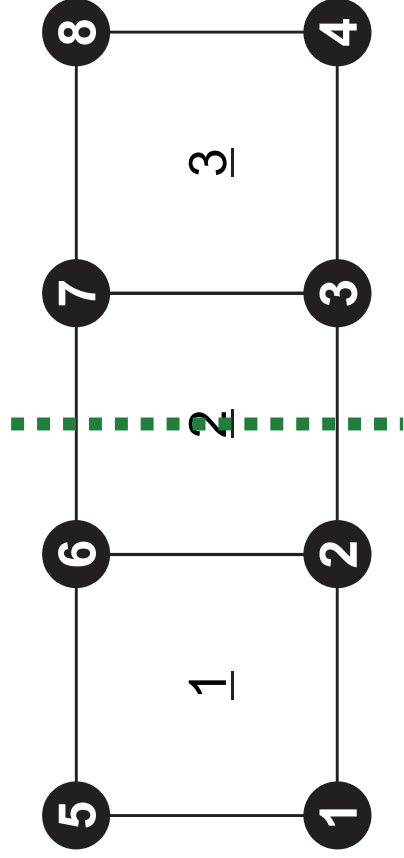


Parallel FEM Procedures

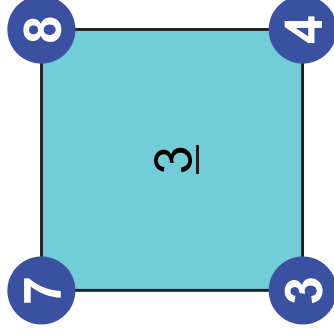
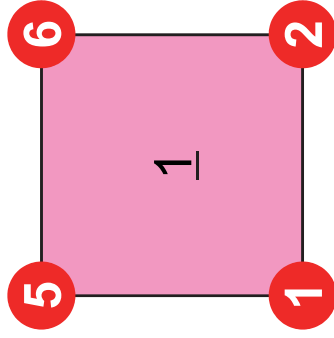
- Design on “Local Data Structure” is important
 - for SPMD-type operations in the previous page
- Matrix Generation
- Preconditioned Iterative Solvers for Linear Equations

Bi-Linear Square Elements

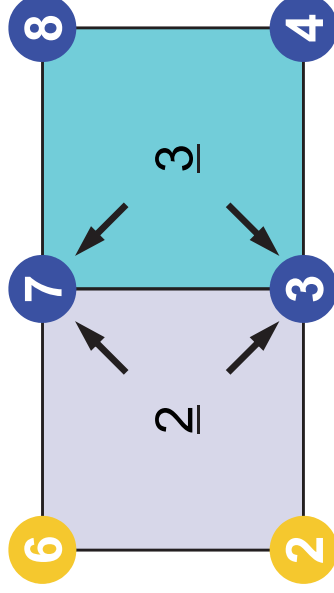
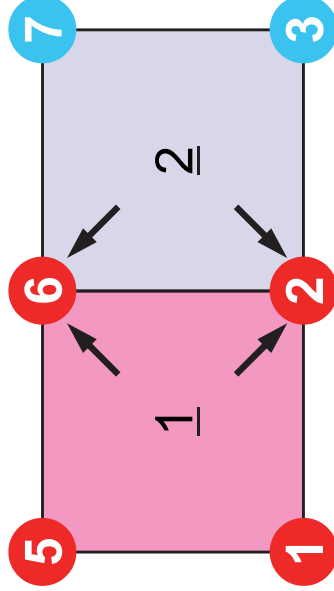
Values are defined on each node



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.



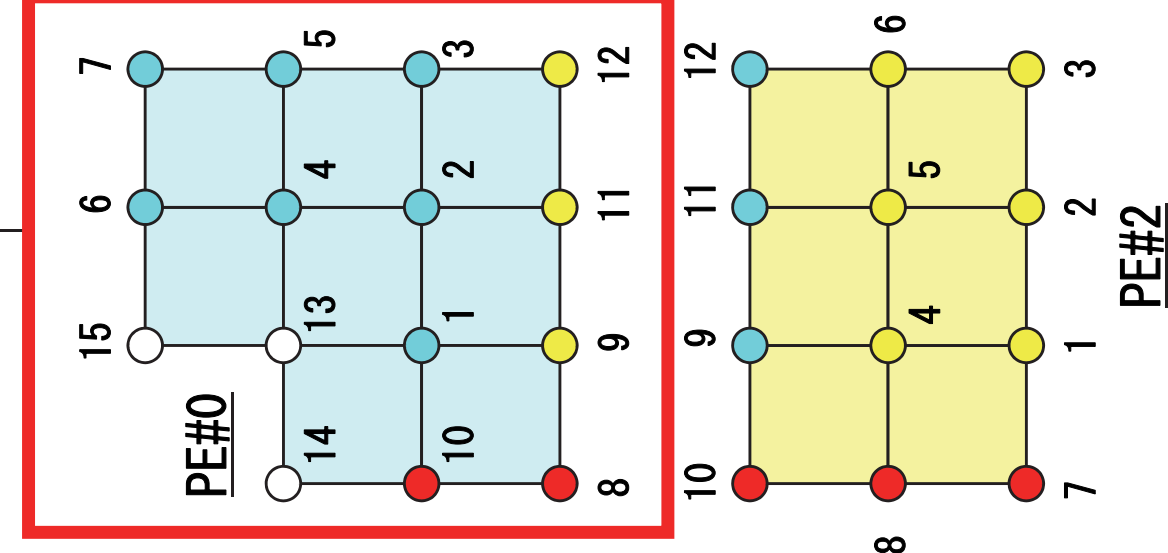
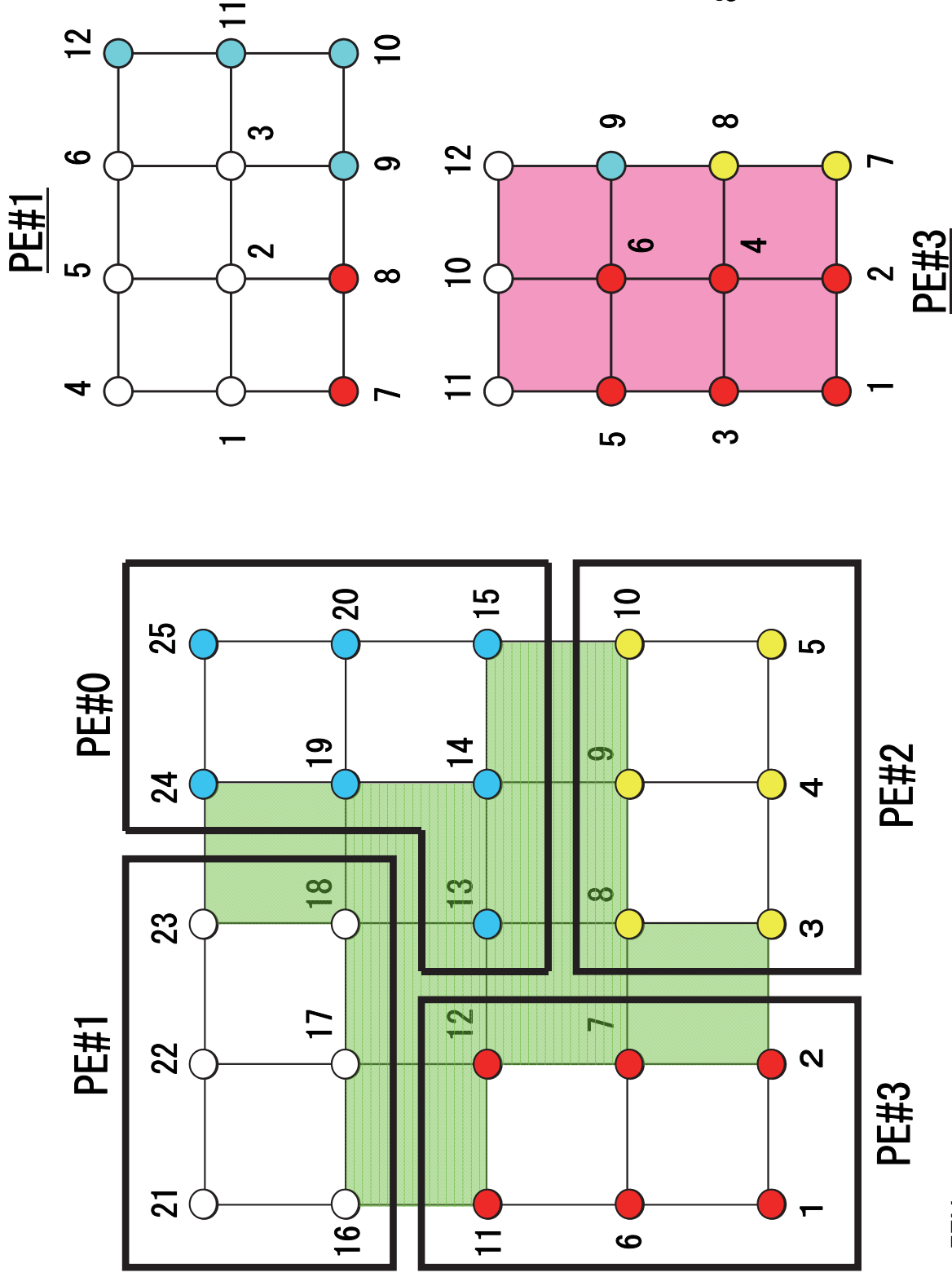


Local Data of Parallel FEM

- **Node-based partitioning for IC/ILU type preconditioning methods**
- Local data includes information for :
 - Nodes originally assigned to the partition/PE
 - Elements which include the nodes : Element-based operations (Matrix Assemble) are allowed for fluid/structure subsystems.
 - 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
- Communication table between partitions
- NO global information required except partition-to-partition connectivity

Node-based Partitioning

internal nodes - elements - external nodes

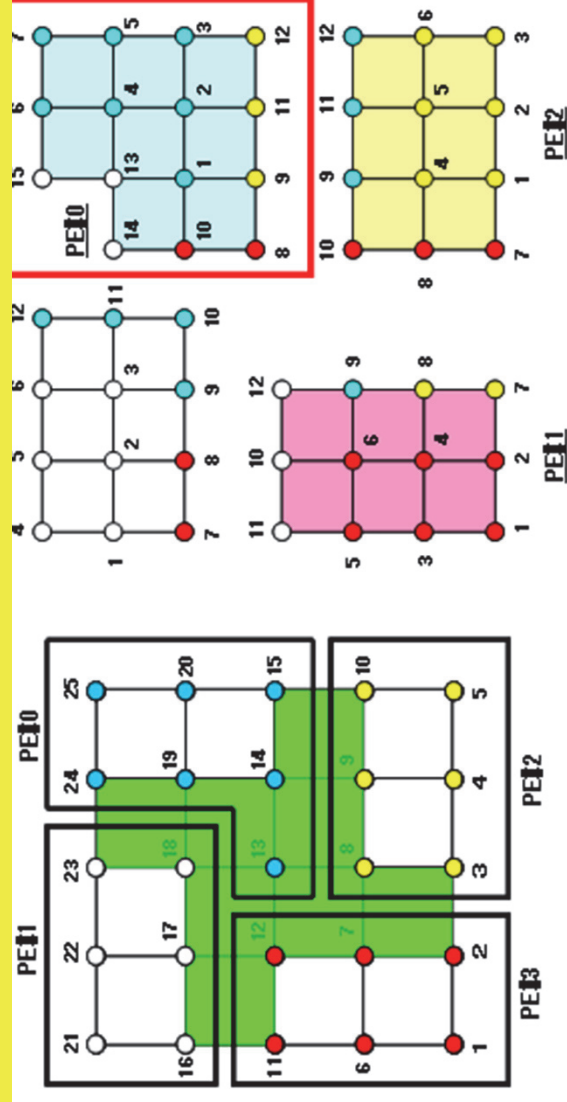
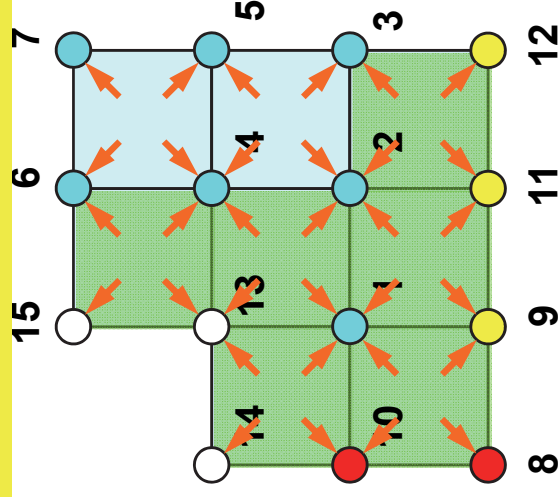


Node-based Partitioning

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.

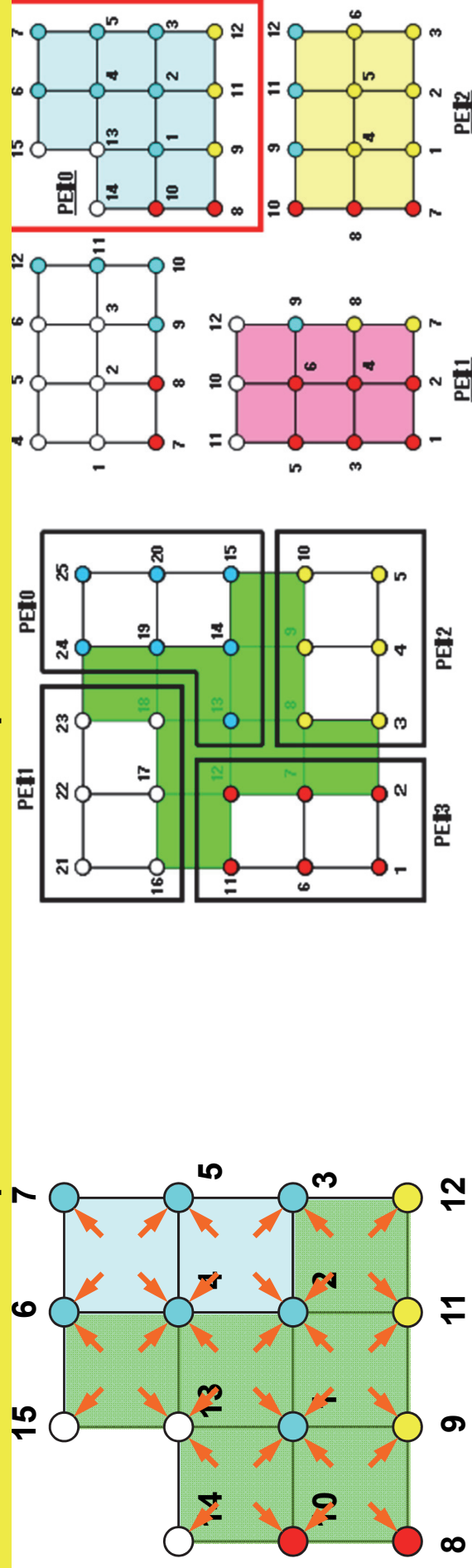
- Info of External Nodes are required for completely local element-based operations on each processor.



