

# Overview of (1D) FEM & Road to Parallel FEM

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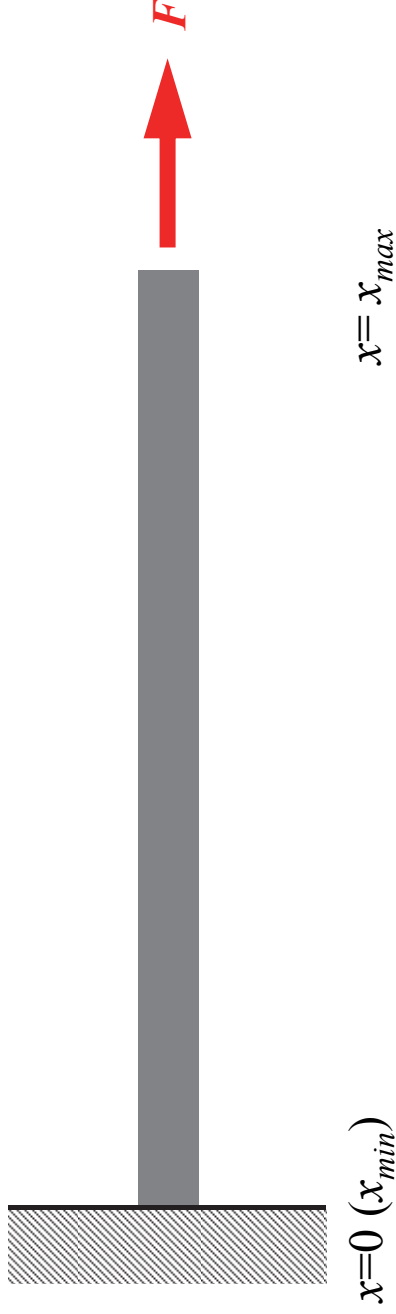
- 1D-code for Static Linear-Elastic Problems by Galerkin FEM
- Sparse Linear Solver
  - Conjugate Gradient Method
  - Preconditioning
- Storage of Sparse Matrices
- Program
- Road to Parallel FEM

# Keywords

- 1D Static Linear Elastic Problems
- Galerkin Method
- Linear Element
- Preconditioned Conjugate Gradient Method

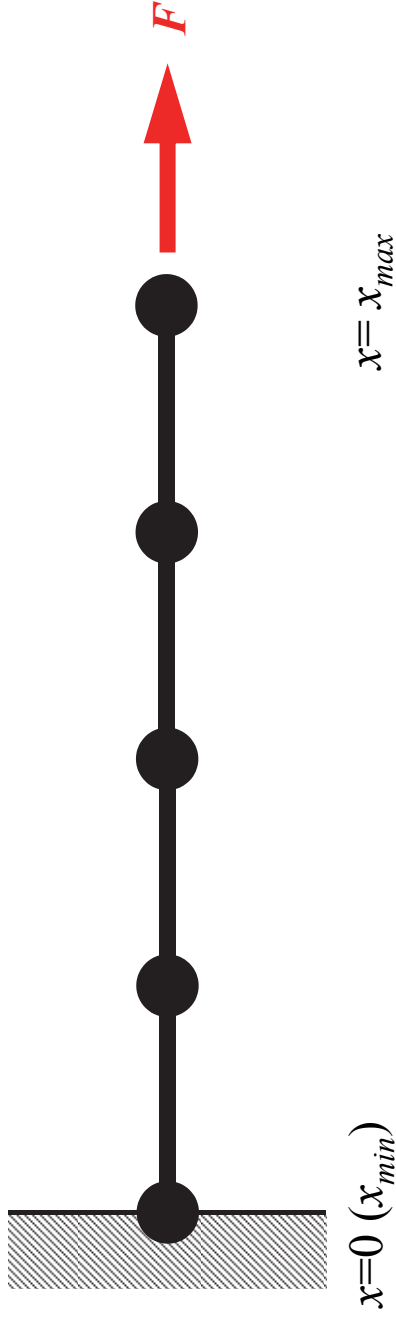
# 1D Static Linear Elastic Problem

## (Truss : トラス)



- Only deforms in  $x$ -direction (displacement:  $u$ )
  - Uniform: Sectional Area  $A$ , Young's Modulus  $E$
  - Boundary Conditions (B.C.)
    - $x=0 \quad : u=0$  (fixed)
    - $x=x_{max} : F$  (axial force)
- Truss: NO bending deformation by G-force

# 1D Static Linear Elastic Problem



Equilibrium  
Equation

$$\frac{\partial \sigma_x}{\partial x} + X = 0$$

Strain~  
Displacement

$$\varepsilon_x = \frac{\partial u}{\partial x}$$

Stress~  
Strain

$$\sigma_x = E \varepsilon_x$$

$$\frac{\partial}{\partial x} \left( E \frac{\partial u}{\partial x} \right) + X = 0$$

Governing Equation  
for  $u$

# Procedures for Computation

- solve equations for displacement  $u$

$$\frac{\partial}{\partial x} \left( E \frac{\partial u}{\partial x} \right) + X = 0$$

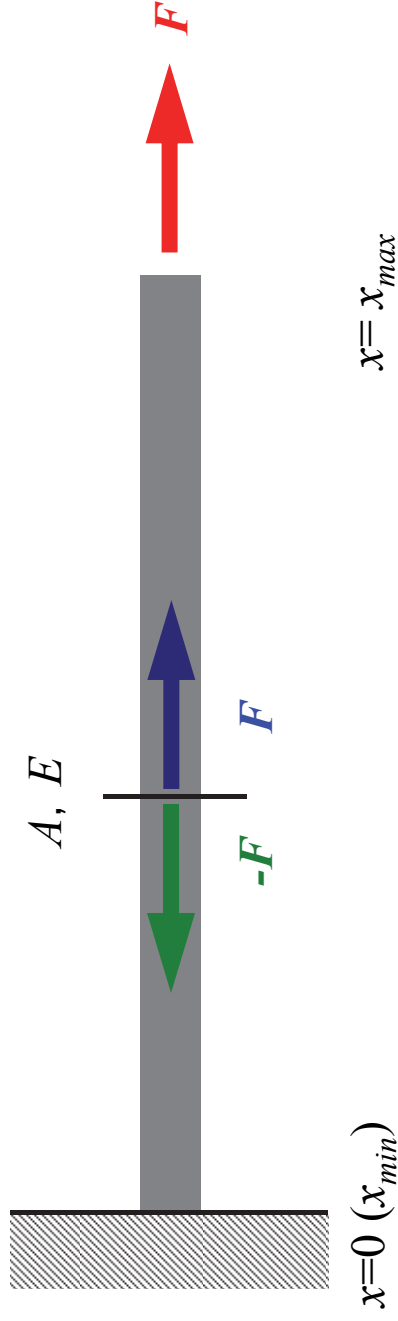
- calc. strain

$$\varepsilon_x = \frac{\partial u}{\partial x}$$

- calc. stress

$$\sigma_x = E \varepsilon_x$$

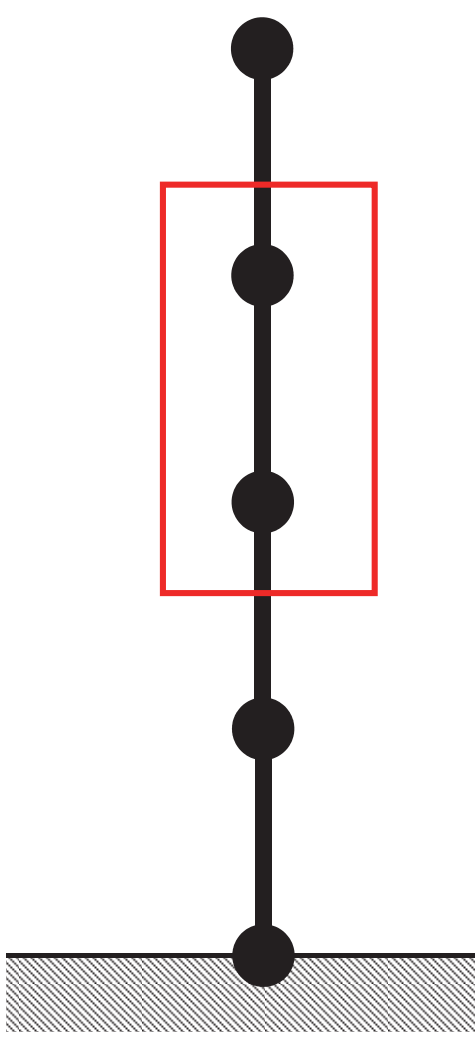
# Results Expected



- $x_{max}=10, F=5, A=2, E=10$ .
- Equilibrium State: Uniform axial force at any section
  - Uniform stress:  $\sigma = F/A = 2.5$
  - Uniform strain:  $\varepsilon = \sigma/E = 0.25$
  - Uniform displacement for each element, if size of each element is uniform (deformation rate=  $\varepsilon$ )  $u = 2.5 @ x = x_{max}$

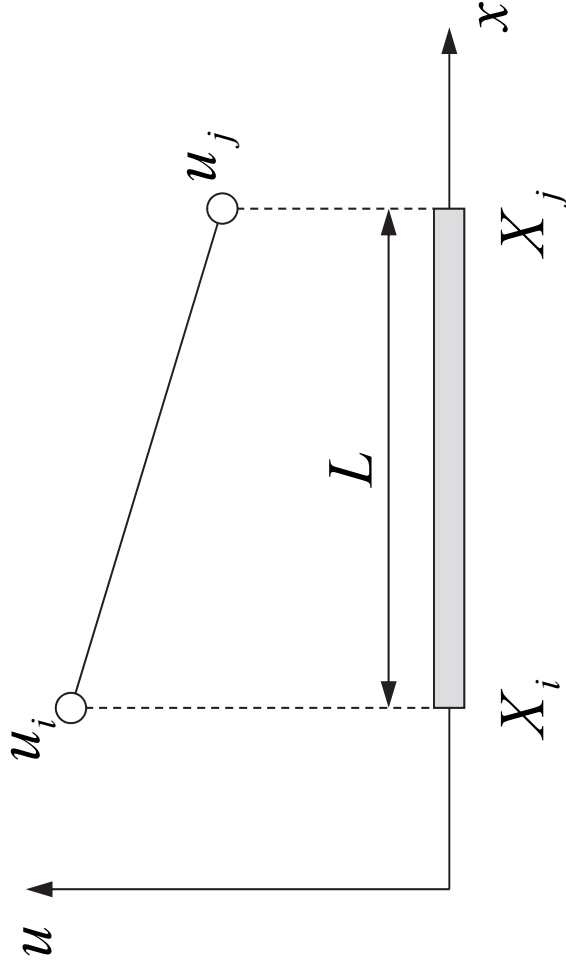
# 1D Linear Element (1/4)

## 一次元線形要素

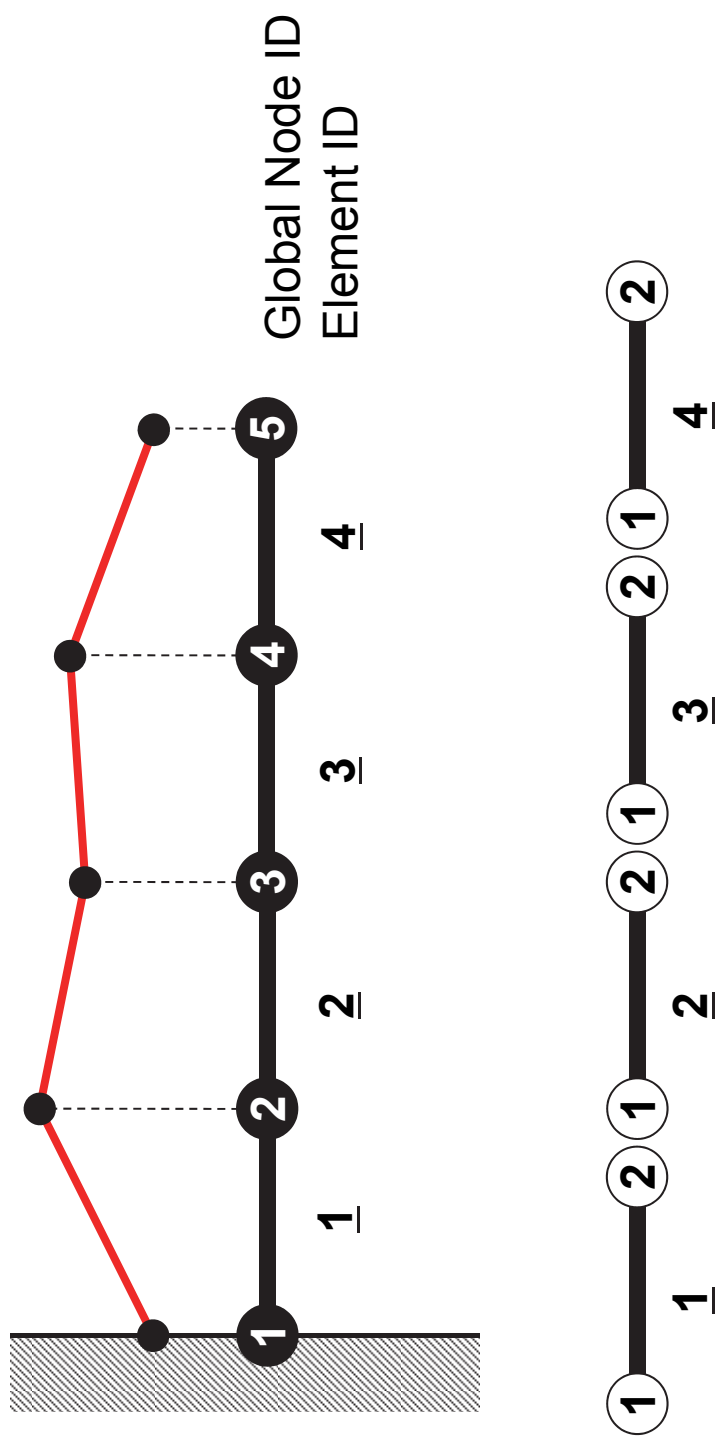


- 1D Linear Element
  - Length =  $L$ 
    - Node (Vertex) (節点)
    - Element (要素)
- $u_i$  Displacement at  $i$
- $u_j$  Displacement at  $j$
- Displacement  $u$  on each element is linear function of  $x$  (Piecewise Linear):

$$u = \alpha_1 + \alpha_2 x$$



# Piecewise Linear



Strain and stress are constant in each element  
(might be discontinuous at each “node”)