We do not need communication during matrix assembly !!

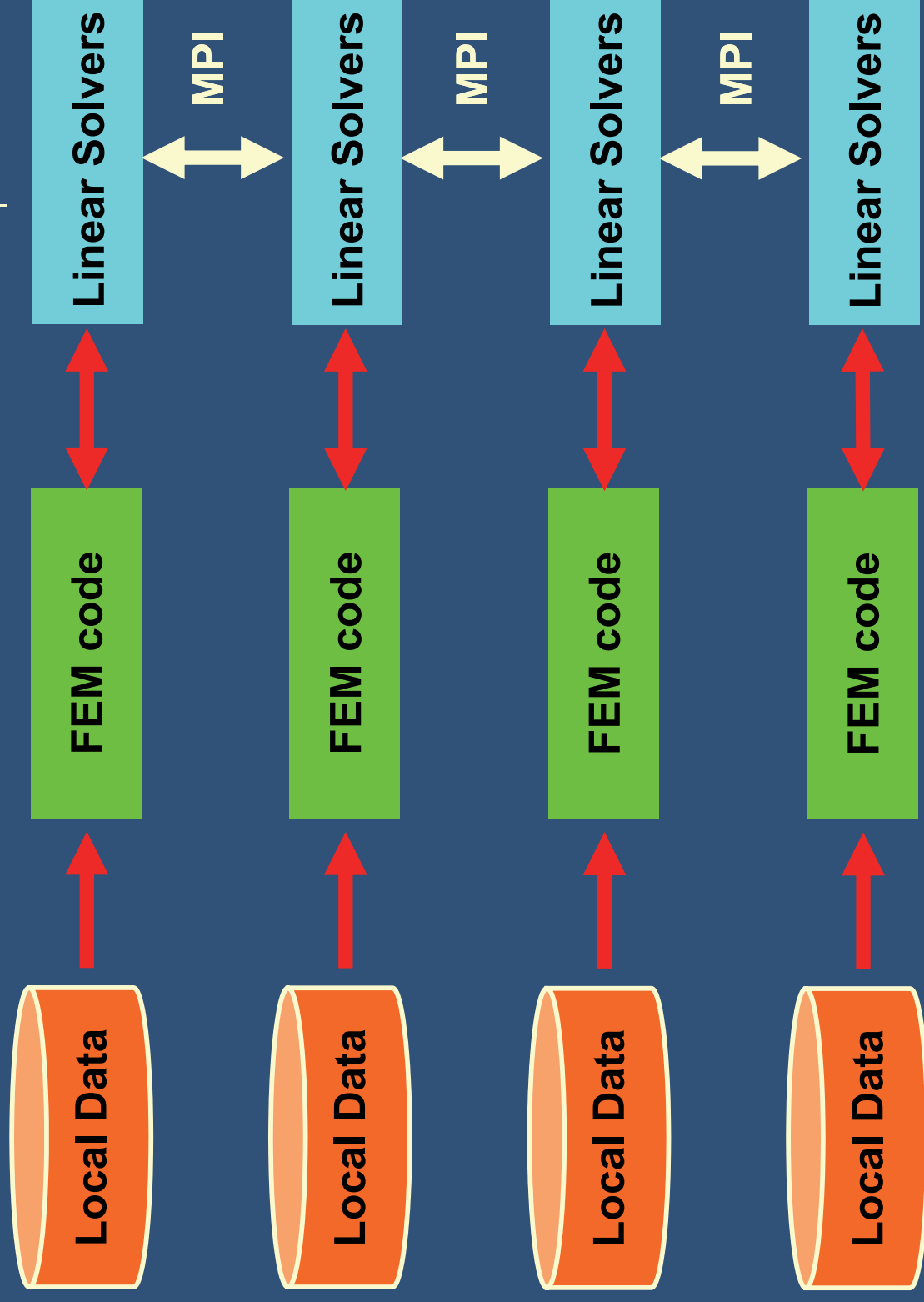
- Partitioned nodes themselves (Internal Nodes)
- Elements which include Internal Nodes
- External Nodes included in the Elements
in overlapped region among partitions.

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



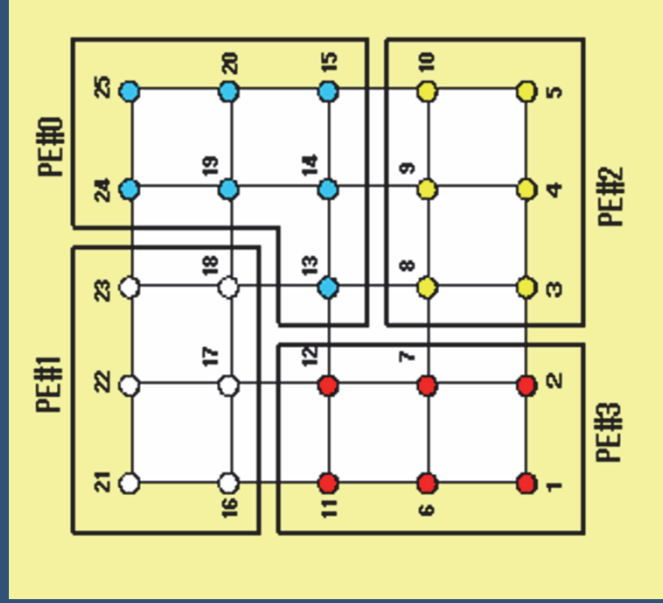
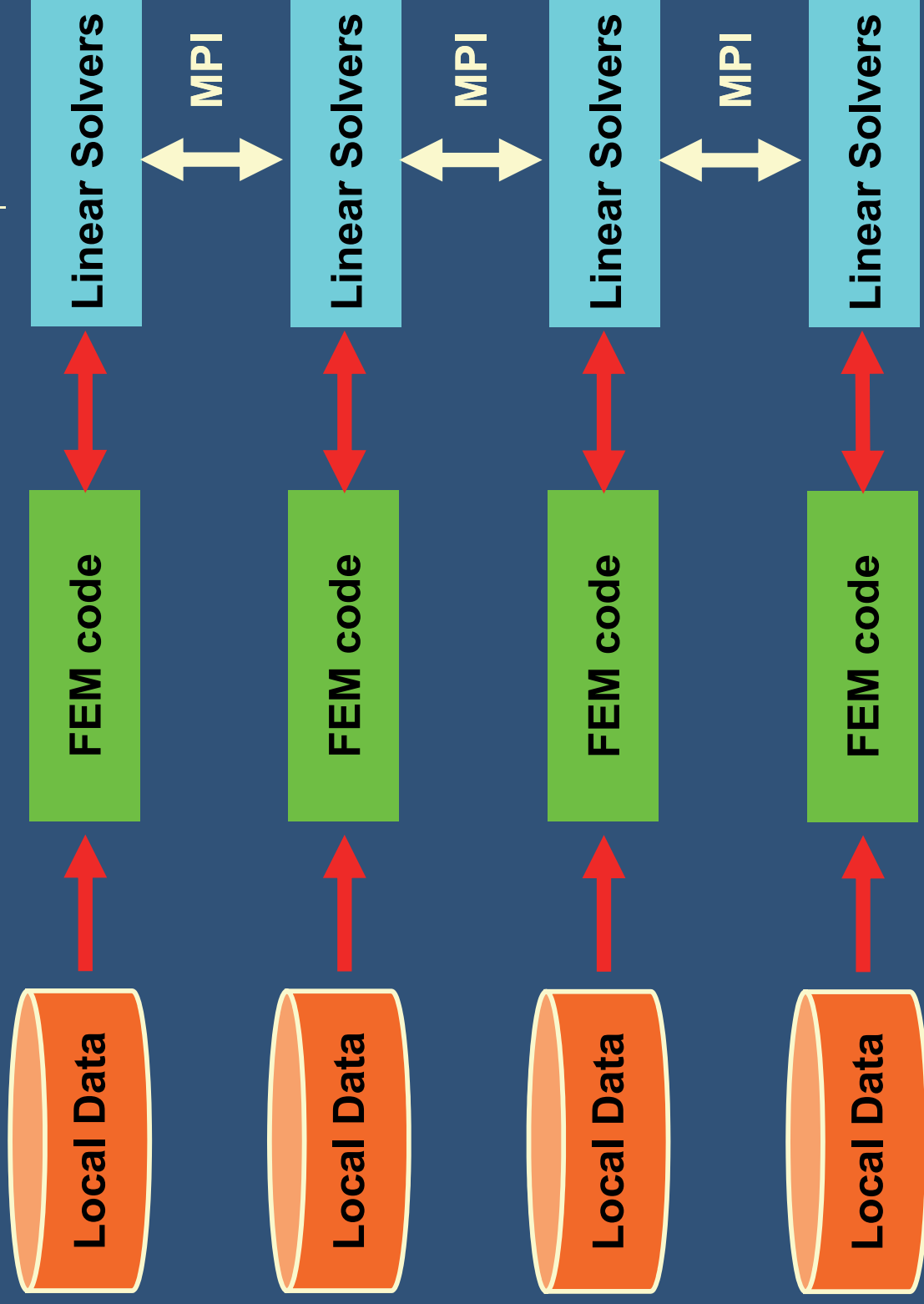
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



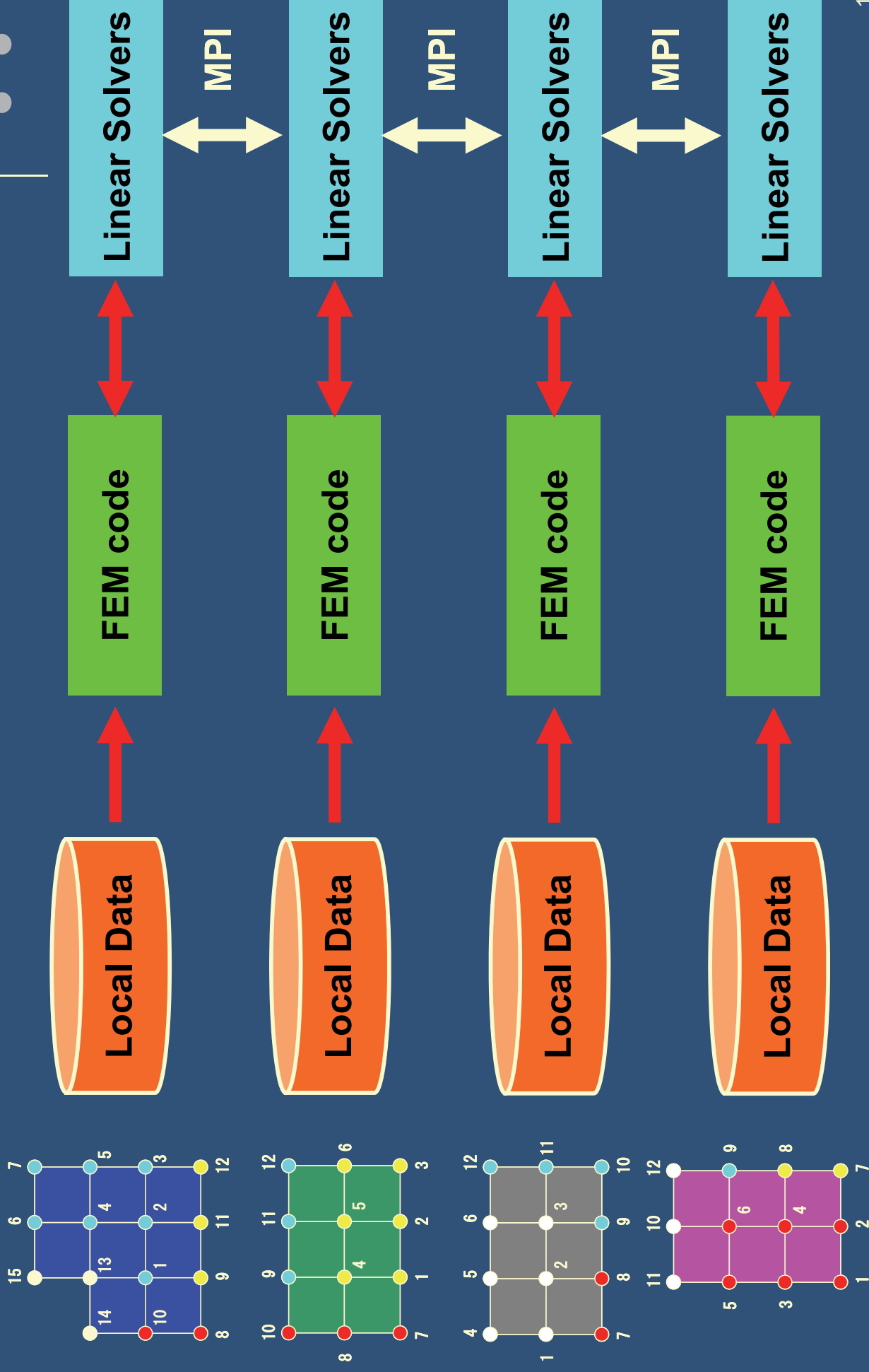
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



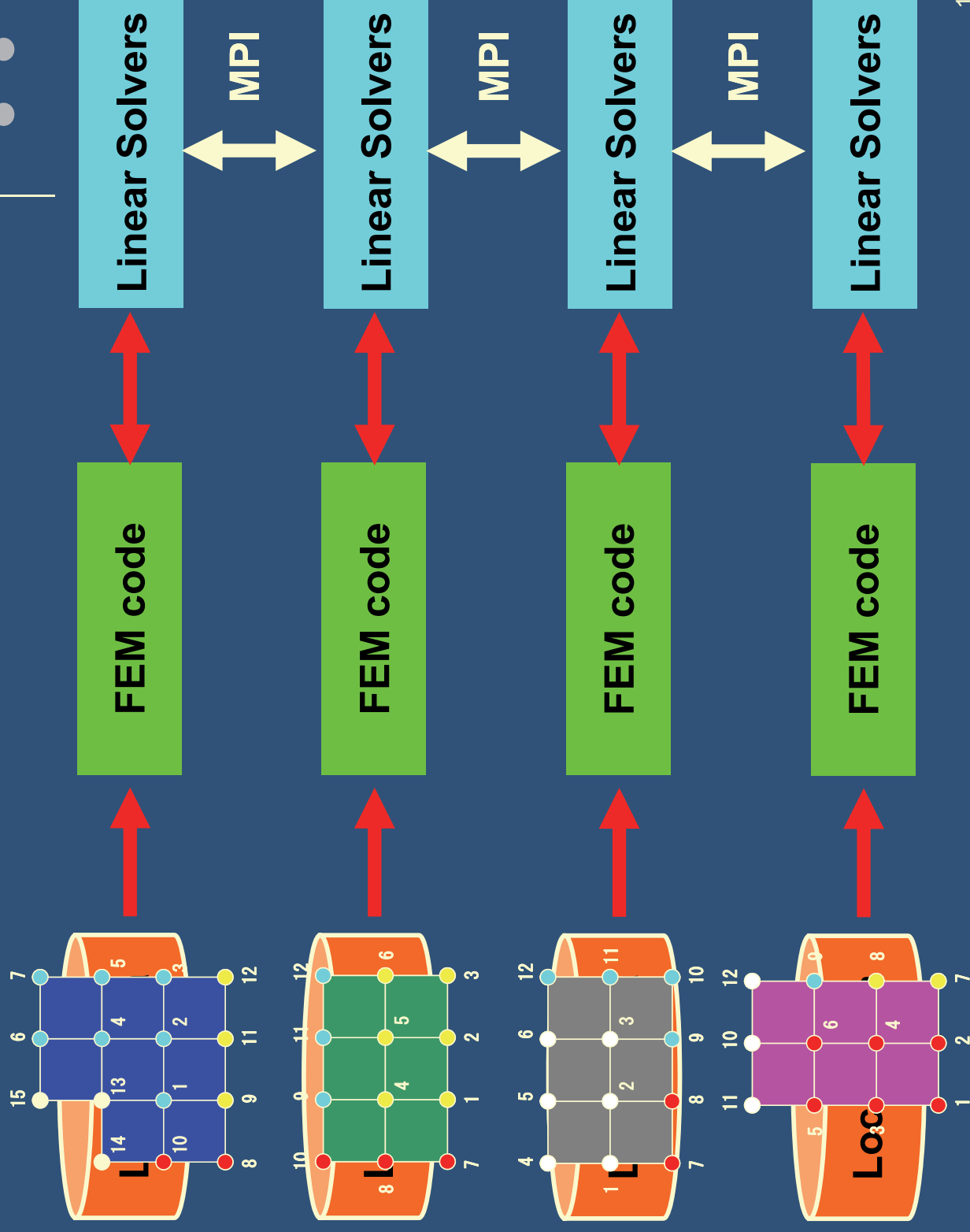
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



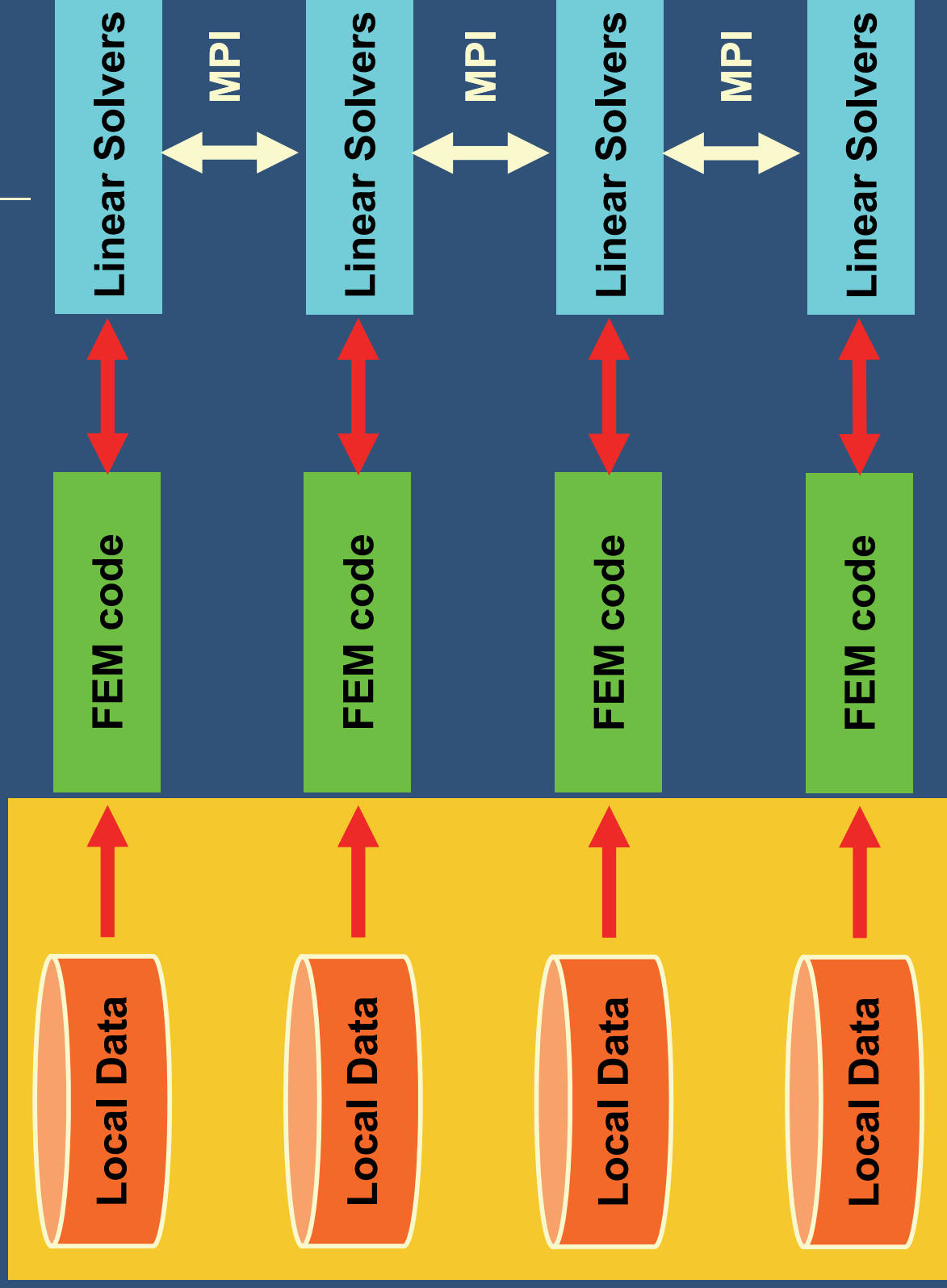
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



Parallel Computing in FEM

SPMD: Single-Program Multiple-Data

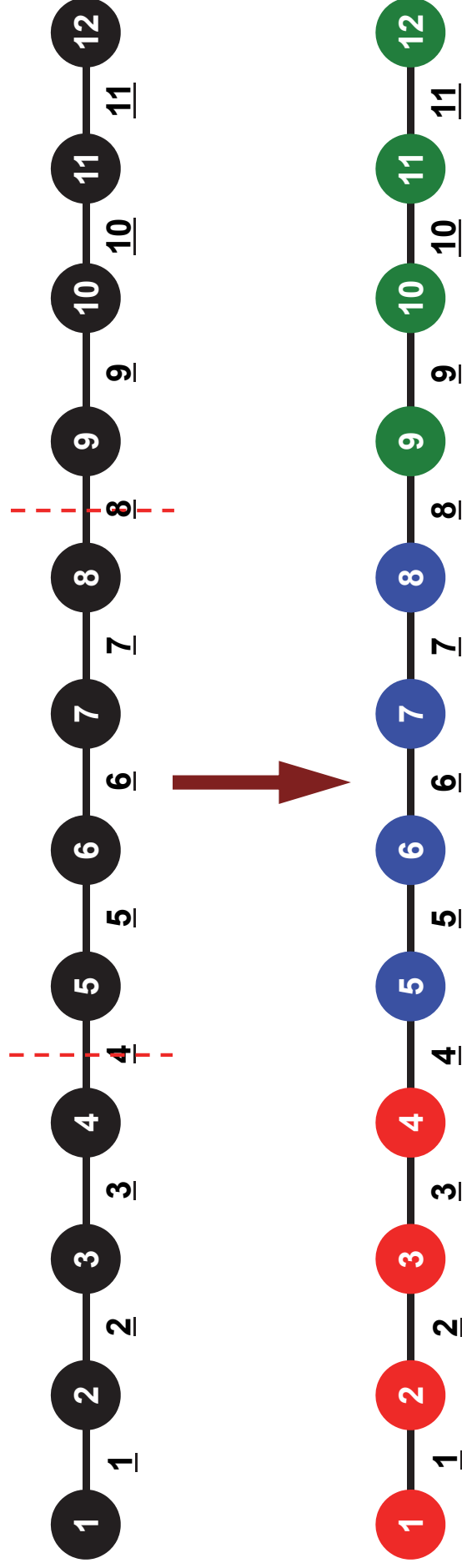


What is Communications ?

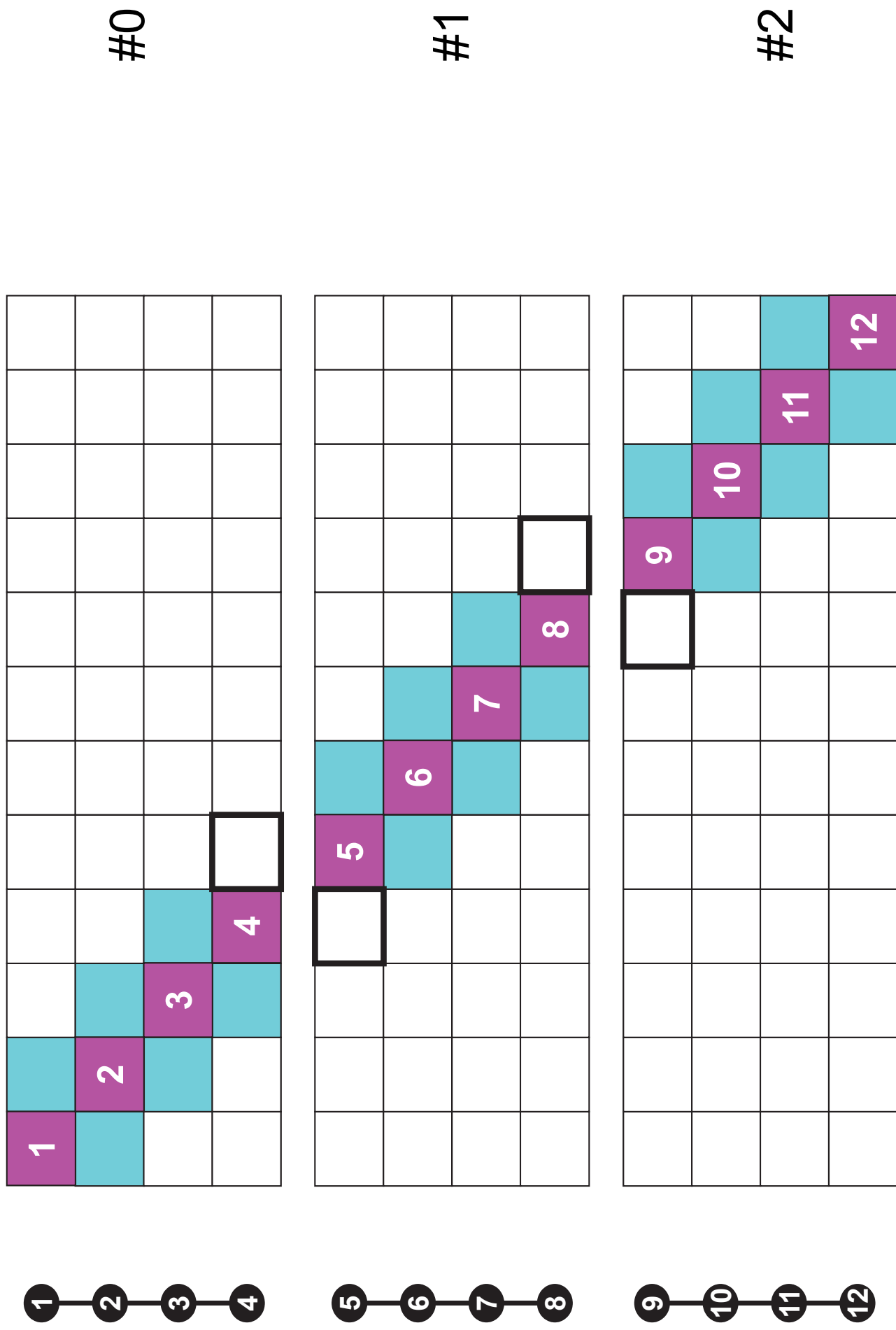


- to get information of “external nodes” from external partitions (local data)
- “Communication tables” contain the information

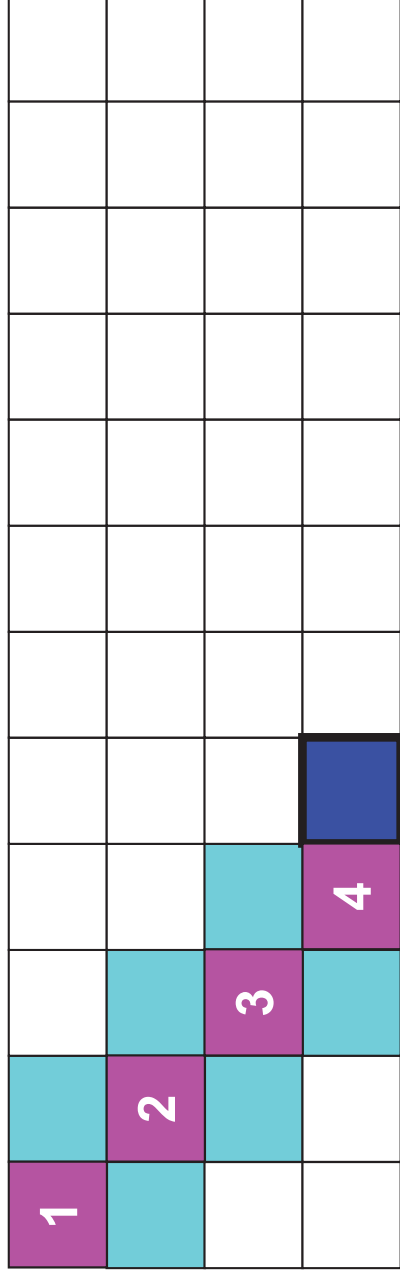
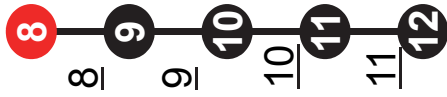
1D FEM: 12 nodes/11 elem's/3 domains