# 1D Linear Elem.: Shape Function (2/4)

- Coef's are calculated based on info. at each node

$$u = u_i @ x = X_i, \quad u = u_j @ x = X_j$$

$$u_i = \alpha_1 + \alpha_2 X_i, \quad u_j = \alpha_1 + \alpha_2 X_j$$

- Coefficients:

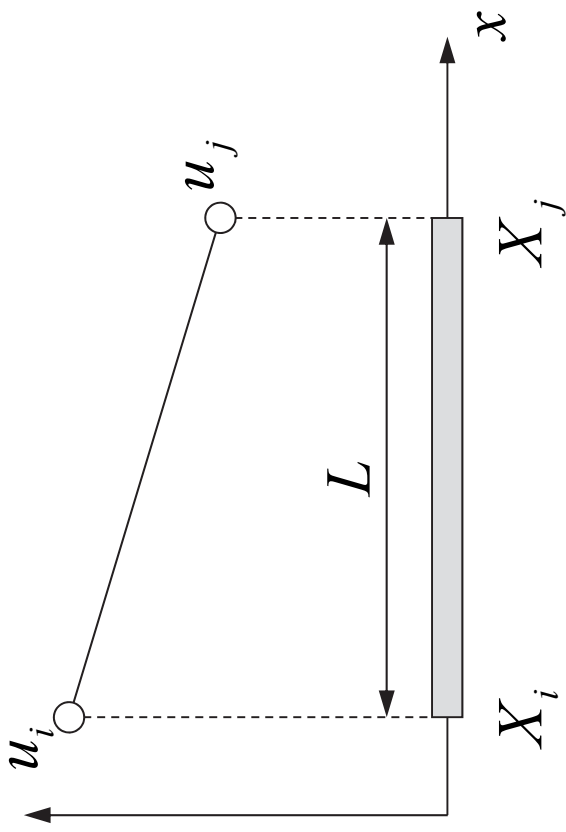
$$\alpha_1 = \frac{u_i X_j - u_j X_i}{L}, \quad \alpha_2 = \frac{u_j - u_i}{L}$$

- $u$  can be written as follows, according to  $u_i$  and  $u_j$ :

$$u = \left( \frac{X_j - x}{L} \right) u_i + \left( \frac{x - X_i}{L} \right) u_j$$

$N_i$   $N_j$

**$N_i, N_j$**   
Shape Function or  
Interpolation Function  
function of  $x$  (only)

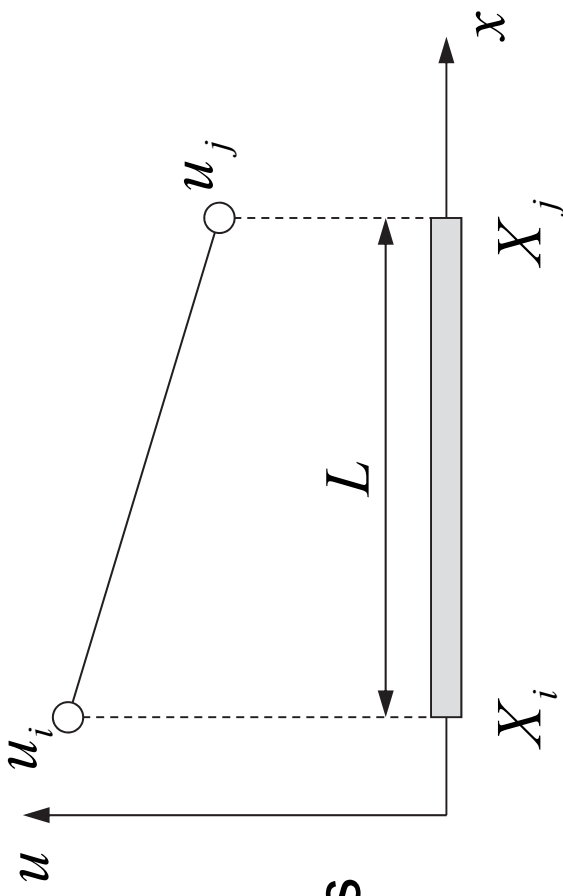


# 1D Linear Elem.: Shape Function (3/4)

- Number of Shape Functions = Number of Vertices of Each Element

- $N_i$ : Function of Position
- A kind of Test/Trial Functions

$$N_i = \left( \frac{X_j - x}{L} \right), \quad N_j = \left( \frac{x - X_i}{L} \right)$$



- Linear combination of shape functions provides displacement “in” each element
  - Coef’s (unknowns): Displacement at each node

$$u = N_i u_i + N_j u_j \longleftrightarrow$$

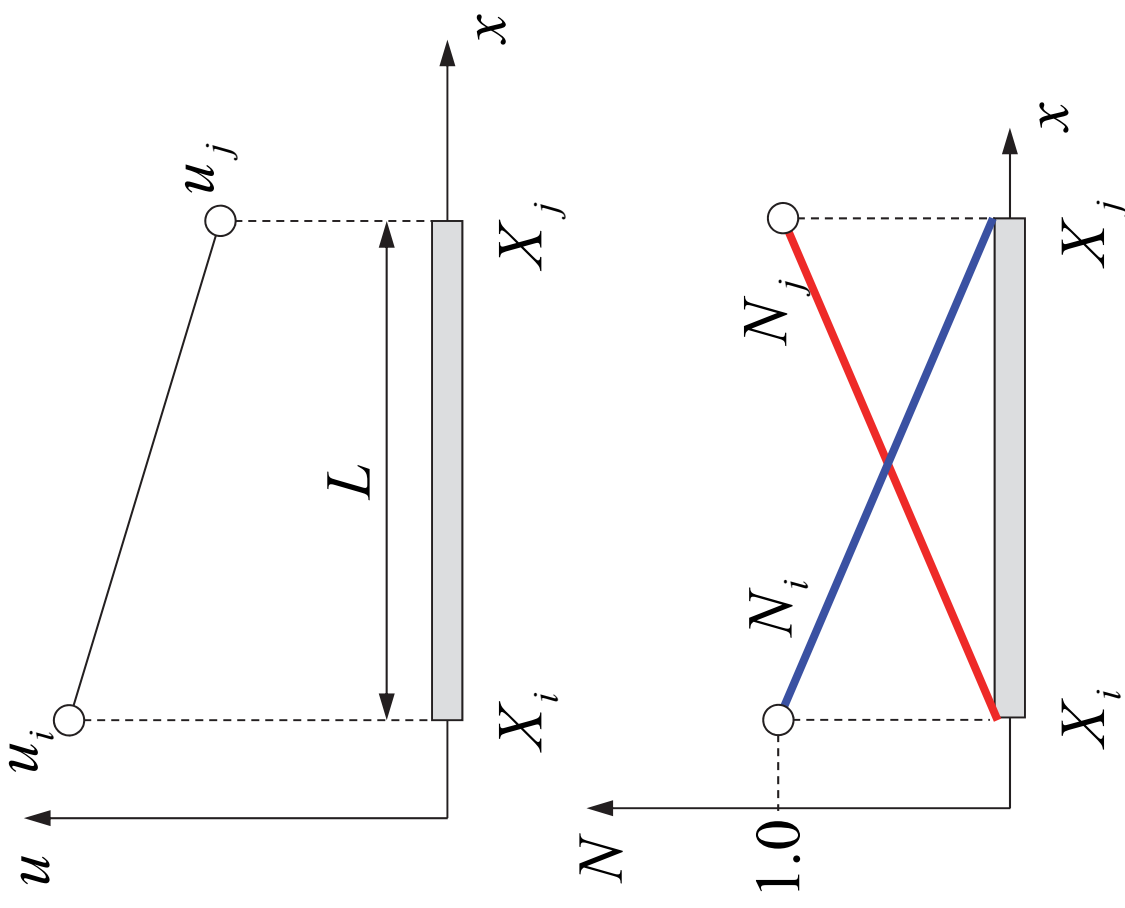
|          |                                                                                                                |
|----------|----------------------------------------------------------------------------------------------------------------|
| $\Psi_i$ | Trial/Test Function (known function of position, defined in domain and at boundary. “Basis” in linear algebra. |
| $a_i$    | Coefficients (unknown)                                                                                         |

$$u_M = \sum_{i=1}^M a_i \Psi_i$$

# 1D Linear Elem.: Shape Function (4/4)

- Value of  $N_i$ 
  - =1 at one of the nodes
  - in element
  - =0 on other nodes

$$N_i = \left( \frac{X_j - x}{L} \right), \quad N_j = \left( \frac{x - X_i}{L} \right)$$



# Galerkin Method (1/4)

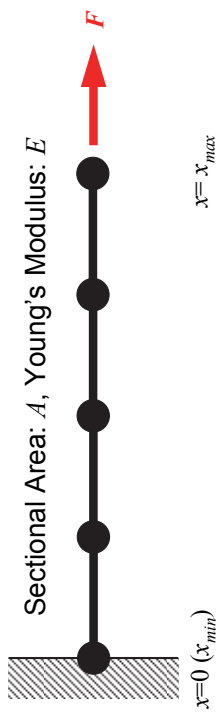
- Governing Equation for 1D Static Linear-Elastic Problems

$$E \left( \frac{d^2 u}{dx^2} \right) + X = 0$$

$$u = [N] \{ \phi \}$$

Distribution of Displacement in Each Elem.

(Matrix Form),  $\phi$  : Displacement at Each Node



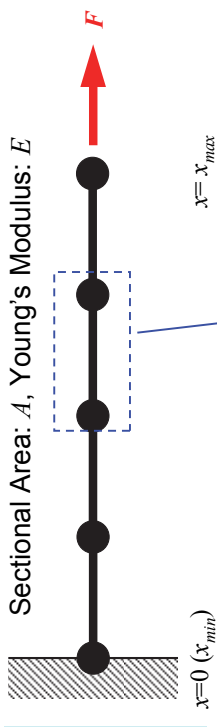
- Following integral equation is obtained at each element by Galerkin method (one of Weighted Residual Methods(WRM)), where  $[N]$ 's are also weighting functions:

$$\int_V [N]^T \left\{ E \left( \frac{d^2 u}{dx^2} \right) + X \right\} dV = 0$$

# Galerkin Method (2/4)

- Green's Theorem (1D)

$$\int_V \left( \frac{d^2 B}{dx^2} \right) dV = \int_S A \frac{dB}{dx} dS - \int_V \left( \frac{dA}{dx} \frac{dB}{dx} \right) dV$$



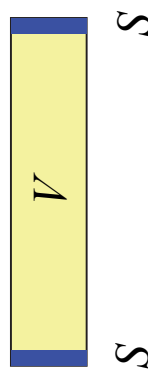
- Apply this to the 1st part of eqn with 2<sup>nd</sup>-order diff.:

$$\int_V E[N]^T \left( \frac{d^2 u}{dx^2} \right) dV = - \int_V E \left( \frac{d[N]^T}{dx} \frac{du}{dx} \right) dV + \int_S E[N]^T \frac{du}{dx} dS$$

- Consider the following terms:

$$u = [N]\{\phi\}, \quad \frac{du}{dx} = \frac{d[N]}{dx} \{\phi\} \quad \bar{\sigma} = E \frac{du}{dx}$$

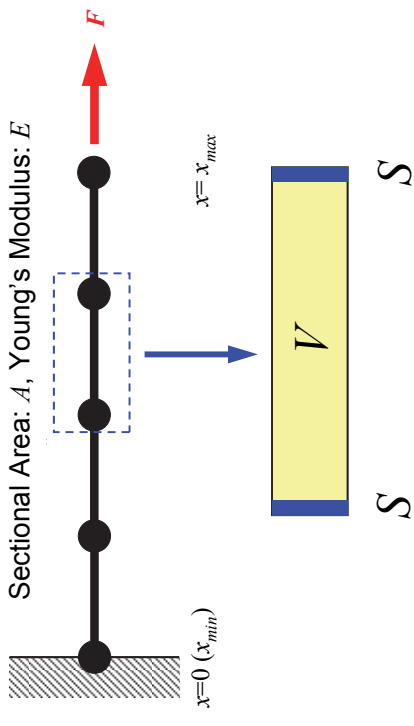
Stress on Surfaces  
of Each Element



# Galerkin Method (3/4)

- Finally following eqn is obtained by considering term due to body forces ( $X$ )

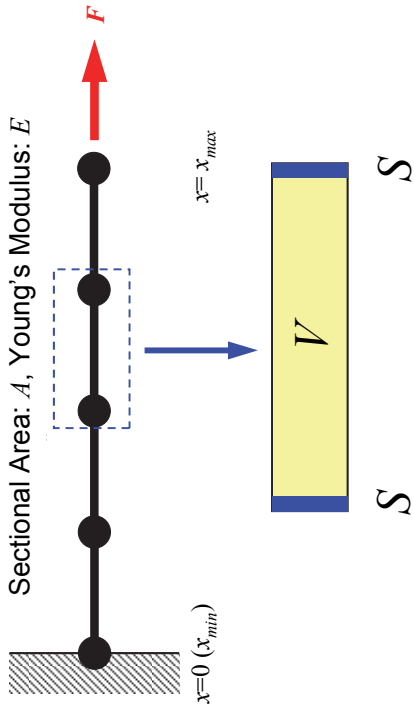
$$-\int_V E \left( \frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV \cdot \{\phi\} + \int_S \bar{\sigma} [N]^T dS + \int_V X [N]^T dV = 0$$



- This is called “weak form (弱形式)” . Original PDE consists of terms with 2<sup>nd</sup>-order diff., but this “weak form” only includes 1<sup>st</sup>-order diff by Green’s theorem.
  - Requirements for shape functions are “weaker” in “weak form”. Linear functions can describe effects of 2<sup>nd</sup>-order differentiation.