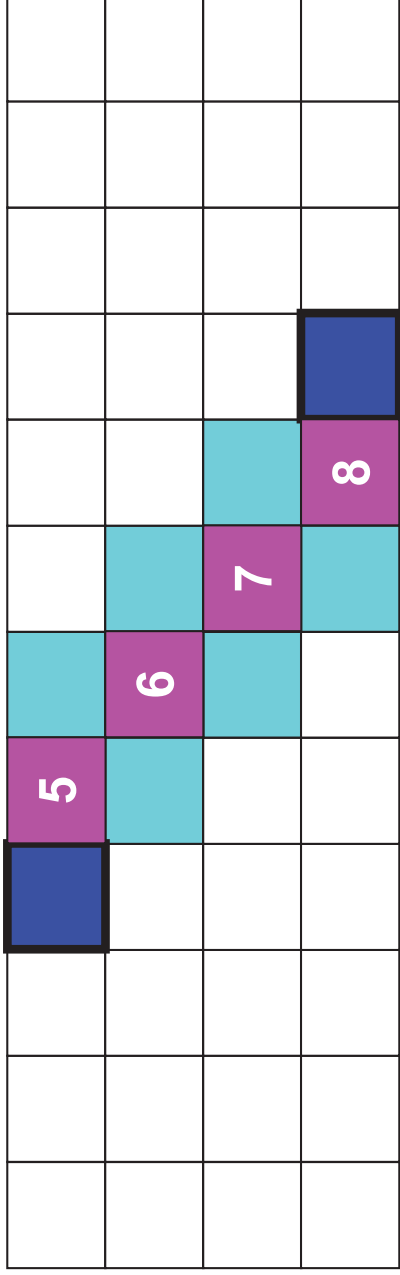
Matrices are incomplete !