# Galerkin Method (4/4)

$$\begin{aligned}
 & - \int_V E \left( \frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV \cdot \{\phi\} \\
 & + \int_S \bar{\sigma}[N]^T dS + \int_V X[N]^T dV = 0
 \end{aligned}$$



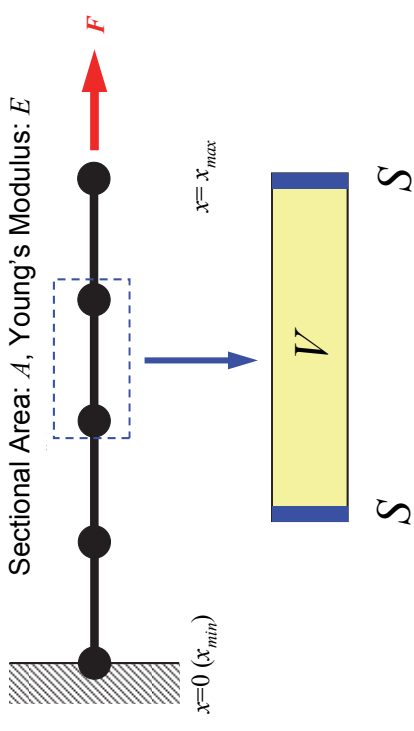
- These terms coincide at element boundaries and disappear. Finally, only terms on the domain boundaries remain.

# Weak Form and Boundary Conditions

- Value of dependent variable is defined (Dirichlet)
  - Weighting Function = 0
  - Principal B.C. (Boundary Condition) (第一種境界条件)
  - Essential B.C. (基本境界条件)

- Derivatives of Unknowns (Neumann)

- Naturally satisfied in weak form
- Secondary B.C. (第二種境界条件)
- Natural B.C (自然境界条件)



$$\begin{aligned}
 & - \int_V E \left( \frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV \cdot \{\phi\} \\
 & + \int_S \bar{\sigma} [N]^T dS + \int_V X [N]^T dV = 0
 \end{aligned}$$

where  $\bar{\sigma} = E \frac{du}{dx}$

Weak Form with B.C.: on each elem.

$$[k]^{(e)} \{\phi\}^{(e)} = \{f\}^{(e)}$$

$$[k]^{(e)} = \int_V E \left( \frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV$$

$$[f]^{(e)} = \int_V X[N]^T dV + \int_S \bar{\sigma} [N]^T dS$$

# Integration over Each Element: $[k]$

$$N_i = \left( \frac{X_j - x}{L} \right), \quad N_j = \left( \frac{x - X_i}{L} \right)$$

$$\frac{dN_i}{dx} = \left( \frac{-1}{L} \right), \quad \frac{dN_j}{dx} = \left( \frac{1}{L} \right)$$

$$\int_V E \left( \frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV$$

$$= E \int_0^L \begin{bmatrix} -1/L \\ 1/L \end{bmatrix} \begin{bmatrix} -1/L & 1/L \end{bmatrix} A \, dx$$

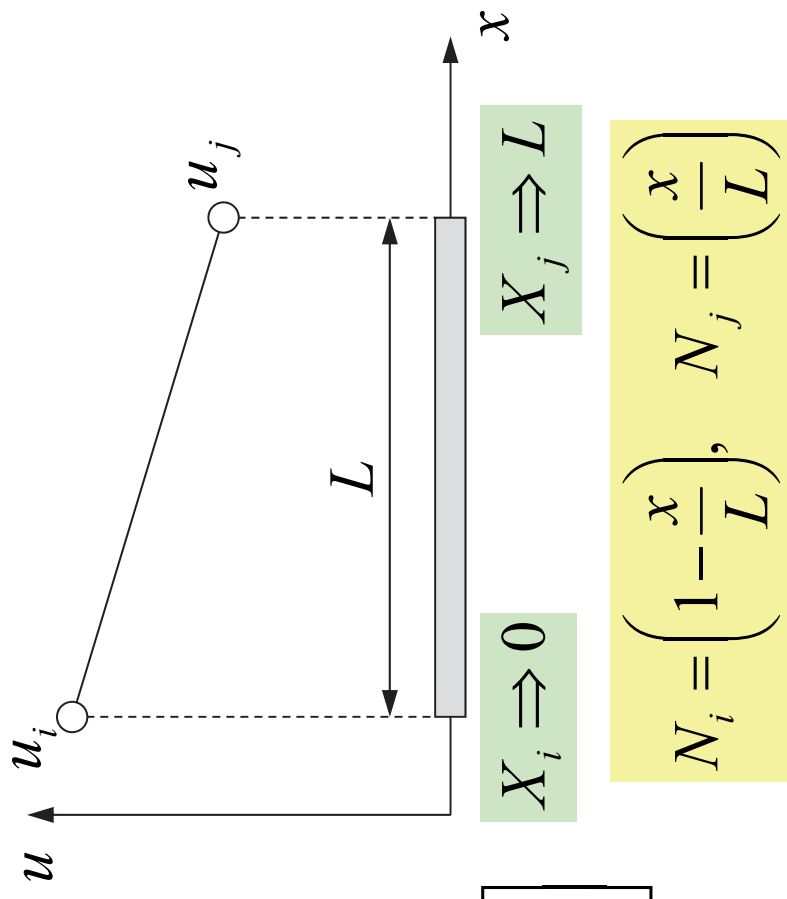
2x1 matrix

1x2 matrix

$$= \frac{EA}{L^2} \int_0^L \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} dx = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

$A$ : Sectional Area

$L$ : Length

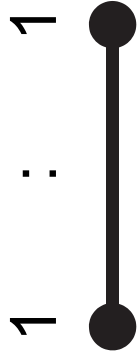


# Integration over Each Element: $\{f\}$ (1/2)

$$N_i = \left( \frac{X_j - x}{L} \right), \quad N_j = \left( \frac{x - X_i}{L} \right), \quad \frac{dN_i}{dx} = \left( \frac{-1}{L} \right), \quad \frac{dN_j}{dx} = \left( \frac{1}{L} \right)$$

$$N_i = \left( 1 - \frac{x}{L} \right), \quad N_j = \left( \frac{x}{L} \right)$$

$$\int_V X[N]^T dV = XA \int_0^L \begin{bmatrix} 1-x/L \\ x/L \end{bmatrix} dx = \frac{XAL}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \quad \text{Body Force}$$



$A$ : Sectional Area

$L$ : Length

# Integration over Each Element: $\{f\}$ (2/2)

$$N_i = \left( \frac{X_j - x}{L} \right), \quad N_j = \left( \frac{x - X_i}{L} \right), \quad \frac{dN_i}{dx} = \left( \frac{-1}{L} \right), \quad \frac{dN_j}{dx} = \left( \frac{1}{L} \right)$$

$$\int_V X[N]^T dV = XA \int_0^L \begin{bmatrix} 1 - x/L \\ x/L \end{bmatrix} dx = \frac{XAL}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \quad \text{Body Force}$$

$$\int_S \bar{\sigma}[N]^T dS = \bar{\sigma}A|_{x=L} = \bar{\sigma}A \begin{Bmatrix} 0 \\ 1 \end{Bmatrix} \quad \text{Surface Force}$$



when surface force acts on only this surface.

# Global Equations

- Accumulate Element Equations:

$$[k]^{(e)} \{\phi\}^{(e)} = \{f\}^{(e)} \quad \text{Element Matrix, Element Equations}$$



$$[K] \cdot \{\Phi\} = \{F\} \quad \text{Global Matrix, Global Equations}$$

$$[K] = \sum [k], \quad \{F\} = \sum \{f\}$$

$\{\Phi\}$ : *global vector of*  $\{\phi\}$

This is the final linear equations  
(global equations) to be solved.

# ECCS 2012 System

## Creating Directory

```
>$ cd Documents      create your directory under this (good for Windows)
>$ mkdir fem1        your favorite name
>$ cd fem1
```

This is your “top” directory, and is called **<\$fem1>** in this class.

## 1D Code for Static Linear-Elastic Problems

```
>$ cd <$fem1>
>$ cp /home03/skengon/Documents/class/fem1/1d.tar .
>$ tar xvf 1d.tar
>$ cd 1d
```

# Compile & GO !

```
>$ cd <$fem1>/1d
>$ cc -O 1d.c          (or g95 -O 1d.f)
>$ ./a.out
```

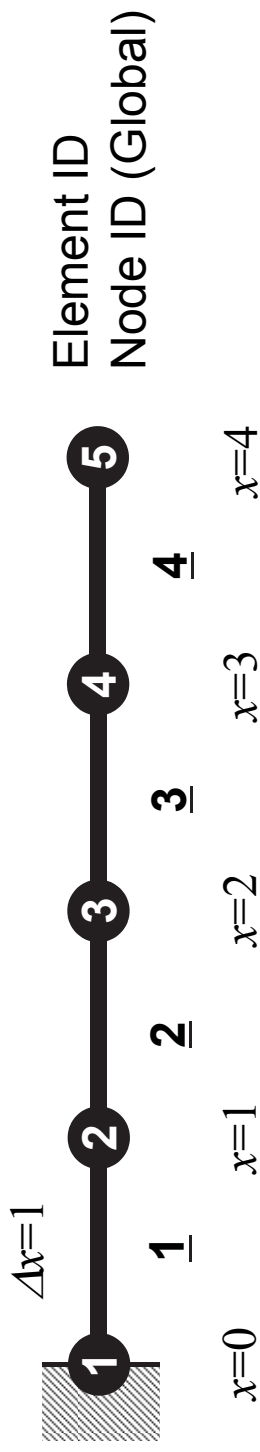
**Control Data**    input.dat

```
4
1.0  1.0  1.0  1.0  1.0
100
1.e-8
```

**NE** (Number of Elements)  
 **$\Delta x$**  (Length of Each Elem.: **L**), **F**, **A**, **E**  
 Number of MAX. Iterations for CG Solver  
 Convergence Criteria for CG Solver

$$\sigma = \frac{F}{A} = \frac{1}{1} = 1$$

$$\frac{du}{dx} = \varepsilon = \frac{\sigma}{E} = \frac{1}{1} = 1$$



# Results

```

>$ ./a.out
4 iters, RESID= 0.000000E+00 U(N)= 4.000000E+00

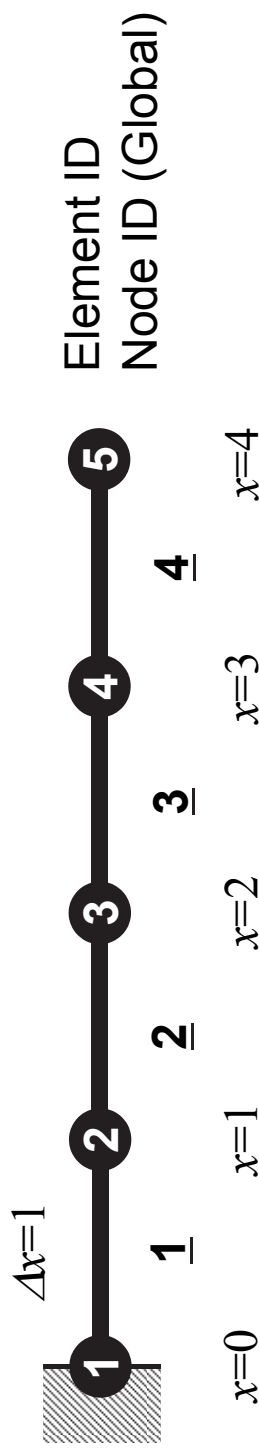
### DISPLACEMENT      at each node (computed)
1  0.000000E+00
2  1.000000E+00
3  2.000000E+00
4  3.000000E+00
5  4.000000E+00

### STRESS              at each element (computed, theoretical)
1  1.000000E+00  1.000000E+00
2  1.000000E+00  1.000000E+00
3  1.000000E+00  1.000000E+00
4  1.000000E+00  1.000000E+00