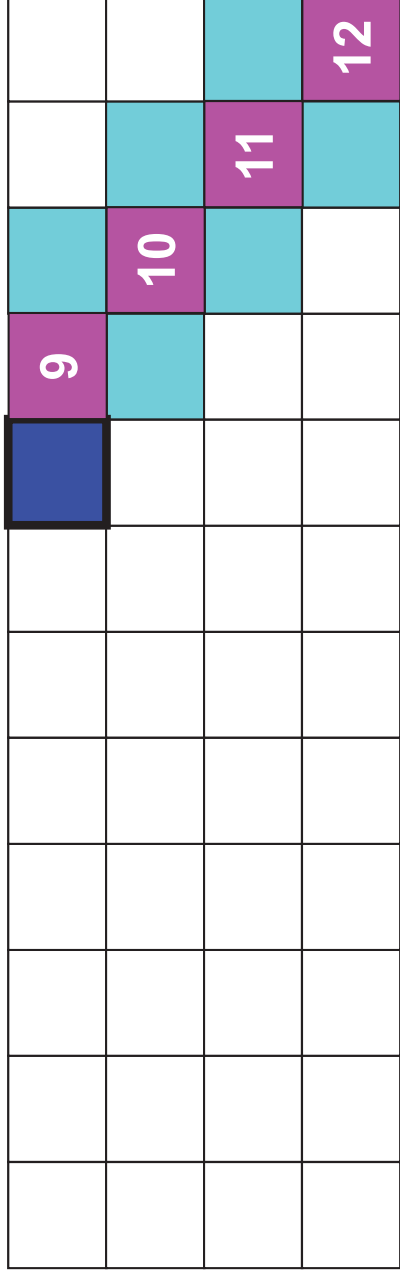
Connected Elements + External Nodes



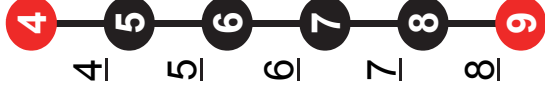
#0



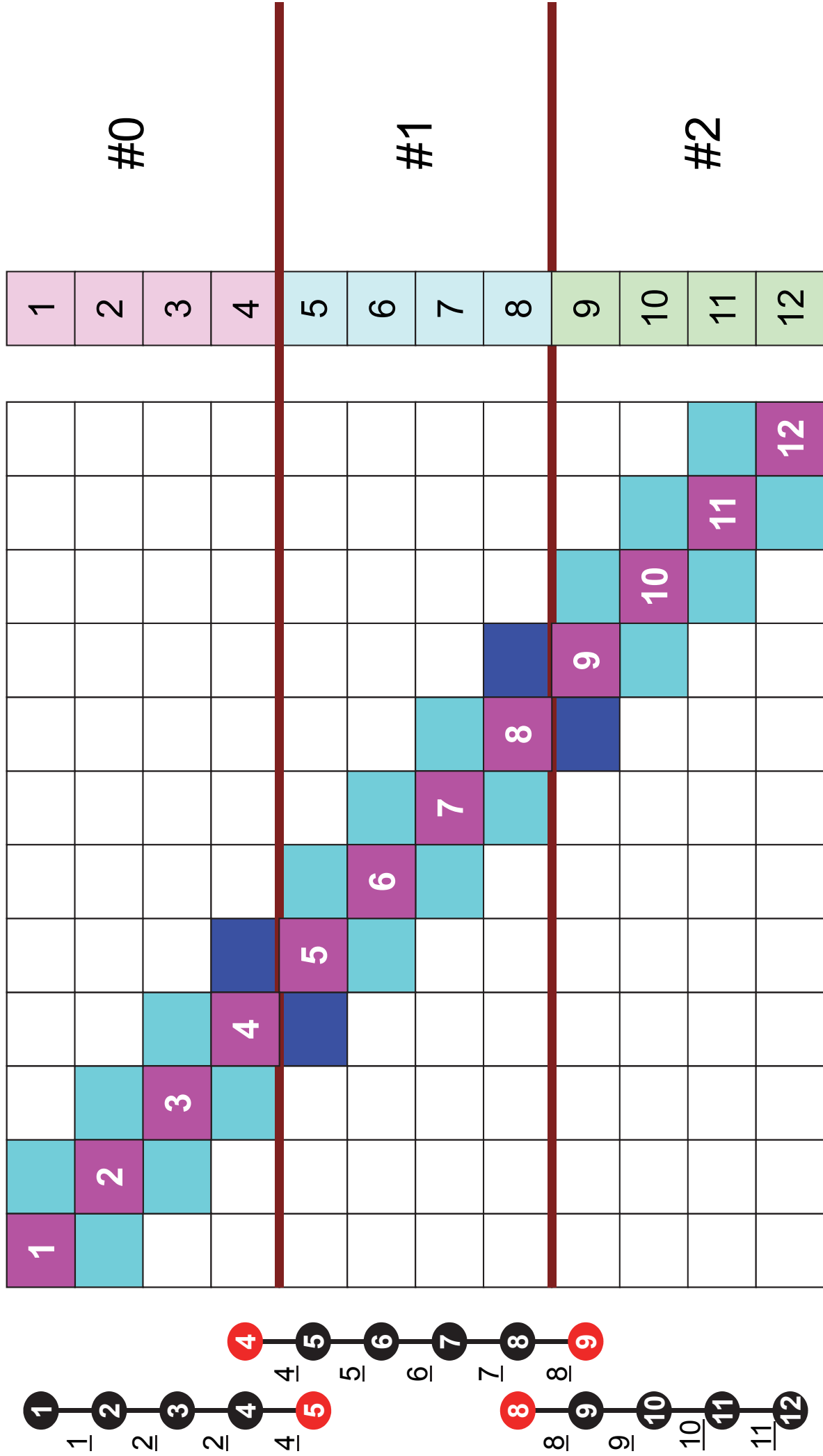
#1



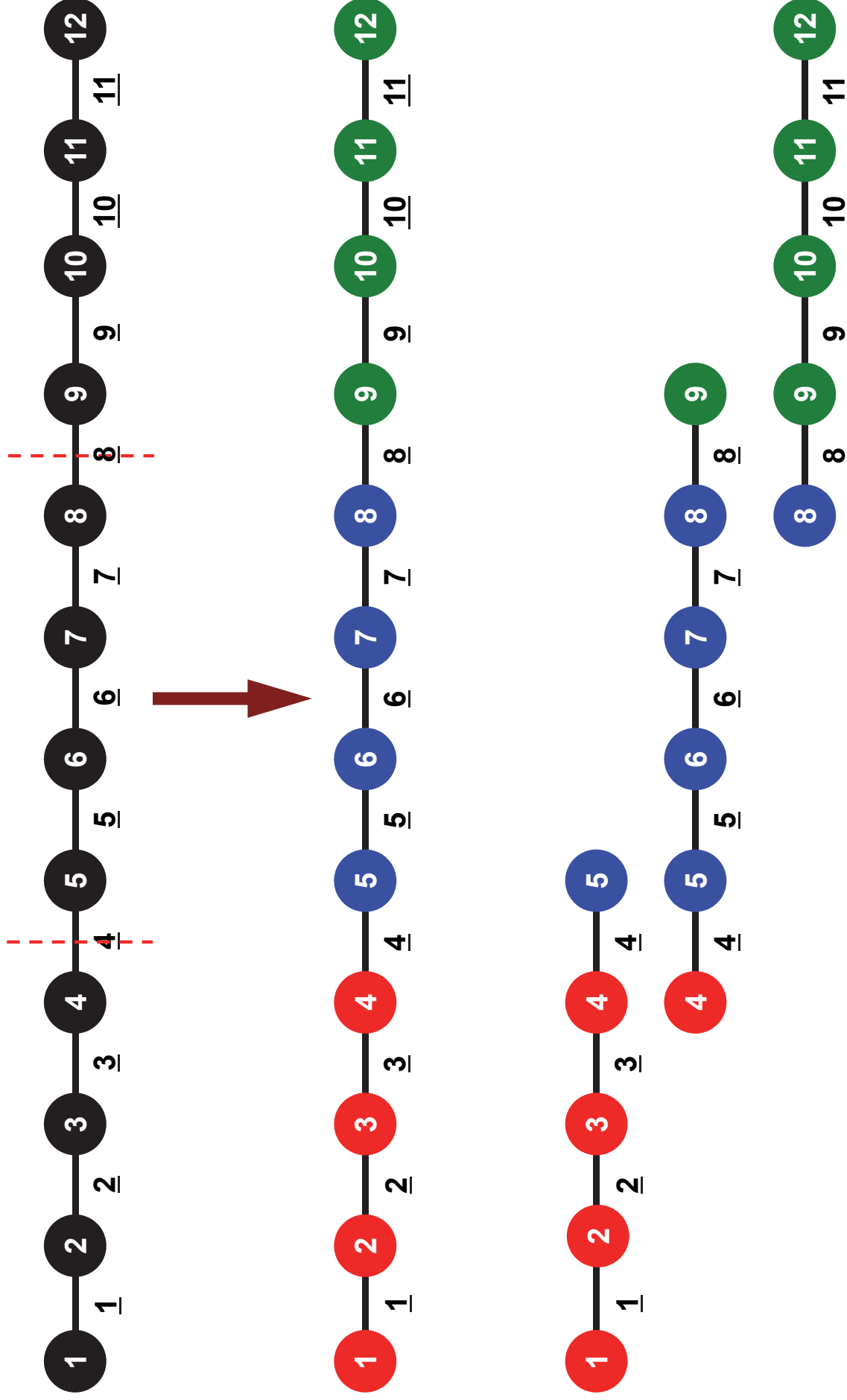
#2



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

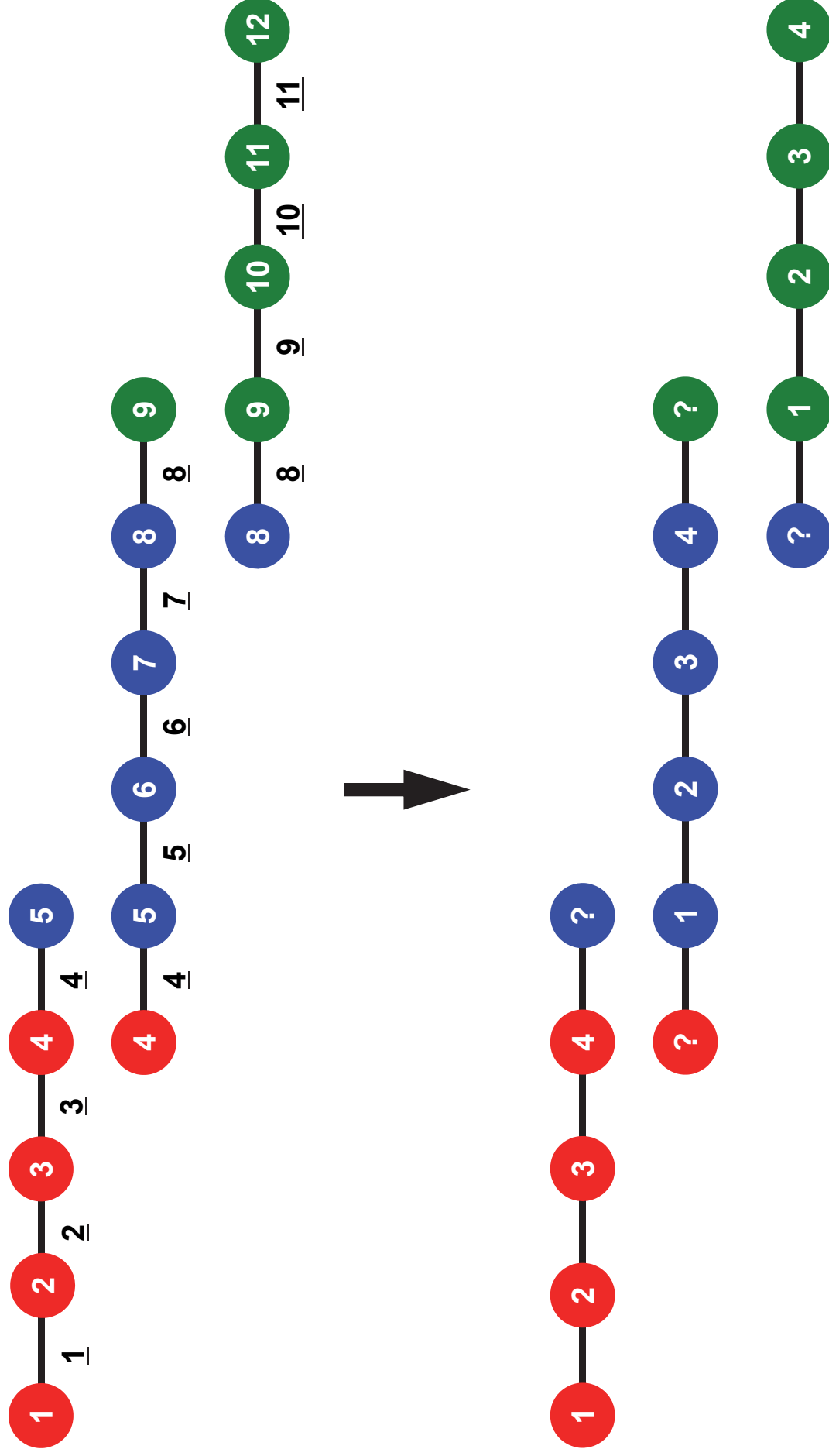


1D FEM: 12 nodes/11 elem's/3 domains



Local Numbering for SPMD

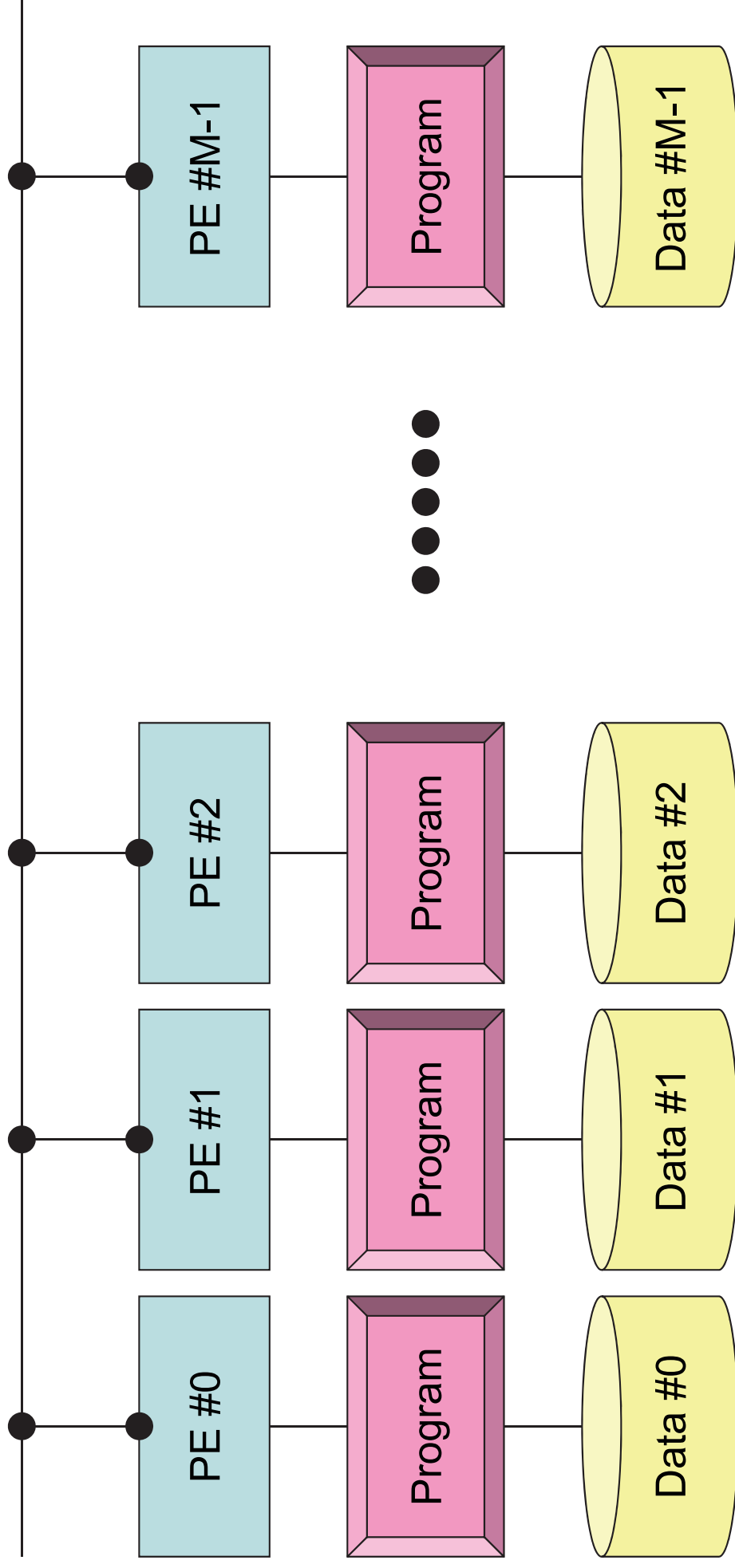
Numbering of internal nodes is 1-N ($0-N-1$), same operations in serial program can be applied. How about numbering of external nodes ?



PE: Processing Element
Processor, Domain, Process

SPMD

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

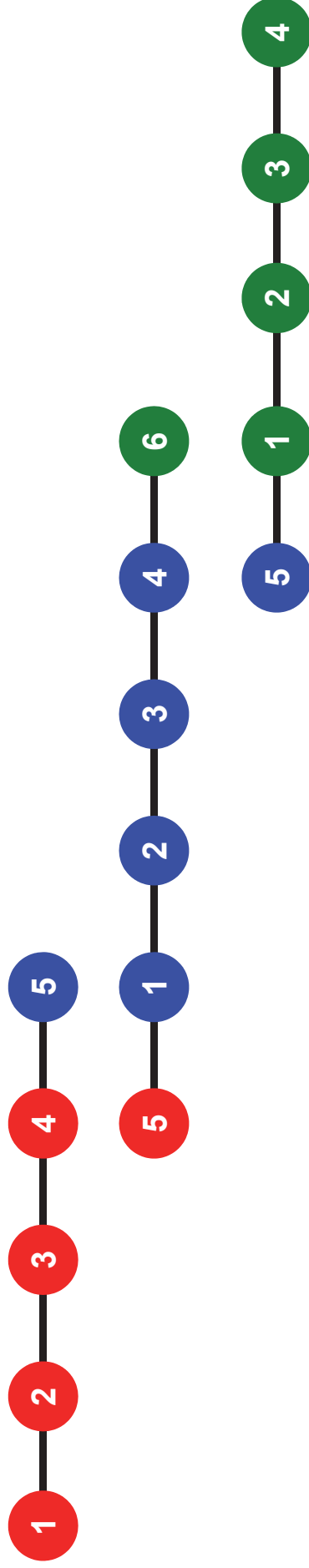


Each process does same operation for different data

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.

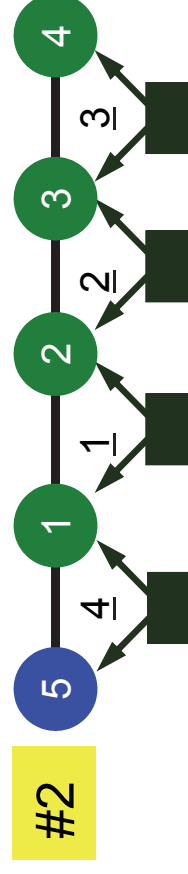
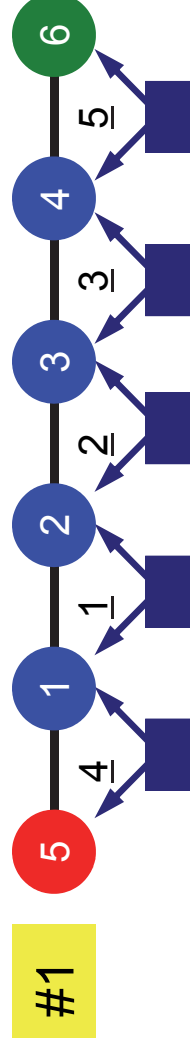
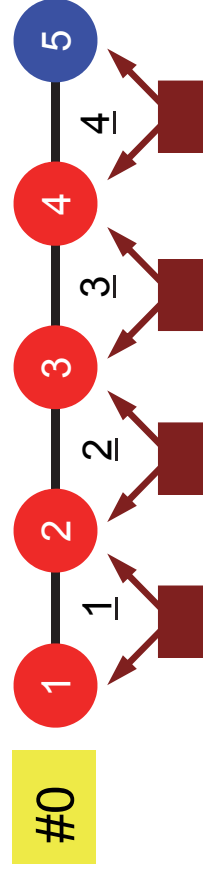
Local Numbering for SPMD

Numbering of external nodes: $N+1$, $N+2$ ($N, N+1$)



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

Integration on each element, element matrix $\rightarrow$ global matrix
 Operations can be done by info. of internal/external nodes
 and elements which include these nodes



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

```

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

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
```

1
2
3
4
5
6
7
8
9
10
11
12

Dot Products

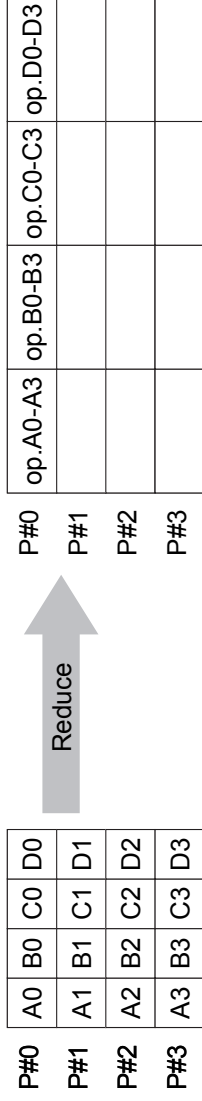
Global Summation needed: Communication ?

```
!C
!C-- ALPHA= RH0 / {p} {q}

C1= 0.d0
do i= 1, N
  C1= C1 + W(i, P)*W(i, Q)
enddo
ALPHA= RH0 / C1
```

1
2
3
4
5
6
7
8
9
10
11
12

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
 - count I number of elements in send/receive buffer
 - datatype I data type of elements of send/receive buffer
- type is defined by "datatype"
- number of elements in send/receive buffer
- data type of elements of send/receive buffer

FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.

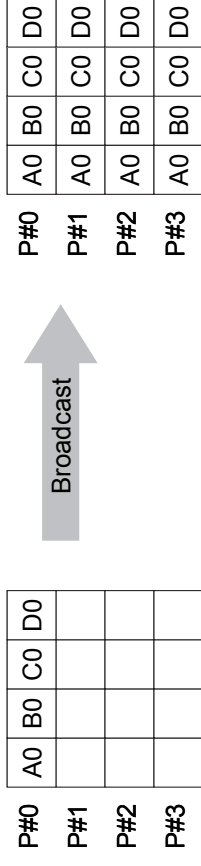
C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc

- 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

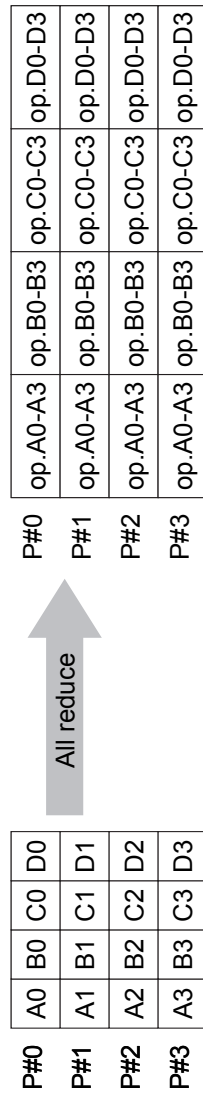
- root I I rank of root process
- comm I I communicator
- ierr I O completion code

MPI_BCAST



- Broadcasts a message from the process with rank "root" to all other processes of the communicator
- call `MPI_BCAST (buffer, count, datatype, root, comm, ierr)`
 - buffer choice I/O starting address of buffer
 type is defined by "datatype"
 - count I I number of elements in send/recv buffer
 - datatype I I data type of elements of send/recv buffer
 FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.
 C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc.
 - root I I rank of root process
 - comm I I communicator
 - ierr I O completion code

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, 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/recv buffer
- **datatype** I I data type of elements in send/recv buffer
- **op** I I reduce operation
- **comm** I I communicator
- **ierr** I O completion code

“op” of MPI_Reduce/Allreduce

Fortran

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

- | | |
|---------------------|--------------------|
| • MPI_MAX, MPI_MIN | Max, Min |
| • MPI_SUM, MPI_PROD | Summation, Product |
| • MPI_LAND | Logical AND |

Matrix-Vector Products

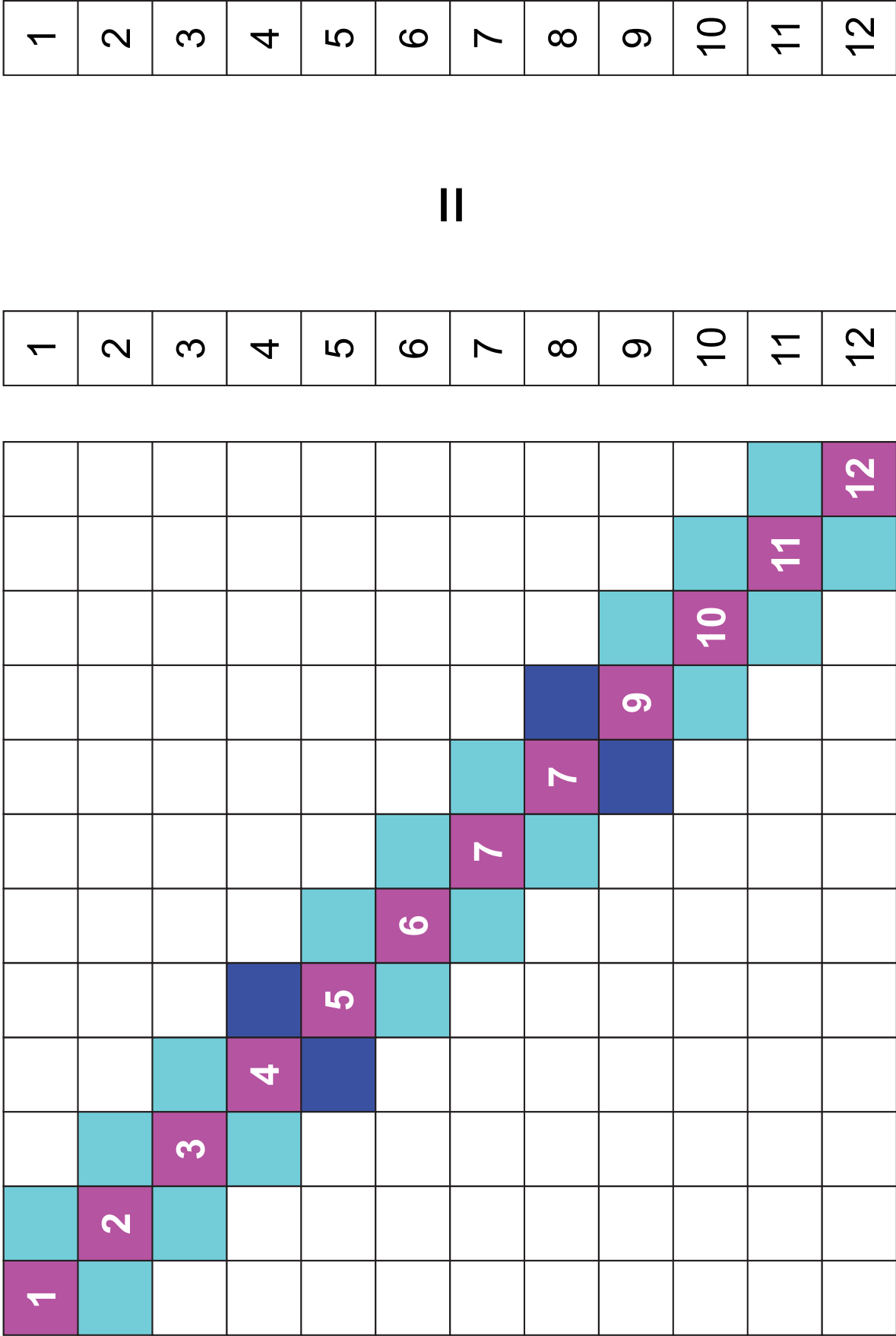
Values at External Points: P-to-P Communication