```

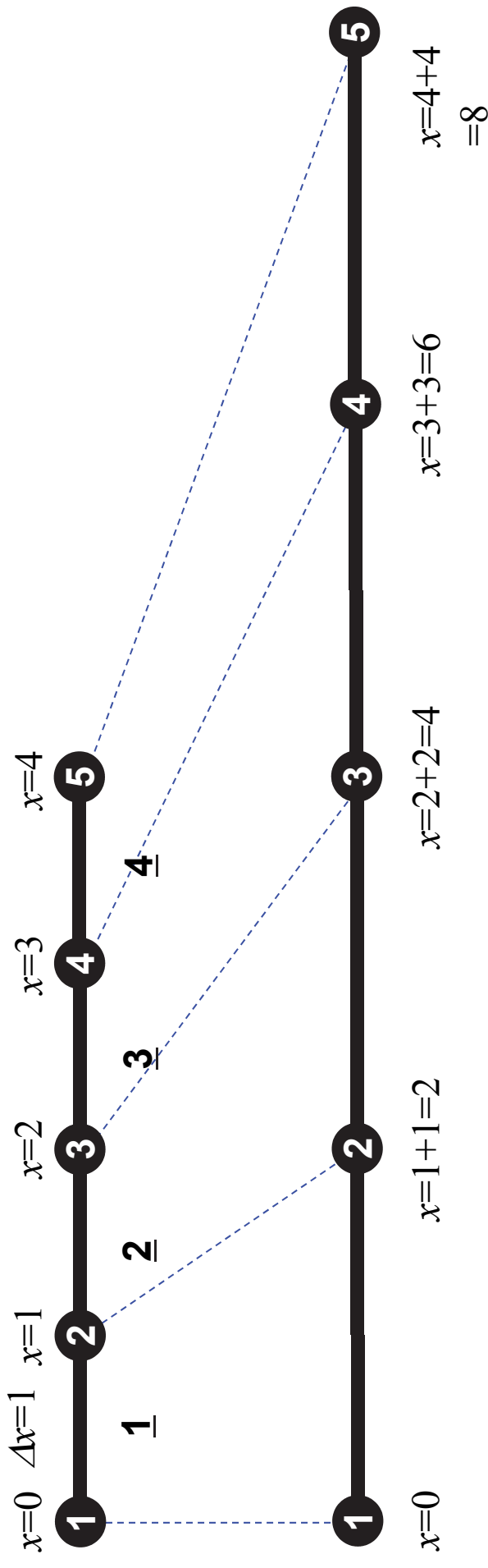
$$\sigma = \frac{F}{A} = \frac{1}{1} = 1$$

$$\frac{du}{dx} = \varepsilon = \frac{\sigma}{E} = \frac{1}{1} = 1$$



# Strain=1.00 (100%)

Length of each element is doubled compared to initial condition

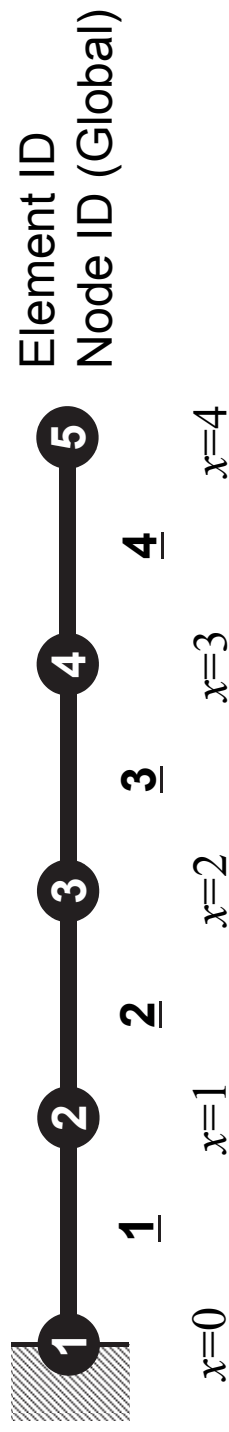


### DISPLACEMENT **at each node (computed)**

|   |              |
|---|--------------|
| 1 | 0.000000E+00 |
| 2 | 1.000000E+00 |
| 3 | 2.000000E+00 |
| 4 | 3.000000E+00 |
| 5 | 4.000000E+00 |

# Element Eqn's/Accumulation (1/3)

- 4 elements, 5 nodes



- $[k]$  and  $\{f\}$  of Element-1:

$$[k]^{(1)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} \quad \{f\}^{(1)} = \frac{XAL}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} + \int_S \bar{\sigma} [N]^T dS = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$$

$X=0$  in this case

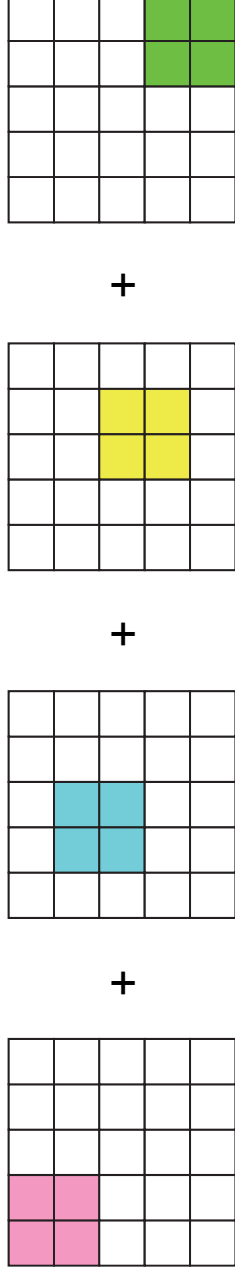
- As for Element-4:

$$[k]^{(4)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} \quad \{f\}^{(4)} = \int_S \bar{\sigma} [N]^T dS = \bar{\sigma} A \begin{Bmatrix} 0 \\ 1 \end{Bmatrix} = \begin{Bmatrix} 0 \\ F \end{Bmatrix}$$

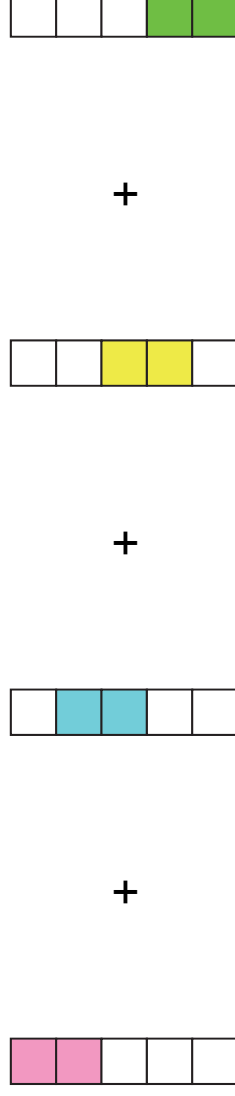
# Element Eqn's/Accumulation (2/3)

- Element-by-Element Accumulation:

$$[K] = \sum_{e=1}^4 [k]^{(e)} =$$



$$\{F\} = \sum_{e=1}^4 \{f\}^{(e)} =$$



# Element Eqn's/Accumulation (3/3)

- Relations to FDM

$$[k]^{(e)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

$$[K] = \sum_{e=1}^4 [k]^{(e)} = \left[ \begin{array}{c|c|c|c} \begin{matrix} +1 & -1 \\ -1 & +1 \end{matrix} & & & \\ \hline & \begin{matrix} +1 & -1 \\ -1 & +1 \end{matrix} & & \\ \hline & & \begin{matrix} +1 & -1 \\ -1 & +1 \end{matrix} & \\ \hline & & & \begin{matrix} +1 & -1 \\ -1 & +1 \end{matrix} \end{array} \right] \times \frac{EA}{L}$$

$$= \begin{bmatrix} +1 & -1 & & \\ -1 & +2 & -1 & \\ & -1 & +2 & -1 \\ & & -1 & +2 \end{bmatrix} \times \frac{EA}{L}$$

$$\begin{aligned} - \int_V \left( \frac{d^2 u}{dx^2} \right) dV &= - \int_V \left( \frac{u_{i+1} - 2u_i + u_{i-1}}{L^2} \right) dV \\ &= - \left( \frac{u_{i+1} - 2u_i + u_{i-1}}{L^2} \right) \cdot AL = -(u_{i+1} - 2u_i + u_{i-1}) \cdot \frac{A}{L} \end{aligned}$$

Something familiar ...

FEM: Coefficient Matrices are generally sparse  
(many ZERO's)

# Element-by-Element Operation

very flexible if each element has different material property, size, etc.

$$[k]^{(e)} = \frac{E^{(e)} A^{(e)}}{L^{(e)}} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

$$[K] = \sum_{e=1}^4 [k^{(e)}] =$$

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 $\times \frac{E^{(1)} A^{(1)}}{L^{(1)}} +$ 

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 $\times \frac{E^{(2)} A^{(2)}}{L^{(2)}} +$ 

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 $\times \frac{E^{(3)} A^{(3)}}{L^{(3)}} +$ 

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 $\times \frac{E^{(4)} A^{(4)}}{L^{(4)}}$

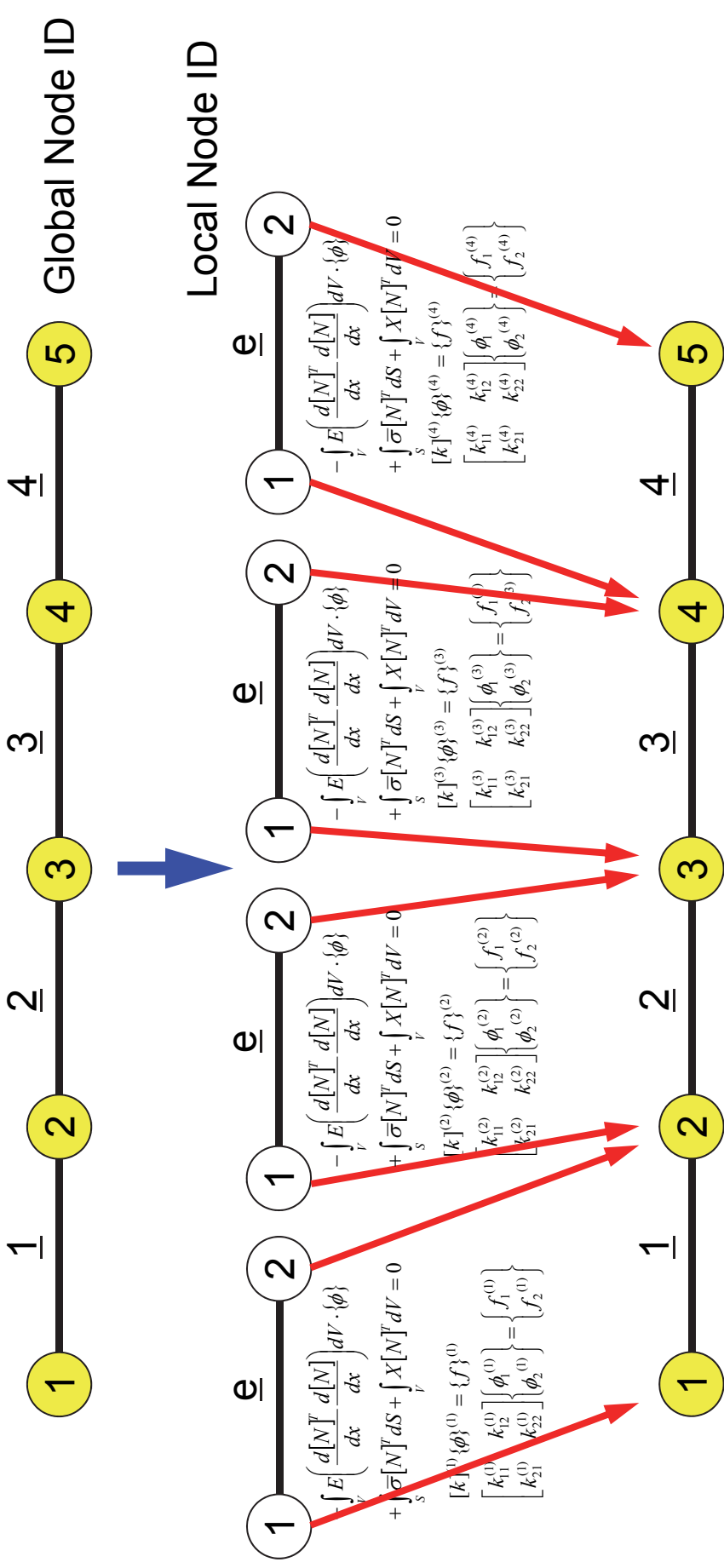
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$$\times \frac{E^{(2)} A^{(2)}}{L^{(2)}}$$

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$$\times \frac{E^{(4)} A^{(4)}}{L^{(4)}}$$

# Element/Global Operations



$$[K] \{\Phi\} = \{F\}$$

$$\begin{bmatrix} D_1 & AU_{11} & & & \\ AL_{21} & D_2 & AU_{21} & & \\ & AL_{31} & D_3 & AU_{31} & \\ & & AL_{41} & D_4 & AU_{41} \\ & & & AL_{51} & D_5 \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \end{bmatrix} = \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \end{bmatrix}$$

Mapping Information needed,  
from element-matrix  
to global-matrix.