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

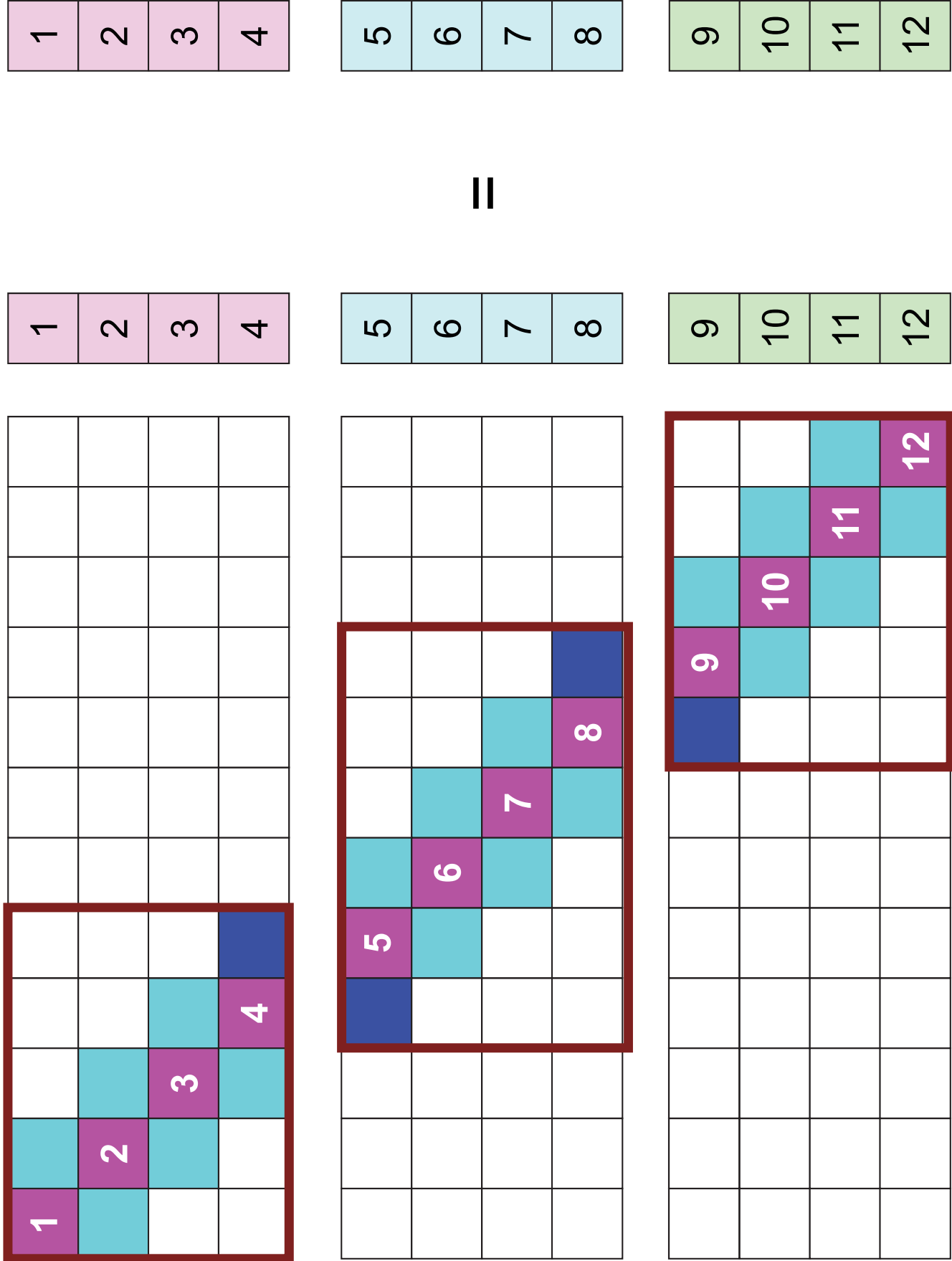
do i= 1, N
  W(i,Q) = DIAG(i)*W(i,P)
  do j= INDEX(i-1)+1, INDEX(i)
    W(i,Q) = W(i,Q) + AMAT(j)*W(ITEM(j),P)
  enddo
enddo
```



Mat-Vec Products: Local Op. Possible



Mat-Vec Products: Local Op. Possible



Mat-Vec Products: Local Op. Possible

1			
	2		
		3	
			4

1	2	3	4
---	---	---	---

1	2	3	4
---	---	---	---

		7	
	6		
5			

5	6	7	8
---	---	---	---

5	6	7	8
---	---	---	---

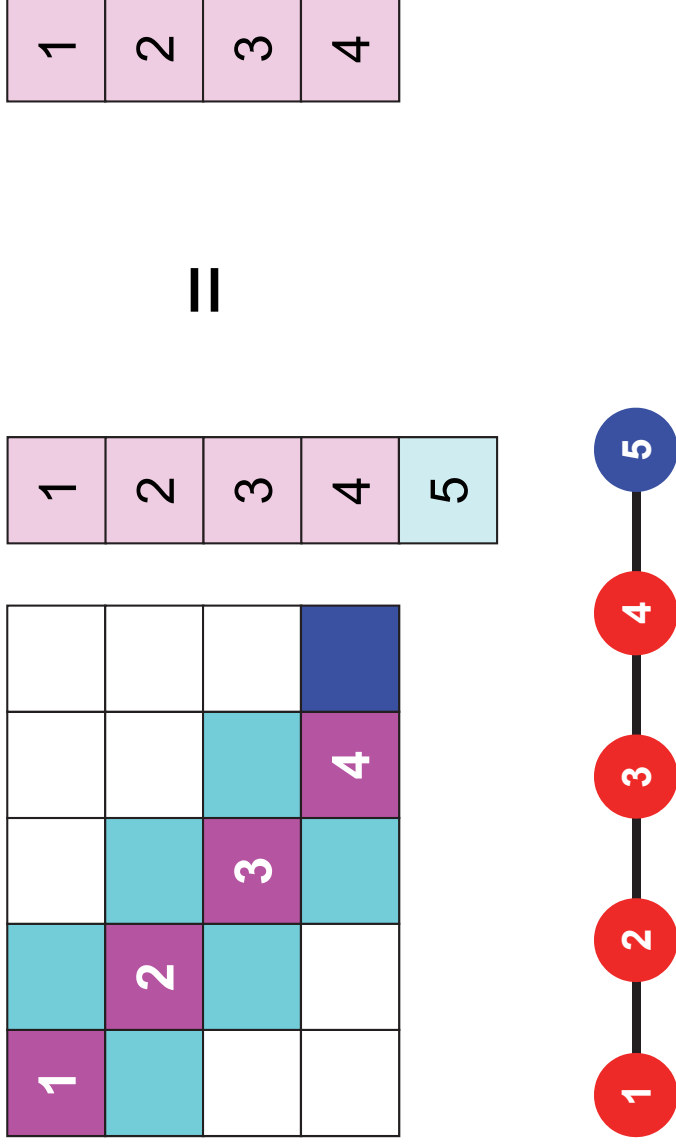
=

			12
		11	
9	10		

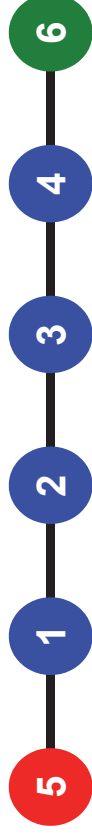
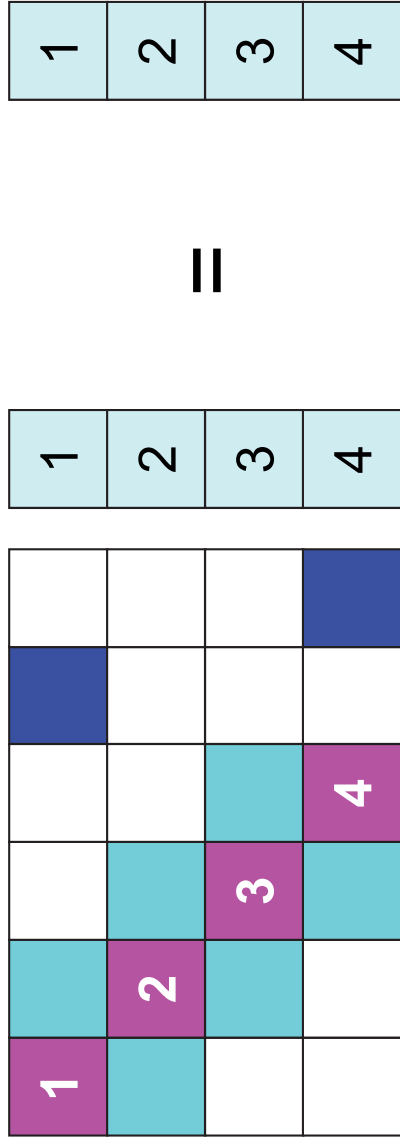
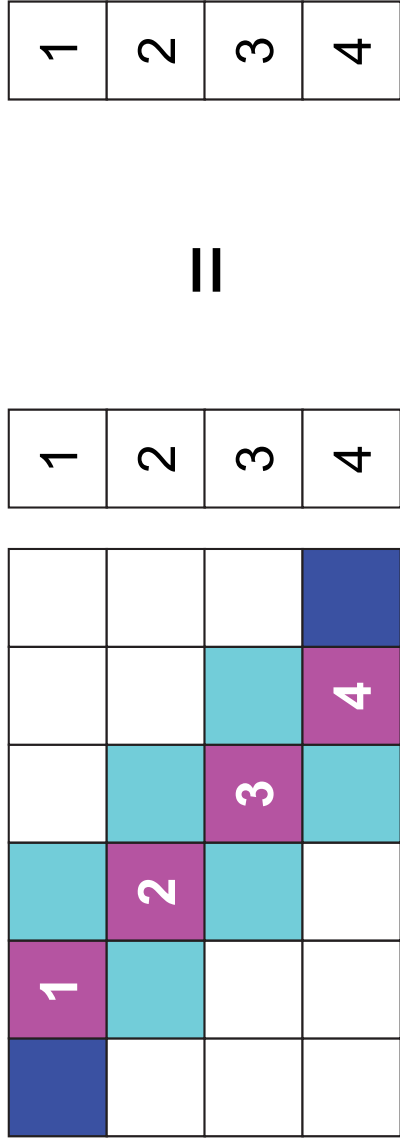
9	10	11	12
---	----	----	----

9	10	11	12
---	----	----	----

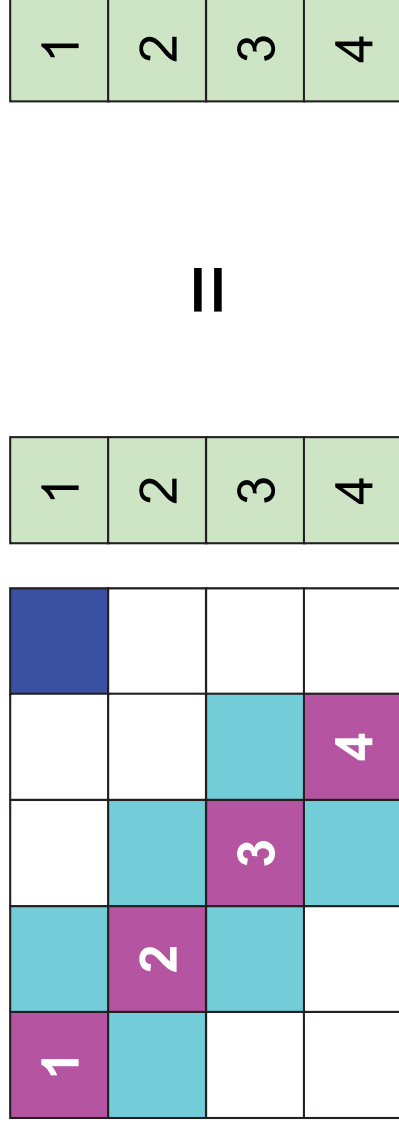
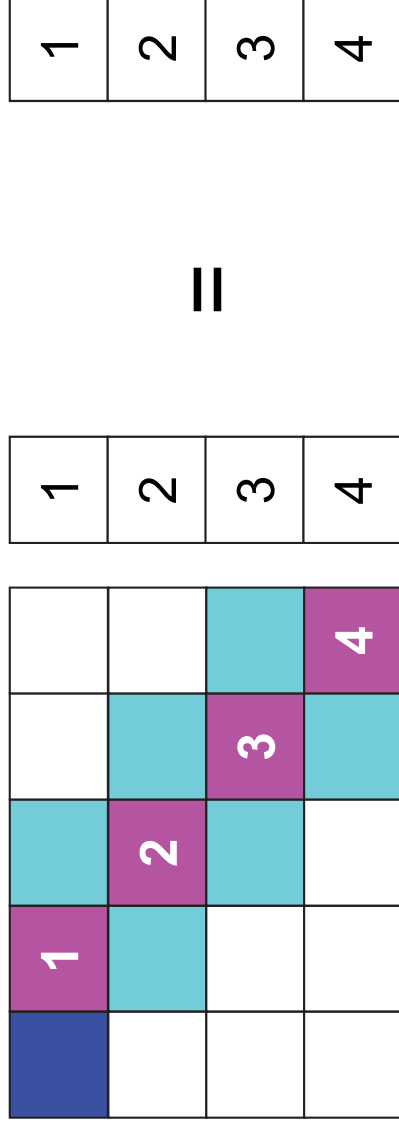
Mat-Vec Products: Local Op. #0



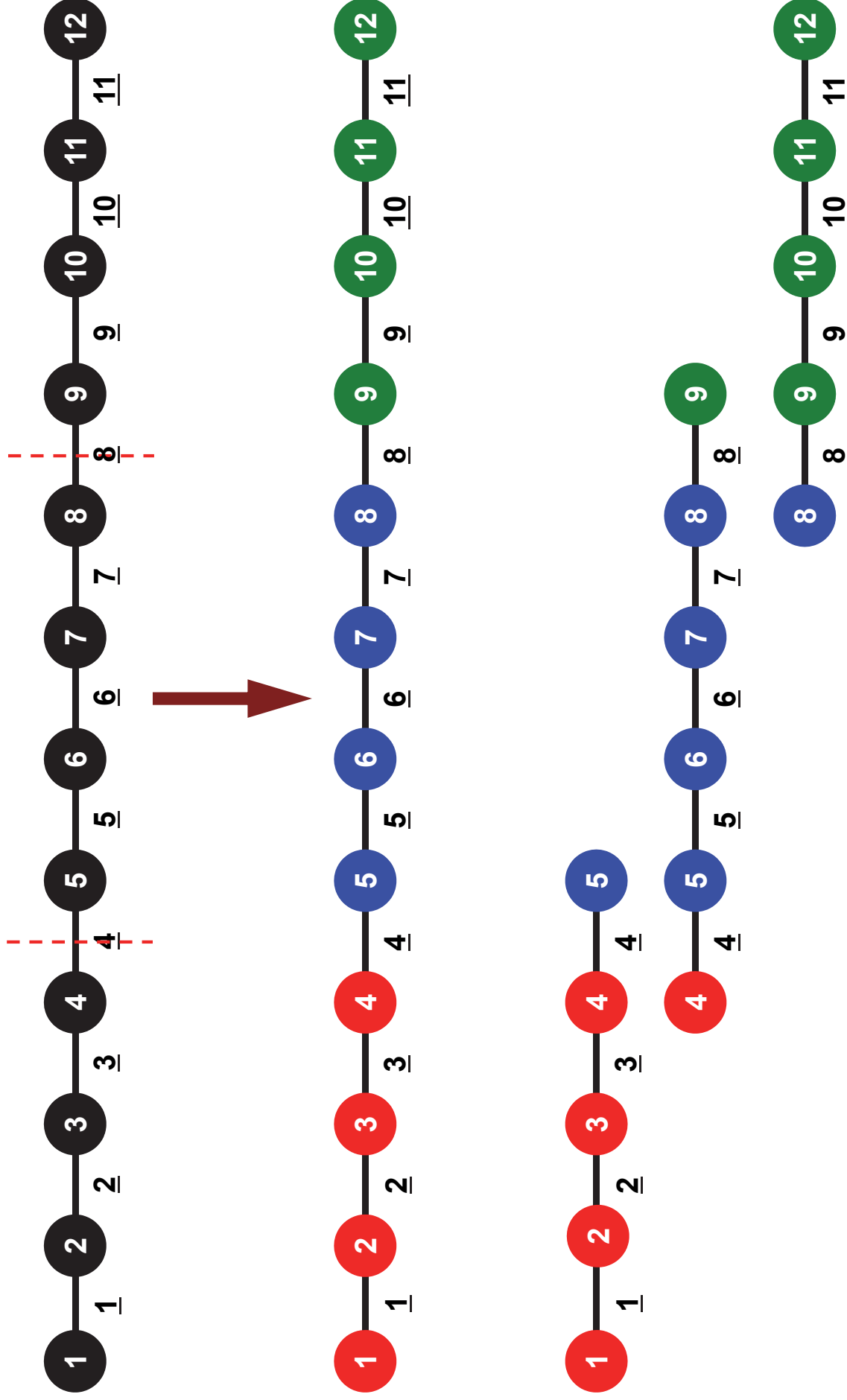
Mat-Vec Products: Local Op. #1



Mat-Vec Products: Local Op. #2

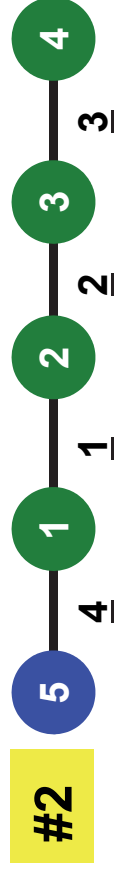


1D FEM: 12 nodes/11 elem's/3 domains



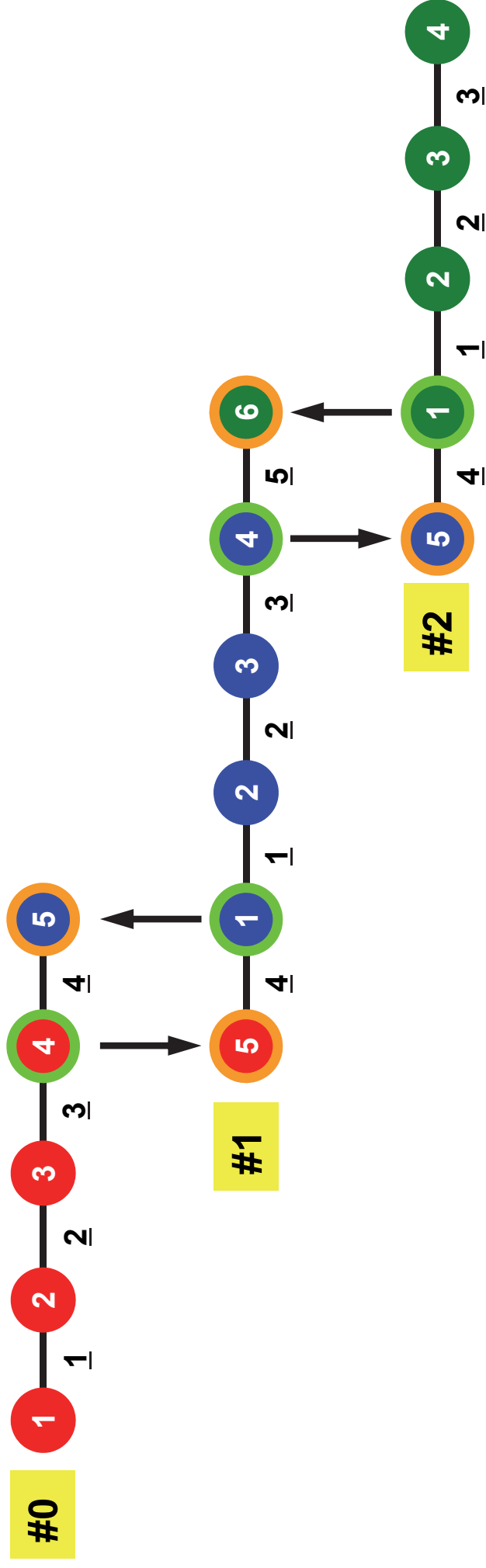
1D FEM: 12 nodes/11 elem's/3 domains

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



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

Internal/External Nodes

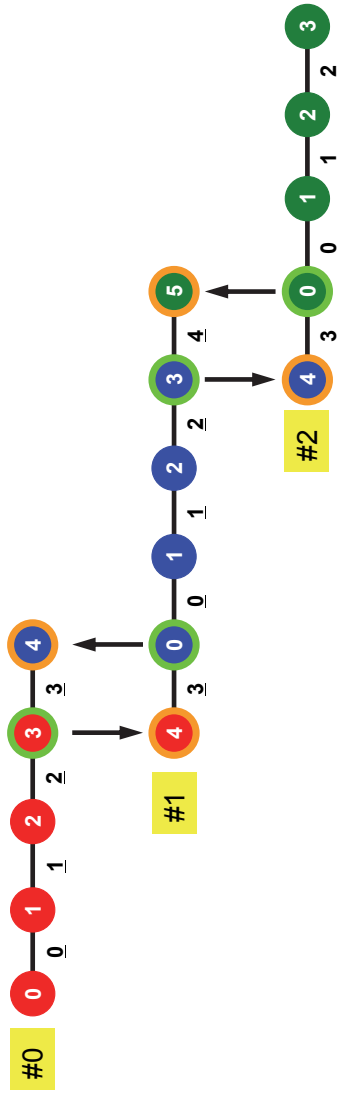


What is Peer-to-Peer Communication ?

- 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-to-Peer/Point-to-Point

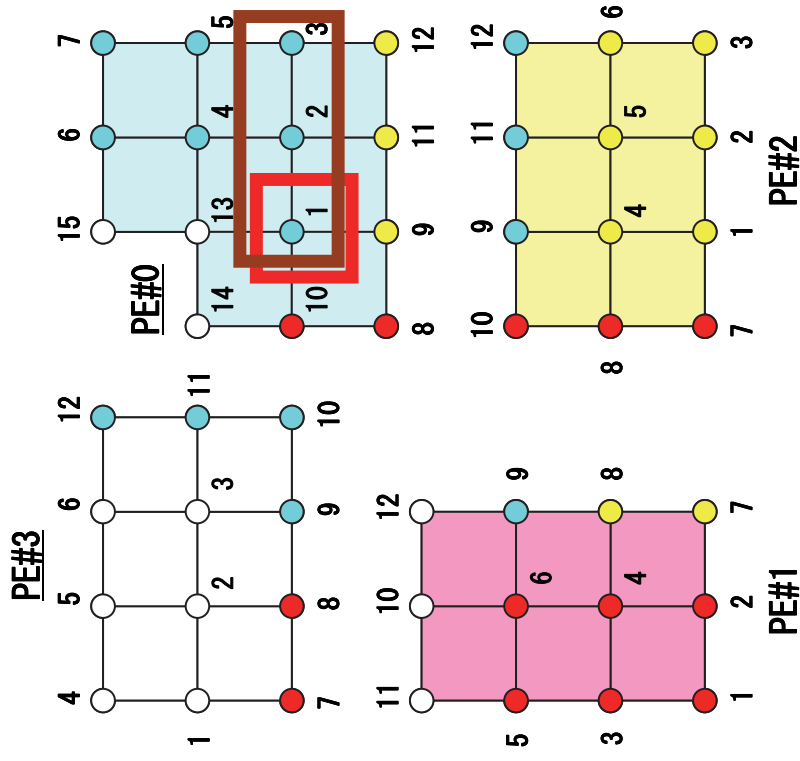
- MPI_Send, MPI_Receive
- Communication with limited processes
 - Neighbors
- Application Area
 - FEM, FDM: Localized Method



SEND: sending from boundary nodes

Send continuous data to send buffer of neighbors

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



MPI_SEND

- 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)`

– <u>sendbuf</u>	choice	I	starting address of sending buffer
– <u>count</u>	I	I	number of elements sent to each process
– <u>datatype</u>	I	I	data type of elements of sending buffer
– <u>dest</u>	I	I	rank of destination
– <u>tag</u>	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),

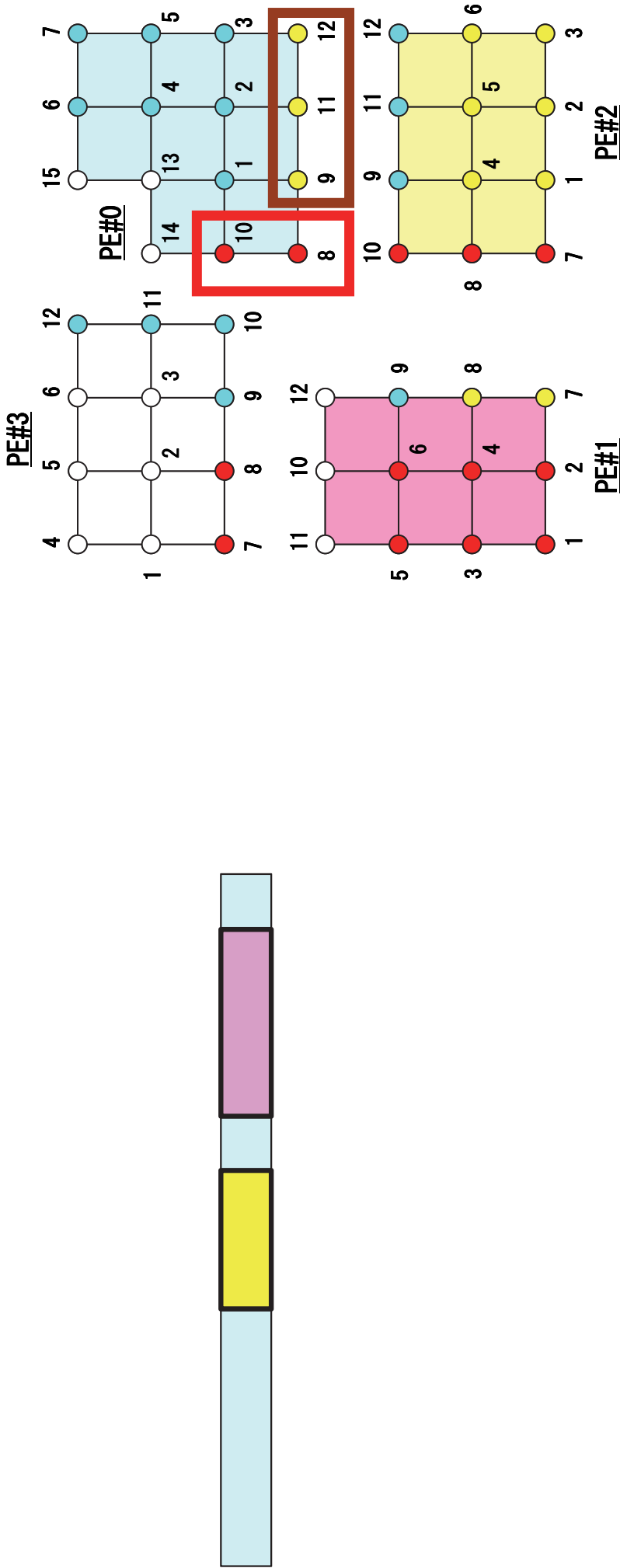
communicator

– <u>comm</u>	I	I	
– <u>request</u>	I	○	communication request array used in <code>MPI_Waitall</code>
– <u>ierr</u>	I	○	completion code

Recv: receiving to external nodes

Recv. continuous data to recv. buffer from neighbors

- `MPI_Irecv`
(`recvbuf`, `count`, `datatype`, `dest`, `tag`, `comm`, `request`)
 - 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



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 `tags` of `MPI_Isend` and `MPI_Irecv` are matched.

Usually tag is set to be “0” (in this class), communicator

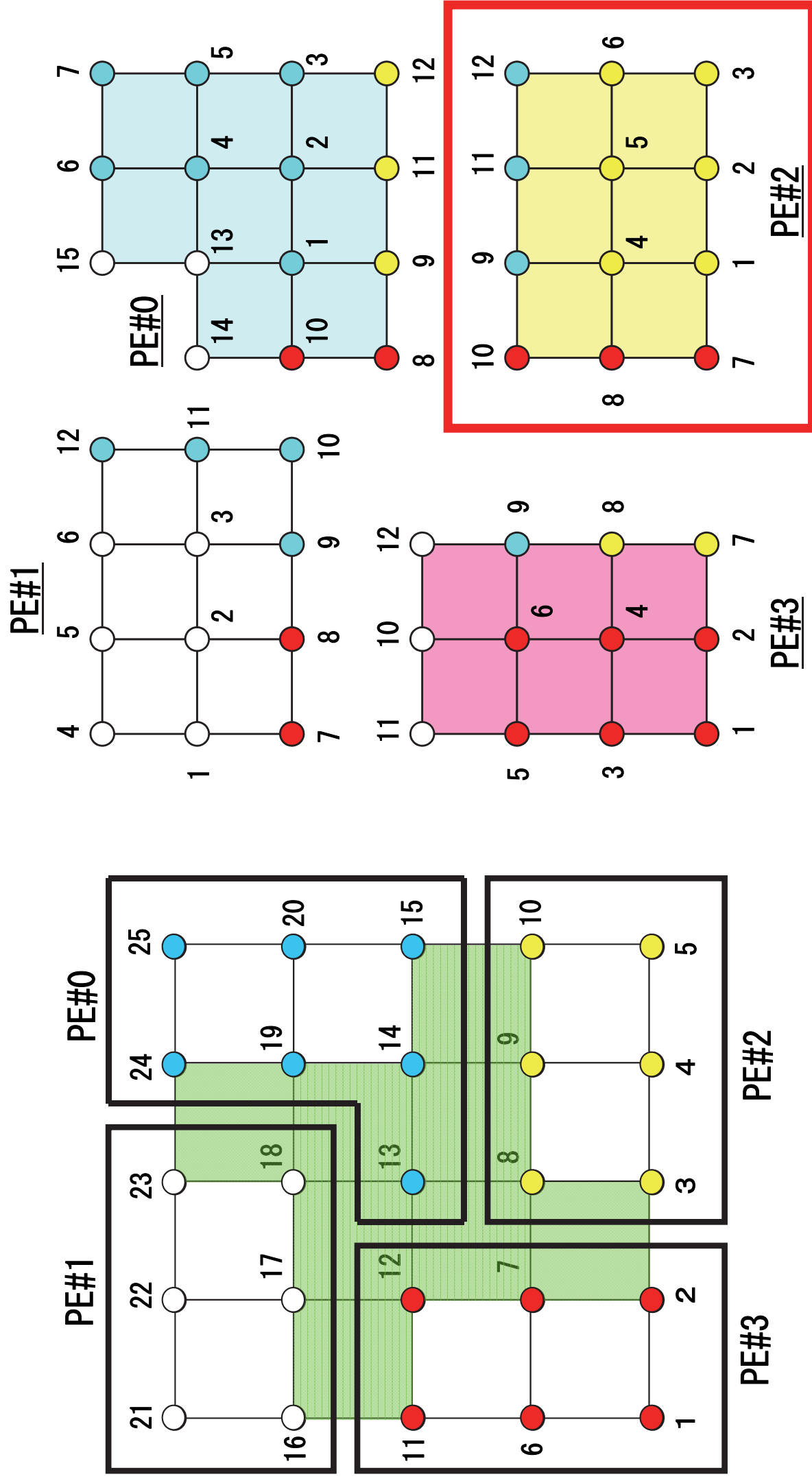
- comm I I
- request I O **communication request used in `MPI_waitall`**
- ierr I O completion code

MPI_WAITALL

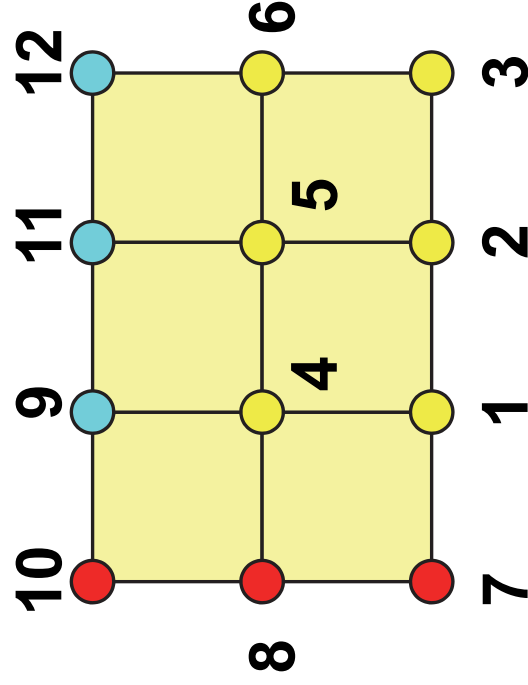
- `MPI_waitall` blocks until all comm's, associated with request in the array, complete. It is used for synchronizing MPI_Isend and MPI_Irecv in this class.
- At sending phase, contents of sending buffer cannot be modified before calling corresponding `MPI_waitall`. At receiving phase, contents of receiving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

Node-based Partitioning

internal nodes - elements - external nodes



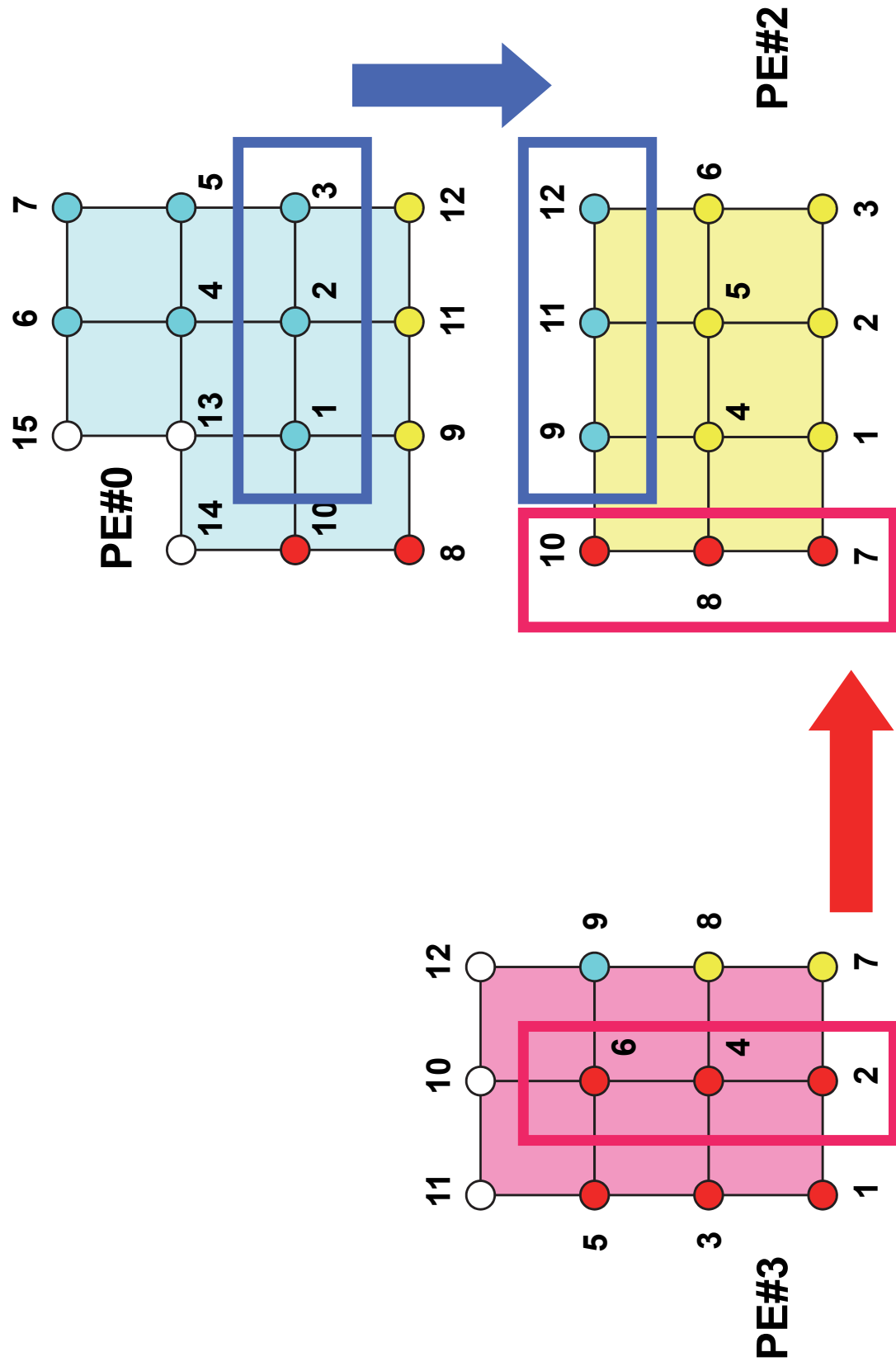
Description of Distributed Local Data



- 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 ?

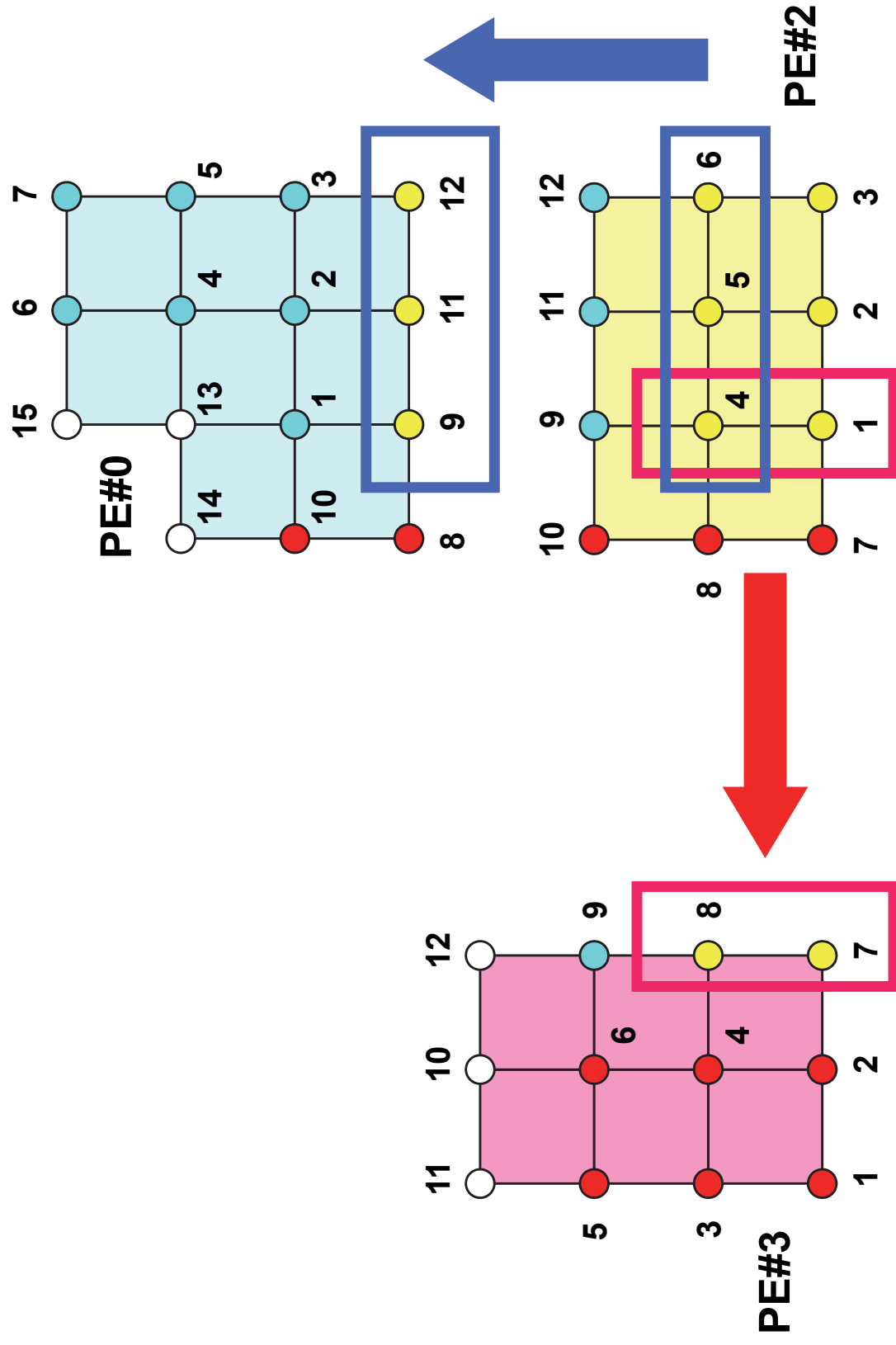
External Nodes (外点) : RECEIVE

PE#2 : receive information for “external nodes”



Boundary Nodes (境界点) : SEND

PE#2 : send information on “boundary nodes”



Distributed Local Data Structure for Parallel Computation

- Distributed local data structure for domain-to-domain 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