- 1D-code for Static Linear-Elastic Problems by Galerkin FEM
- **Sparse Linear Solver**
  - **Conjugate Gradient Method**
  - **Preconditioning**
- Storage of Sparse Matrices
- Program
- Road to Parallel FEM

# Large-Scale Linear Equations in Scientific Applications

- Solving large-scale linear equations  $Ax=b$  is the most important and expensive part of various types of scientific computing.
  - for both linear and nonlinear applications
- Various types of methods proposed & developed.
  - for dense and sparse matrices
  - classified into direct and iterative methods
- Dense Matrices: 密行列: Globally Coupled Problems
  - BEM, Spectral Methods, MO/MD (gas, liquid)
- Sparse Matrices: 疎行列: Locally Defined Problems
  - **FEM**, FDM, DEM, MD (solid), BEM w/FMM

# Conjugate Gradient Method

## 共役勾配法

- Conjugate Gradient: CG
  - Most popular “non-stationary” iterative method
- for Symmetric Positive Definite (SPD) Matrices
  - 対称正定
  - $\{x\}^T[A]\{x\} > 0$  for arbitrary  $\{x\}$
  - All of diagonal components, eigenvalues and leading principal minors  $> 0$  (主小行列式・首座行列式)
  - Matrices of Galerkin-based FEM: heat conduction, Poisson, static linear elastic problems

### • Algorithm

- “Steepest Descent Method”
- $\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + \alpha_i \mathbf{p}^{(i)}$ 
  - $\mathbf{x}^{(i)}$ : solution,  $\mathbf{p}^{(i)}$ : search direction,  $\alpha_i$ : coefficient
- Solution  $\{x\}$  minimizes  $\{x-y\}^T[A]\{x-y\}$ , where  $\{y\}$  is exact solution.

$$\det \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & a_{24} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdots & a_{3n} \\ a_{41} & a_{42} & a_{43} & a_{44} & \cdots & a_{4n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & a_{n4} & \cdots & a_{nn} \end{bmatrix}$$

# Procedures of Conjugate Gradient

```

Compute  $r^{(0)} = b - [A] x^{(0)}$ 
for  $i = 1, 2, \dots$ 
     $z^{(i-1)} = r^{(i-1)}$ 
     $\rho_{i-1} = r^{(i-1)} z^{(i-1)}$ 
    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

```

- Mat-Vec. Multiplication
- Dot Products
- DAXPY

$x^{(i)}$  : Vector  
 $\alpha_i$  : Scalar

# Preconditioning for Iterative Solvers

- Convergence rate of iterative solvers strongly depends on the spectral properties (eigenvalue distribution) of the coefficient matrix  $\mathbf{A}$ .
  - Eigenvalue distribution is small, eigenvalues are close to 1
  - In “ill-conditioned” problems, “condition number” (ratio of max/min eigenvalue if  $\mathbf{A}$  is symmetric) is large (条件数).
- A preconditioner  $\mathbf{M}$  (whose properties are similar to those of  $\mathbf{A}$ ) transforms the linear system into one with more favorable spectral properties (前处理)
  - $\mathbf{M}$  transforms  $\mathbf{Ax}=\mathbf{b}$  into  $\mathbf{A}'\mathbf{x}=\mathbf{b}'$  where  $\mathbf{A}'=\mathbf{M}^{-1}\mathbf{A}$ ,  $\mathbf{b}'=\mathbf{M}^{-1}\mathbf{b}$
  - If  $\mathbf{M}\sim\mathbf{A}$ ,  $\mathbf{M}^{-1}\mathbf{A}$  is close to identity matrix.
  - If  $\mathbf{M}^{-1}=\mathbf{A}^{-1}$ , this is the best preconditioner (Gaussian Elim.)
  - Generally,  $\mathbf{A}'\mathbf{x}=\mathbf{b}'$  where  $\mathbf{A}'=\mathbf{M}_L^{-1}\mathbf{A}\mathbf{M}_R^{-1}$ ,  $\mathbf{b}'=\mathbf{M}_L^{-1}\mathbf{b}$ ,  $\mathbf{x}'=\mathbf{M}_R\mathbf{x}$
  - $\mathbf{M}_L/\mathbf{M}_R$ : Left/Right Preconditioning (左/右前处理)

# Preconditioned CG Solver

```

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

```

# ILU(0), IC(0)

- Widely used Preconditioners for Sparse Matrices
  - Incomplete LU Factorization
  - Incomplete Cholesky Factorization (for Symmetric Matrices)
- Incomplete Direct Method
  - Even if original matrix is sparse, inverse matrix is not necessarily sparse.
  - fill-in
  - ILU(0)/IC(0) without fill-in have same non-zero pattern with the original (sparse) matrices

# Diagonal Scaling, Point-Jacobi

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

- **solve**  $[M] \mathbf{z}^{(i-1)} = \mathbf{r}^{(i-1)}$  is very easy.
- Provides fast convergence for simple problems.
- 1d.f, 1d.c

- 1D-code for Static Linear-Elastic Problems by Galerkin FEM
- Sparse Linear Solver
  - Conjugate Gradient Method
  - Preconditioning
- **Storage of Sparse Matrices**
- Program
- Road to Parallel FEM

# Coef. Matrix derived from FEM

- Sparse Matrix
  - Many “0”s
- Storing all components (e.g.  $A(i,j)$ ) is not efficient for sparse matrices
  - $A(i,j)$  is suitable for dense matrices

$$\begin{bmatrix}
 D & X & & & & & & & & & & & & & & \\
 X & D & X & & & & & & & & & & & & & \\
 & X & D & X & & & & & & & & & & & & \\
 & & X & D & X & & & & & & & & & & & \\
 & & & X & D & & & & & & & & & & & \\
 & & & & D & X & & & & & & & & & & \\
 & & & & X & D & X & & & & & & & & & \\
 & & & & X & X & & & & & & & & & & \\
 & & & & X & X & X & & & & & & & & & \\
 & & & & X & X & X & D & X & & & & & & & \\
 & & & & X & X & X & X & D & X & & & & & & \\
 & & & & X & X & X & X & X & D & X & & & & & \\
 & & & & X & X & X & X & X & X & D & X & & & & \\
 & & & & X & X & X & X & X & X & X & D & X & & & \\
 & & & & X & X & X & X & X & X & X & X & D & X & & \\
 & & & & X & X & X & X & X & X & X & X & X & D & X & \\
 & & & & X & X & X & X & X & X & X & X & X & X & D & \\
 & & & & X & X & X & X & X & X & X & X & X & X & X & D
 \end{bmatrix}
 =
 \begin{bmatrix}
 \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \\ \Phi_6 \\ \Phi_7 \\ \Phi_8 \\ \Phi_9 \\ \Phi_{10} \\ \Phi_{11} \\ \Phi_{12} \\ \Phi_{13} \\ \Phi_{14} \\ \Phi_{15} \\ \Phi_{16}
 \end{bmatrix}
 =
 \begin{bmatrix}
 F_1 \\ F_2 \\ F_3 \\ F_4 \\ F_5 \\ F_6 \\ F_7 \\ F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \\ F_{16}
 \end{bmatrix}$$

- Number of non-zero off-diagonal components is  $O(100)$  in FEM
  - If number of unknowns is  $10^8$ :
    - $A(i,j)$ :  $O(10^{16})$  words
    - Actual Non-zero Components:  $O(10^{10})$  words
- Only (really) non-zero off-diag. components should be stored on memory

# Variables/Arrays in 1d.f, 1d.c related to coefficient matrix

| name             | type | size         | description                                                            |
|------------------|------|--------------|------------------------------------------------------------------------|
| <b>N</b>         | I    | -            | # Unknowns                                                             |
| <b>NPLU</b>      | I    | -            | # Non-Zero Off-Diagonal Components                                     |
| <b>Diag (:)</b>  | R    | N            | Diagonal Components                                                    |
| <b>U (:)</b>     | R    | N            | Unknown Vector                                                         |
| <b>Rhs (:)</b>   | R    | N            | RHS Vector                                                             |
| <b>Index (:)</b> | I    | 0 : N<br>N+1 | Off-Diagonal Components (Number of Non-Zero Off-Diagonals at Each ROW) |
| <b>Item (:)</b>  | I    | NPLU         | Off-Diagonal Components (Corresponding Column ID)                      |
| <b>AMat (:)</b>  | R    | NPLU         | Off-Diagonal Components (Value)                                        |

Only non-zero components are stored according to “Compressed Row Storage” .

# Mat-Vec. Multiplication for Sparse Matrix

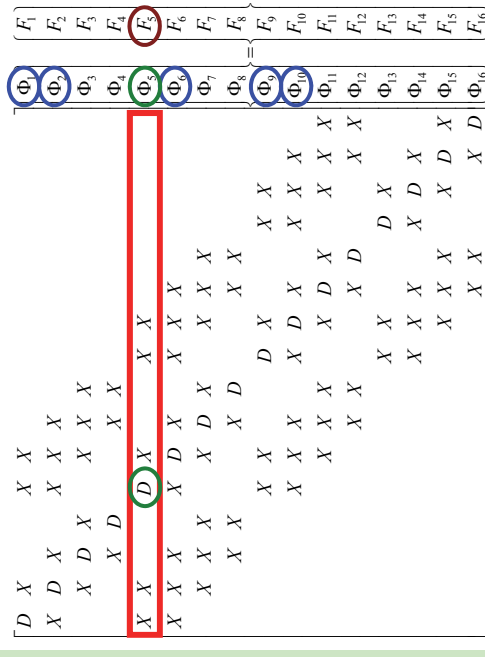
## Compressed Row Storage (CRS)

**Diag (i)** Diagonal Components (REAL,  $i=1 \sim N$ )  
**Index (i)** Number of Non-Zero Off-Diagonals at Each ROW (INT,  $i=0 \sim N$ )  
**Item (k)** Off-Diagonal Components (Corresponding Column ID)  
 (INT,  $k=1, \text{index}(N)$ )  
**Amat (k)** Off-Diagonal Components (Value)  
 ( REAL,  $k=1, \text{index}(N)$  )

```

{Y} = [A] {X}

do i= 1, N
  Y(i)= Diag(i)*X(i)
  do k= Index(i-1)+1, Index(i)
    Y(i)= Y(i) + Amat(k)*X(Item(k))
  enddo
enddo
  
```



# Mat-Vec. Multiplication for Dense Matrix

## Very Easy, Straightforward

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1,N-1} & a_{1,N} \\ a_{21} & a_{22} & & a_{2,N-1} & a_{2,N} \\ \dots & & \dots & & \\ a_{N-1,1} & a_{N-1,2} & & a_{N-1,N-1} & a_{N-1,N} \\ a_{N,1} & a_{N,2} & \dots & a_{N,N-1} & a_{N,N} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N-1} \\ x_N \end{Bmatrix} = \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N-1} \\ y_N \end{Bmatrix}$$

```
{Y} = [A] {X}
```

```
do j= 1, N
  Y(j)= 0. d0
  do i= 1, N
    Y(j)= Y(j) + A(i, j)*X(i)
  enddo
enddo
```

# Compressed Row Storage (CRS): C

|   |           |             |             |              |
|---|-----------|-------------|-------------|--------------|
| 0 | 1.1<br>⊙  | 2.4<br>①,0  | 3.2<br>④,1  |              |
| 1 | 3.6<br>①  | 4.3<br>⊙,2  | 2.5<br>③,3  | 3.7<br>⑤,4   |
| 2 | 5.7<br>②  | 1.5<br>④,6  | 3.1<br>⑥,7  | 9.1<br>⑦,5   |
| 3 | 9.8<br>③  | 4.1<br>①,8  | 2.5<br>④,9  | 2.7<br>⑤,10  |
| 4 | 11.5<br>④ | 3.1<br>⊙,11 | 9.5<br>①,12 | 10.4<br>②,13 |
| 5 | 12.4<br>⑤ | 6.5<br>②,15 | 9.5<br>⑥,16 |              |
| 6 | 23.1<br>⑥ | 6.4<br>①,17 | 2.5<br>②,18 | 1.4<br>⑤,19  |
| 7 | 51.3<br>⑦ | 9.5<br>①,21 | 1.3<br>②,22 | 13.1<br>⑦,20 |
|   |           |             | 9.6<br>③,23 | 3.1<br>⑤,24  |

**Diag (i)** Diagonal Components (REAL,  $i=1\sim N$ )

**Index (i)** Number of Non-Zero Off-Diagonals at Each ROW (INT,  $i=0\sim N$ )

**Item (k)** Off-Diagonal Components (Corresponding Column ID) (INT,  $k=1, \text{index}(N)$ )

**AMat (k)** Off-Diagonal Components (Value) (REAL,  $k=1, \text{index}(N)$ )

```
{Y}=[A] {X}

for (i=0; i<N; i++) {
    Y[i] = Diag[i] * X[i];
    for (k=Index[i]; k<Index[i+1]; k++) {
        Y[i] += AMat[k]*X[Index[k]];
    }
}
```

- 1D-code for Static Linear-Elastic Problems by Galerkin FEM
- Sparse Linear Solver
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# 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
- Calculation of Stress

# Program: 1d.c (1/7)

## variables and arrays

```

/*
//
// 1D Solid Mechanics for Truss Elements solved by
// CG (Conjugate Gradient) Method
//
// d/dx (EdU/dx) + F = 0
// U=0@x=0
//
*/

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

int main() {
    int NE, N, NPLU, IterMax, errno;
    int R, Z, Q, P, DD;

    double dX, Resid, Eps, Area, F, Young;
    double X1, X2, U1, U2, DL, Strain, Sigma, Ck;
    double *U, *Rhs, *X;
    double *Diag, *AMat;
    double **W;

    int *Index, *Item, *Icelnod;
    double Kmat[2][2], Emat[2][2];

    int i, j, in1, in2, k, icel, k1, k2, jS;
    int iter;
    FILE *fp;
    double BNorm2, Rho, Rho1=0.0, C1, Alpha, DNorm2;
    int ierr = 1;

```

# Variable/Arrays (1/2)

| Name                  | Type | Size | I/O | Definition                           |
|-----------------------|------|------|-----|--------------------------------------|
| <b>NE</b>             | I    |      | I   | # Element                            |
| <b>N</b>              | I    |      | O   | # Node                               |
| <b>NPLU</b>           | I    |      | O   | # Non-Zero Off-Diag. Components      |
| <b>IterMax</b>        | I    |      | I   | MAX Iteration Number for CG          |
| <b>errno</b>          | I    |      | O   | ERROR flag                           |
| <b>R, Z, Q, P, DD</b> | I    |      | O   | Name of Vectors in CG                |
| <b>dx</b>             | R    |      | I   | Length of Each Element               |
| <b>Resid</b>          | R    |      | O   | Residual for CG                      |
| <b>Eps</b>            | R    |      | I   | Convergence Criteria for CG          |
| <b>Area</b>           | R    |      | I   | Sectional Area of Element            |
| <b>F</b>              | R    |      | I   | Axial Force F at X=Xmax              |
| <b>Young</b>          | R    |      | I   | Young's Modulus                      |
| <b>x1, x2, u1, u2</b> | R    |      | O   | Location/Displacement at Local Nodes |

# Variable/Arrays (2/2)

| Name                  | Type | Size        | I/O | Definition                                        |
|-----------------------|------|-------------|-----|---------------------------------------------------|
| <b>DL, Ck</b>         | R    |             | ○   | Coef's for Element Matrix                         |
| <b>Strain, Stress</b> | R    |             | ○   | Element Strain, Element Stress                    |
| <b>X</b>              | R    | N           | ○   | Location of Each Node                             |
| <b>U</b>              | R    | N           | ○   | Displacement of Each Node                         |
| <b>Rhs</b>            | R    | N           | ○   | RHS Vector                                        |
| <b>Diag</b>           | R    | N           | ○   | Diagonal Components                               |
| <b>W</b>              | R    | [ 4 ] [N]   | ○   | Work Array for CG                                 |
| <b>Amat</b>           | R    | NPLU        | ○   | Off-Diagonal Components (Value)                   |
| <b>Index</b>          | I    | N+1         | ○   | Number of Non-Zero Off-Diagonals at Each ROW      |
| <b>I tem</b>          | I    | NPLU        | ○   | Off-Diagonal Components (Corresponding Column ID) |
| <b>Icelnod</b>        | I    | 2*NE        | ○   | Node ID for Each Element                          |
| <b>Kmat</b>           | R    | [ 2 ] [ 2 ] | ○   | Element Matrix [k]                                |
| <b>Emat</b>           | R    | [ 2 ] [ 2 ] | ○   | Element Matrix                                    |

# Program: 1d.c (2/7)

## Initialization, Allocation of Arrays

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

```
fp = fopen("input.dat", "r");
assert(fp != NULL);
fscanf(fp, "%d", &NE);
fscanf(fp, "%lf %lf %lf", &dX, &F, &Area, &Young);
fscanf(fp, "%d", &IterMax);
fscanf(fp, "%lf", &Eps);
fclose(fp);
```

```
N= NE + 1;
```

```
U = calloc(N, sizeof(double));
X = calloc(N, sizeof(double));
Diag = calloc(N, sizeof(double));
```

```
AMat = calloc(2*N-2, sizeof(double));
```

```
Rhs = calloc(N, sizeof(double));
Index= calloc(N+1, sizeof(int));
Item = calloc(2*N-2, sizeof(int));
```

```
Icelnod= calloc(2*NE, sizeof(int));
```

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



**NE: # Element**  
**N : # Node (NE+1)**

# Program: 1d.c (2/7)

## Initialization, Allocation of Arrays

```

/*
//  +-----+
//  | INIT. |
//  +-----+
//
*/

fp = fopen("input.dat", "r");
assert(fp != NULL);
fscanf(fp, "%d", &NE);
fscanf(fp, "%lf %lf %lf", &dX, &F, &Area, &Young);
fscanf(fp, "%d", &IterMax);
fscanf(fp, "%lf", &Eps);
fclose(fp);

N= NE + 1;

U   = calloc(N, sizeof(double));
X   = calloc(N, sizeof(double));
Diag = calloc(N, sizeof(double));

AMat = calloc(2*N-2, sizeof(double));

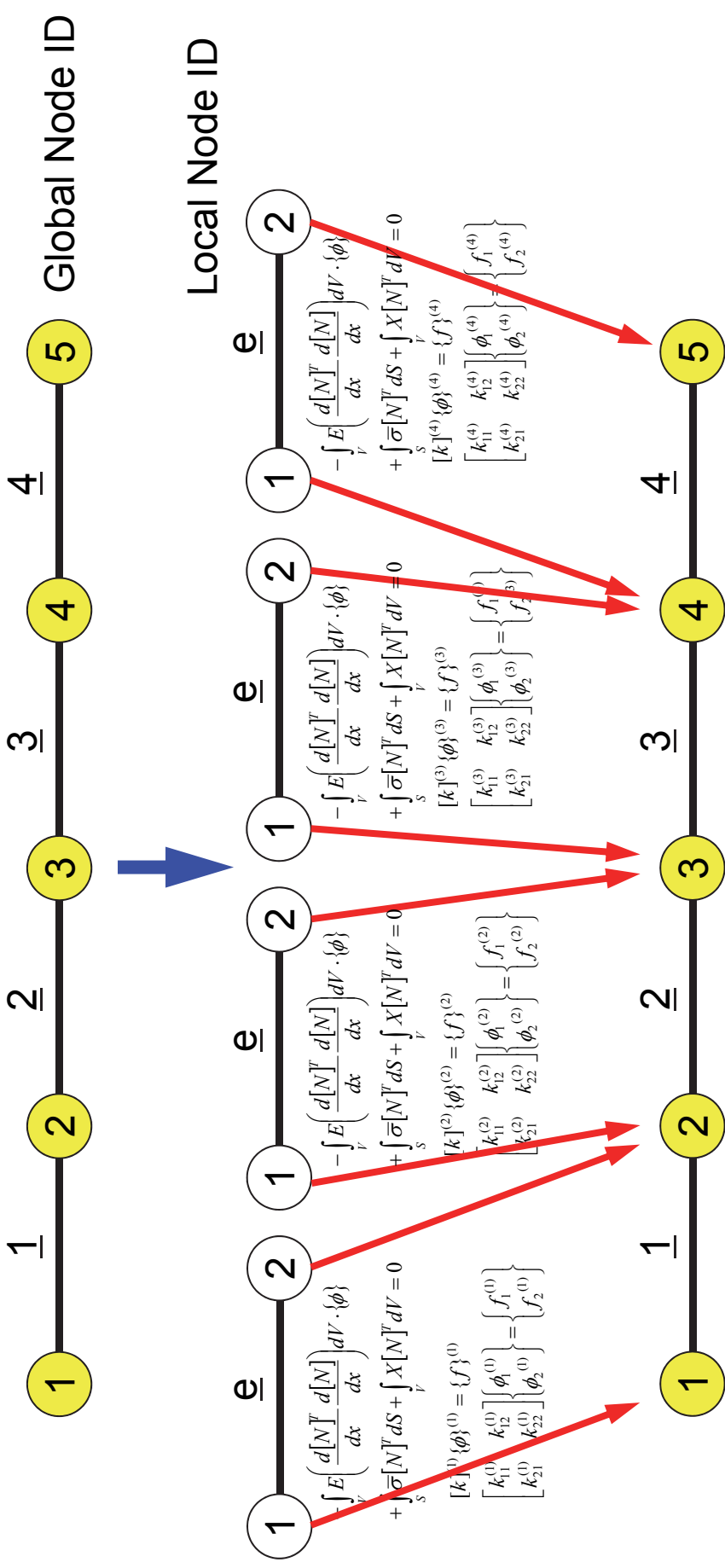
Rhs = calloc(N, sizeof(double));
Index= calloc(N+1, sizeof(int));
Item = calloc(2*N-2, sizeof(int));

Icelnod= calloc(2*NE, sizeof(int));

```

**Amat:** Non-Zero Off-Diag. Comp.  
**Item:** Corresponding Column ID

# Element/Global Operations



$$[K] \{\Phi\} = \{F\}$$

$$\begin{bmatrix} D_1 & AU_{11} & & & \\ AL_{21} & D_2 & AU_{21} & & \\ & AL_{31} & D_3 & AU_{31} & \\ & & AL_{41} & D_4 & AU_{41} \\ & & & AL_{51} & D_5 \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \end{Bmatrix} = \begin{Bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5 \end{Bmatrix}$$

Number of non-zero off-diag. components is 2 for each node. This number is 1 at boundary nodes).

# Program: 1d.c (2/7)

## Initialization, Allocation of Arrays

```

/*
//  +-----+
//  | INIT. |
//  +-----+
//
*/

fp = fopen("input.dat", "r");
assert(fp != NULL);
fscanf(fp, "%d", &NE);
fscanf(fp, "%lf %lf %lf", &dX, &F, &Area, &Young);
fscanf(fp, "%d", &IterMax);
fscanf(fp, "%lf", &Eps);
fclose(fp);

N= NE + 1;

U   = calloc(N, sizeof(double));
X   = calloc(N, sizeof(double));
Diag = calloc(N, sizeof(double));

AMat = calloc(2*N-2, sizeof(double));

Rhs = calloc(N, sizeof(double));
Index= calloc(N+1, sizeof(int));
Item = calloc(2*N-2, sizeof(int));

Icelnod= calloc(2*NE, sizeof(int));

```

**Amat:** Non-Zero Off-Diag. Comp.  
**Item:** Corresponding Column ID

Number of non-zero off-diag.  
 components is 2 for each node. This  
 number is 1 at boundary nodes).

**Total Number of Non-Zero Off-Diag.  
 Components:**  
 $2 * (N-2) + 1 + 1 = 2 * N - 2$

# Program: 1d.c (3/7)

## Initialization, Allocation of Arrays (cont.)

```

W = (double **)malloc(sizeof(double *)*4);
if(W == NULL) {
    fprintf(stderr, "Error: %s\n", strerror(errno));
    return -1;
}
for(i=0; i<4; i++) {
    W[i] = (double *)malloc(sizeof(double)*N);
    if(W[i] == NULL) {
        fprintf(stderr, "Error: %s\n", strerror(errno));
        return -1;
    }
}

for(i=0; i<N; i++)
    U[i] = 0.0;
for(i=0; i<N; i++)
    Diag[i] = 0.0;
for(i=0; i<N; i++)
    RhS[i] = 0.0;
for(k=0; k<2*N-2; k++)
    AMat[k] = 0.0;
for(i=0; i<N; i++)
    X[i] = i*dX;
for(ice1=0; ice1<NE; ice1++) {
    ice1nod[2*ice1] = ice1;
    ice1nod[2*ice1+1] = ice1+1;
}

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

```

# Program: 1d.c (3/7)

## Initialization, Allocation of Arrays (cont.)

```

W = (double **)malloc(sizeof(double *)*4);
if(W == NULL) {
    fprintf(stderr, "Error: %s\n", strerror(errno));
    return -1;
}
for(i=0; i<4; i++) {
    W[i] = (double *)malloc(sizeof(double)*N);
    if(W[i] == NULL) {
        fprintf(stderr, "Error: %s\n", strerror(errno));
        return -1;
    }
}

for(i=0; i<N; i++)
    U[i] = 0.0;
for(i=0; i<N; i++)
    Diag[i] = 0.0;
for(i=0; i<N; i++)
    Rhs[i] = 0.0;
for(k=0; k<2*N-2; k++)
    AMat[k] = 0.0;
for(i=0; i<N; i++)
    X[i] = i*dX;
for(ice1=0; ice1<NE; ice1++) {
    ice1nod[2*ice1] = ice1;
    ice1nod[2*ice1+1] = ice1+1;
}

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

```

**x:** X-coordinate  
component of each node

# Program: 1d.c (3/7)

## Initialization, Allocation of Arrays (cont.)

```

W = (double **)malloc(sizeof(double *)*4);
if(W == NULL) {
    fprintf(stderr, "Error: %s\n", strerror(errno));
    return -1;
}
for(i=0; i<4; i++) {
    W[i] = (double *)malloc(sizeof(double)*N);
    if(W[i] == NULL) {
        fprintf(stderr, "Error: %s\n", strerror(errno));
        return -1;
    }
}

for(i=0; i<N; i++) U[i] = 0.0;
for(i=0; i<N; i++) Diag[i] = 0.0;
for(i=0; i<N; i++) Rhs[i] = 0.0;
for(k=0; k<2*N-2; k++) AMat[k] = 0.0;
for(i=0; i<N; i++) X[i] = i*dX;
for(ice1=0; ice1<NE; ice1++) {
    ice1nod[2*ice1] = ice1;
    ice1nod[2*ice1+1] = ice1+1;
}

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

```



# Program: 1d.c (3/7)

## Initialization, Allocation of Arrays (cont.)

```

W = (double **)malloc(sizeof(double *)*4);
if(W == NULL) {
    fprintf(stderr, "Error: %s\n", strerror(errno));
    return -1;
}
for(i=0; i<4; i++) {
    W[i] = (double *)malloc(sizeof(double)*N);
    if(W[i] == NULL) {
        fprintf(stderr, "Error: %s\n", strerror(errno));
        return -1;
    }
}

for(i=0; i<N; i++) U[i] = 0.0;
for(i=0; i<N; i++) Diag[i] = 0.0;
for(i=0; i<N; i++) Rhs[i] = 0.0;
for(k=0; k<2*N-2; k++) AMat[k] = 0.0;
for(i=0; i<N; i++) X[i] = i*dX;
for(ice1=0; ice1<NE; ice1++) {
    ice1nod[2*ice1] = ice1;
    ice1nod[2*ice1+1] = ice1+1;
}

```

```

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

```

$$[k]^{(e)} = \int_V E \left( \frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

[Kmat]

# Program: 1d.c (4/7)

## Global Matrix: Column ID for Non-Zero Off-Diag's

```
/*
//  +-----+
//  | CONNECTIVITY |
//  +-----+
*/
```

```
for (i=0; i<N+1; i++)  Index[i] = 2;
Index[0]= 0;
Index[1]= 1;
Index[N]= 1;
```

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

```
NPLU= Index[N];
```

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

Number of non-zero off-diag. components is 2 for each node. This number is 1 at boundary nodes).

Total Number of Non-Zero Off-Diag. Components:

$$2*(N-2)+1+1 = 2*N-2 = \text{NPLU} = \text{Index}[N]$$

|  | 0         | 1        | 2        | 3         | 4         | 5 | 6 | 7 | # Non-Zero Off-Diag. | Index[0]= |
|--|-----------|----------|----------|-----------|-----------|---|---|---|----------------------|-----------|
|  | 1.1<br>⊙  | 2.4<br>① | 3.2<br>④ |           |           |   |   |   | 2                    | 0         |
|  | 3.6<br>①  | 4.3<br>⊙ | 2.5<br>③ | 3.7<br>⑤  | 9.1<br>⑦  |   |   |   | 4                    | 2         |
|  | 5.7<br>②  | 1.5<br>④ | 3.1<br>⑥ |           |           |   |   |   | 2                    | 6         |
|  | 9.8<br>③  | 4.1<br>① | 2.5<br>④ | 2.7<br>⑤  |           |   |   |   | 3                    | 8         |
|  | 11.5<br>④ | 3.1<br>⊙ | 9.5<br>① | 10.4<br>② | 4.3<br>⑥  |   |   |   | 4                    | 11        |
|  | 12.4<br>⑤ | 6.5<br>② | 9.5<br>⑥ |           |           |   |   |   | 2                    | 15        |
|  | 23.1<br>⑥ | 6.4<br>① | 2.5<br>② | 1.4<br>⑤  | 13.1<br>⑦ |   |   |   | 4                    | 17        |
|  | 51.3<br>⑦ | 9.5<br>① | 1.3<br>② | 9.6<br>③  | 3.1<br>⑤  |   |   |   | 4                    | 21        |
|  |           |          |          |           |           |   |   |   |                      | 25        |

(Index[i])<sup>th</sup> ~ (Index[i+1])<sup>th</sup> :  
Non-Zero Off-Diag. Components corresponding to *i*-th row.

# Program: 1d.c (4/7)

## Global Matrix: Column ID for Non-Zero Off-Diag's

```

/*
//  +-----+
//  | CONNECTIVITY |
//  +-----+
//
*/

for (i=0; i<N+1; i++)   Index[i] = 2;
Index[0]= 0;
Index[1]= 1;
Index[N]= 1;

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

NPLU= Index[N];

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

```

|  | 0        | 1        | 2        | 3        | 4         | 5         | 6         | 7         | # Non-Zero<br>Off-Diag. | Index[0] = 0 | Index[1] = 2 | Index[2] = 6 | Index[3] = 8 | Index[4] = 11 | Index[5] = 15 | Index[6] = 17 | Index[7] = 21 | Index[8] = 25 |
|--|----------|----------|----------|----------|-----------|-----------|-----------|-----------|-------------------------|--------------|--------------|--------------|--------------|---------------|---------------|---------------|---------------|---------------|
|  | 1.1<br>⊙ | 3.6<br>① | 5.7<br>② | 9.8<br>③ | 11.5<br>④ | 12.4<br>⑤ | 23.1<br>⑥ | 51.3<br>⑦ |                         |              |              |              |              |               |               |               |               |               |
|  | 2.4<br>① | 4.3<br>⊙ | 1.5<br>④ | 4.1<br>① | 3.1<br>⊙  | 6.5<br>②  | 6.4<br>①  | 9.5<br>①  |                         |              |              |              |              |               |               |               |               |               |
|  | 3.2<br>④ | 2.5<br>③ | 3.1<br>⑥ | 2.5<br>④ | 9.5<br>①  | 9.5<br>⑥  | 2.5<br>②  | 1.3<br>②  |                         |              |              |              |              |               |               |               |               |               |
|  |          | 9.1<br>⑦ |          | 2.7<br>⑤ | 10.4<br>② |           | 1.4<br>⑤  | 9.6<br>③  |                         |              |              |              |              |               |               |               |               |               |
|  |          |          |          |          | 4.3<br>⑥  |           | 13.1<br>⑦ | 3.1<br>⑤  |                         |              |              |              |              |               |               |               |               |               |

(Index[i])<sup>th</sup> ~ (Index[i+1])<sup>th</sup>:

Non-Zero Off-Diag. Components corresponding to i-th row.



# Program: 1d.c (5/7)

## Element Matrix ~ Global Matrix

```

/*
//
//  |-----+
//  | MATRIX assemble |
//  |-----+
//
*/

for (icel=0; icel<NE; icel++) {
    in1= Icelnod[2*icel];
    in2= Icelnod[2*icel+1];
    X1 = X[in1];
    X2 = X[in2];
    DL = fabs(X2-X1);

    Ck= Area*Young/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 (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];
}

```



# Program: 1d.c (5/7)

## Element Matrix ~ Global Matrix

```

/*
//
//
//
//
*/
+-----+
| MATRIX assemble |
+-----+

for (icel=0; icel<NE; icel++) {
    in1= Icelnod[2*icel];
    in2= Icelnod[2*icel+1];
    X1 = X[in1];
    X2 = X[in2];
    DL = fabs(X2-X1);

```

```

Ck= Area*Young/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 (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];
}

```



$$[Emat] = [k]^{(e)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} = \frac{EA}{L} [Kmat]$$

# Program: 1d.c (5/7)

## Element Matrix ~ Global Matrix

```

/*
//
//
//
//
*/
+-----+
| MATRIX assemble |
+-----+

for (icel=0; icel<NE; icel++) {
    in1= Icelnod[2*icel];
    in2= Icelnod[2*icel+1];
    X1 = X[in1];
    X2 = X[in2];
    DL = fabs(X2-X1) ;

    Ck= Area*Young/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 (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];
}

```



$$[Emat] = [k]^{(e)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

# Program: 1d.c (5/7)

## Element Matrix ~ Global Matrix

```

/*
//
//
//
//
*/
+-----+
| MATRIX assemble |
+-----+

for (icel=0; icel<NE; icel++) {
    in1= Icelnod[2*icel];
    in2= Icelnod[2*icel+1];
    X1 = X[in1];
    X2 = X[in2];
    DL = fabs(X2-X1);

    Ck= Area*Young/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 (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];
}

```



Non-zero Off-Diag. at  $i$ -th row:

Index[i] , Index[i]+1



$$[Emat] = [k]^{(e)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

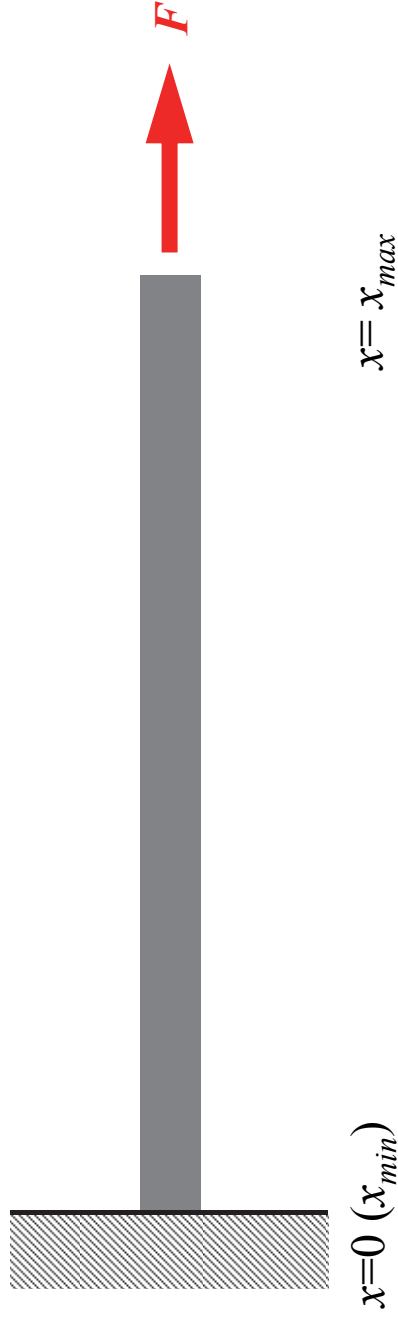
k2

# Program: 1d.c (6/7)

## Boundary Conditions

```
/*  
// +-----+  
// | BOUNDARY conditions |  
// +-----+  
*/  
  
/* X=Xmin */  
    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;  
        }}  
  
/* X=Xmax */  
    i=N-1;  
    Rhs[i]= F;
```

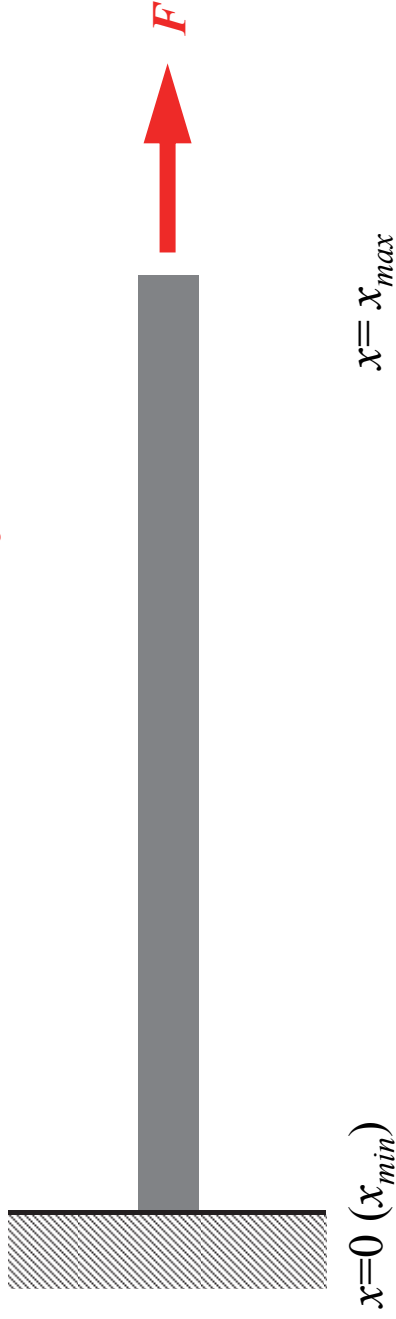
# 1D Static Linear Elastic Problem



- Only deforms in  $x$ -direction (displacement:  $u$ )
  - Uniform: Sectional Area  $A$ , Young's Modulus  $E$
  - Boundary Conditions (B.C.)
    - $x=0 : u=0$  (fixed)
    - $x=x_{max} : F$  (axial force)
- Truss: NO bending deformation by G-force

# (Linear) Equation at $x=0$

$$u_l = 0 \text{ (or } u_0 = 0)$$



- Only deforms in  $x$ -direction (displacement:  $u$ )
  - Uniform: Sectional Area  $A$ , Young's Modulus  $E$
  - Boundary Conditions (B.C.)
    - $x=0$  :  $u=0$  (fixed)
    - $x=x_{max}$  :  $F$  (axial force)
- Truss: NO bending deformation by G-force

# Program: 1d.c (6/7)

## Boundary Conditions

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

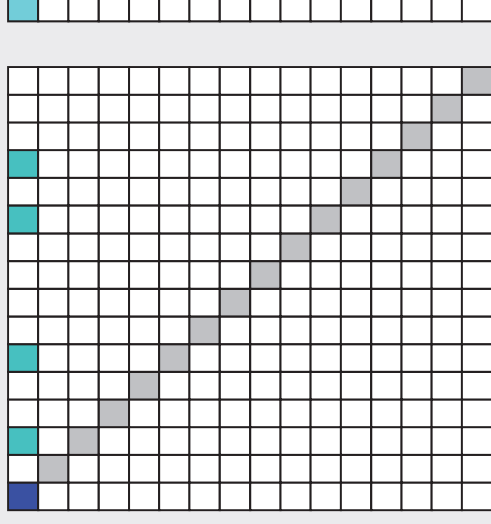
```
/* X=Xmin */
i=0;
jS= Index[i];
AMat[jS]= 0.0;
Diag[i ]= 1.0;
Rhs [i ]= 0.0;
```

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

```
/* X=Xmax */
i=N-1;
Rhs[i]= F;
```

$u_1=0$

Diagonal Component=1  
RHS=0  
Off-Diagonal Components= 0.



# Program: 1d.c (6/7)

## Boundary Conditions

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

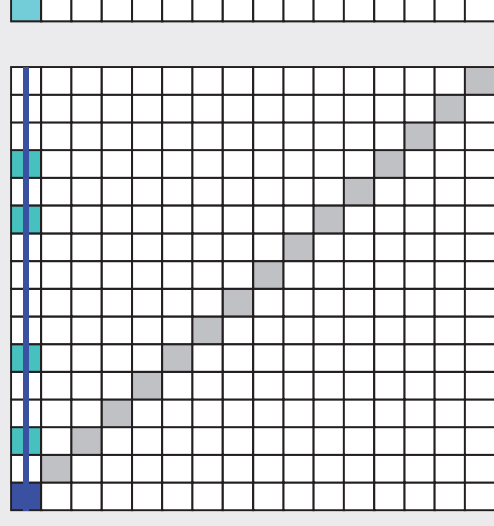
```
/* X=Xmin */
i=0;
jS= Index[i];
AMat[jS]= 0.0;
Diag[i ]= 1.0;
Rhs [i ]= 0.0;
```

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

```
/* X=Xmax */
i=N-1;
Rhs[i]= F;
```

$u_1=0$

Diagonal Component=1  
RHS=0  
Off-Diagonal Components= 0.



**Erase !**

# Program: 1d.c (6/7)

## Boundary Conditions

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

```
/* X=Xmin */
i=0;
jS= Index[i];
AMat[jS]= 0.0;
Diag[i ]= 1.0;
Rhs [i ]= 0.0;
```

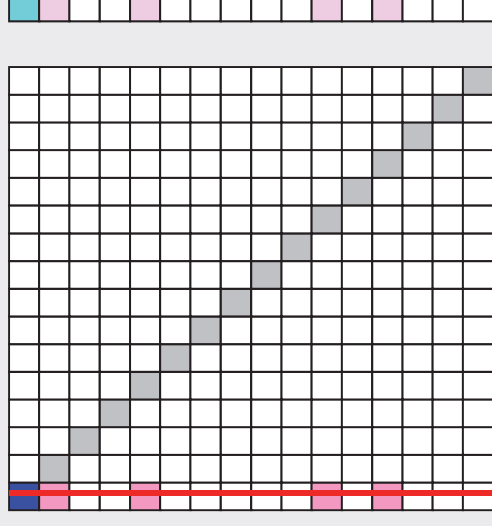
```
for (k=0;k<NPLU;k++) {
  if (Item[k]==0) {AMat[k]=0.0;
  }}
```

```
/* X=Xmax */
i=N-1;
Rhs[i]= F;
```

$u_1=0$

Diagonal Component=1  
RHS=0  
Off-Diagonal Components= 0.

### Elimination and Erase



Column components of boundary nodes (Dirichlet B.C.) are moved to RHS and eliminated for keeping symmetrical feature of the matrix (in this case just erase off-diagonal components)

# Program: 1d.c (6/7)

## Boundary Conditions

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

```
/* X=Xmin */
i=0;
jS= Index[i];
AMat[jS]= 0.0;
Diag[i ]= 1.0;
Rhs [i ]= 0.0;
```

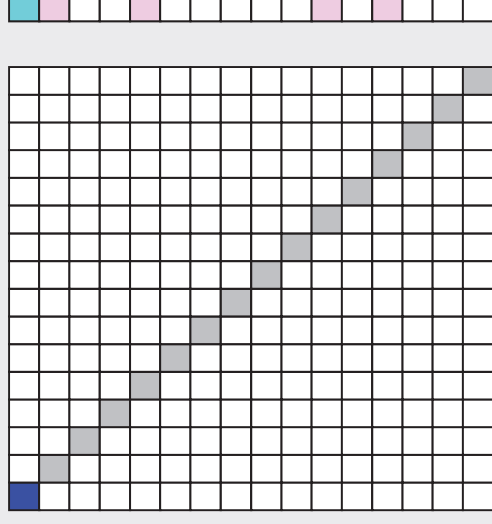
```
for (k=0;k<NPLU;k++) {
  if (Item[k]==0) {AMat[k]=0.0;
  }}
```

```
/* X=Xmax */
i=N-1;
Rhs[i]= F;
```

$u_1=0$

Diagonal Component=1  
RHS=0  
Off-Diagonal Components= 0.

### Elimination and Erase



Column components of boundary nodes (Dirichlet B.C.) are moved to RHS and eliminated for keeping symmetrical feature of the matrix (in this case just erase off-diagonal components)

if  $u_1 \neq 0$

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

/* X=Xmin */
i=0;
jS= Index[i];
AMat[jS]= 0.0;
Diag[i ]= 1.0;
Rhs [i ]= Umin;
```

Column components of boundary nodes (Dirichlet B.C.) are moved to RHS and eliminated for keeping symmetrical feature of the matrix.

```
for (j=1; j<N; j++) {
  for (k=Index[j]; k<Index[j+1]; k++) {
    if (Item[k]==0) {
      Rhs [j]= Rhs[j] - Amat[k]*Umin;
      AMat[k]= 0.0;
    }
  }
}
```

$$\text{Diag } u_j + \sum_{k=\text{Index}[j], k \neq k_s}^{\text{Index}[j-1]} \text{Amat}_k u_{\text{Item}[k]}$$

$$= \text{Rhs}_j - \text{Amat}_{k_s} u_{\text{Item}[k_s]} = \text{Rhs}_j - \text{Amat}_{k_s} u_{\min} \quad \text{where } \text{Item}[k_s] = 0$$

# Program: 1d.c (6/7)

## Boundary Conditions

```

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

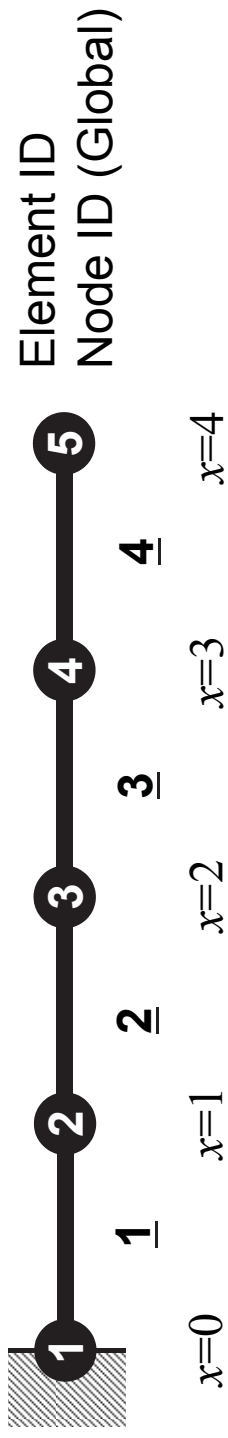
/* X=Xmin */
i=0;
jS= Index[i];
AMat[jS]= 0.0;
Diag[i ]= 1.0;
Rhs [i ]= 0.0;

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

/* X=Xmax */
i= N-1;
Rhs[i]= F;

```

# Element Eqn's/Accumulation



- As for Element-4:

$$[k]^{(4)} = \frac{EA}{L} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} \quad \{f\}^{(4)} = \int_S \bar{\sigma} [N]^T dS = \bar{\sigma} A \begin{Bmatrix} 0 \\ 1 \end{Bmatrix} = \begin{Bmatrix} 0 \\ F \end{Bmatrix}$$

$$[K] = \sum_{e=1}^4 [k]^{(e)} =$$

$$\{F\} = \sum_{e=1}^4 \{f\}^{(e)} =$$

# Preconditioned CG Solver

```

Compute  $r^{(0)} = b - [A]x^{(0)}$ 
for  $i = 1, 2, \dots$ 
    solve  $[M]z^{(i-1)} = r^{(i-1)}$ 
     $\rho_{i-1} = r^{(i-1)} \cdot z^{(i-1)}$ 
    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

```

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

# Diagonal Scaling, Point-Jacobi

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

- **solve**  $[M] \mathbf{z}^{(i-1)} = \mathbf{r}^{(i-1)}$  is very easy.
- Provides fast convergence for simple problems.
- 1d.f, 1d.c

# CG Solver (1/6)

```
/*
//      +-----+
//      | CG iterations |
//      +-----+
*/
```

```
R = 0;
Z = 1;
Q = 1;
P = 2;
DD= 3;
```

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

Reciprocal numbers (逆数) of diagonal components are stored in  $W[DD][i]$ .  
Computational cost for division is usually expensive.

# CG Solver (1/6)

```
/*
// +-----+
// | CG iterations |
// +-----+
*/
```

```
R = 0;
Z = 1;
Q = 1;
P = 2;
DD= 3;
```

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

```
W[0][i] = W[R][i]      ⇒ {r}
W[1][i] = W[Z][i]      ⇒ {z}
W[1][i] = W[Q][i]      ⇒ {q}
W[2][i] = W[P][i]      ⇒ {p}
W[3][i] = W[DD][i]     ⇒ 1/{D}
```

```
Compute  $r^{(0)} = b - [A]x^{(0)}$ 
for  $i = 1, 2, \dots$ 
    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 (7/7)

## Element Stress

```

/*
// +-----+
// | STRESS recovery |
// +-----+
*/

printf ("%s\n", "### STRESS");

for (icel=0; icel<NE; icel++) {
    in1= Icelnod[2*icel];
    in2= Icelnod[2*icel+1];
    X1 = X[in1];
    X2 = X[in2];
    U1 = U[in1];
    U2 = U[in2];
    DL = fabs(X2-X1);

    Strain= (U2-U1)/DL;
    Sigma = Young*Strain;

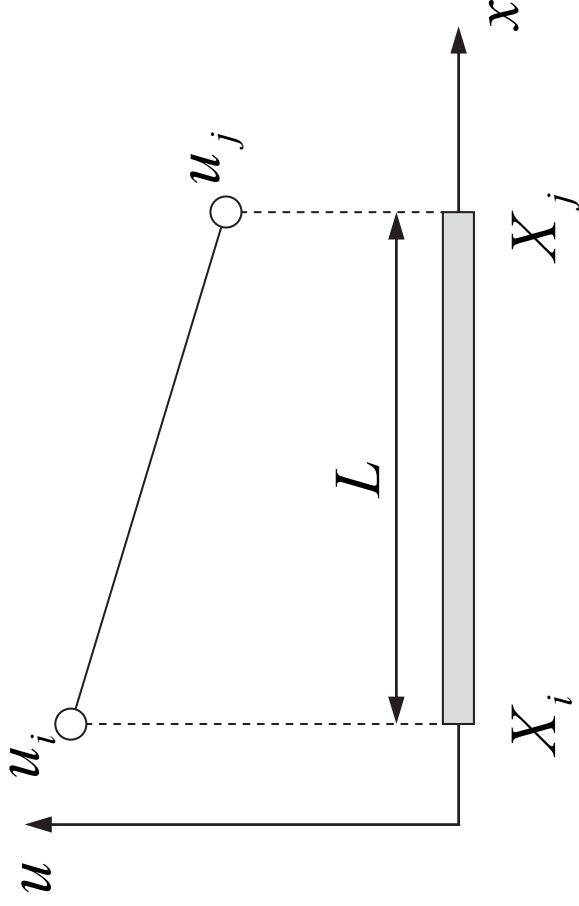
    printf ("%8d%16.6E\n", icel+1, Sigma, F/Area);
}

```

# Element Stress

Constant for 1D linear element: Constant Strain

$$N_i = \left( \frac{X_j - x}{L} \right), \quad N_j = \left( \frac{x - X_i}{L} \right), \quad \frac{dN_i}{dx} = \left( \frac{-1}{L} \right), \quad \frac{dN_j}{dx} = \left( \frac{1}{L} \right)$$



$$u = N_i u_i + N_j u_j$$

$$\varepsilon = \frac{du}{dx} = \frac{d}{dx} (N_i u_i + N_j u_j)$$

$$= \frac{dN_i}{dx} u_i + \frac{dN_j}{dx} u_j$$

$$= \left( -\frac{1}{L} \right) u_i + \left( \frac{1}{L} \right) u_j = \boxed{\frac{u_j - u_i}{L}}$$

# 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
- Calculation of Stress

- 1D-code for Static Linear-Elastic Problems by Galerkin FEM
- Sparse Linear Solver
  - Conjugate Gradient Method
  - Preconditioning
- Storage of Sparse Matrices
- Program
- **Road to Parallel FEM**

# Parallel Computing

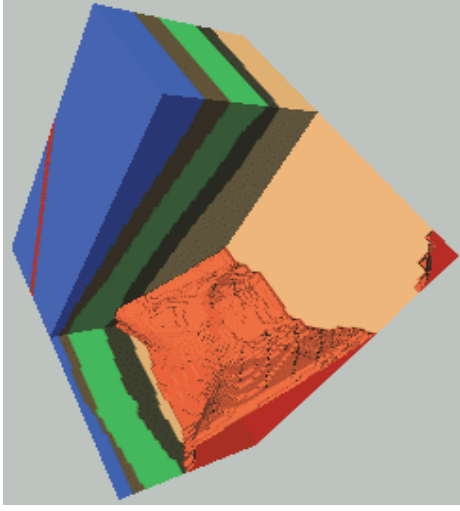
- **Faster, Larger & More Complicated**
- Scalability
  - Solving  $N^x$  scale problem using  $N^x$  computational resources during same computation time
    - for large-scale problems: **Weak Scaling**
    - e.g. CG solver: more iterations needed for larger problems
  - Solving a problem using  $N^x$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

# What is Parallel Computing ? (1/2)

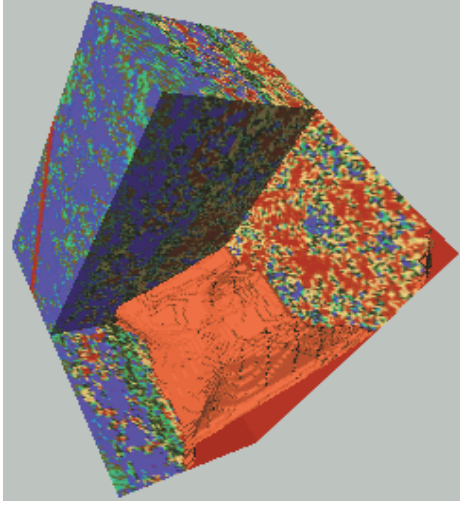
- to solve larger problems faster

## Homogeneous/Heterogeneous Porous Media

Lawrence Livermore National Laboratory



Homogeneous

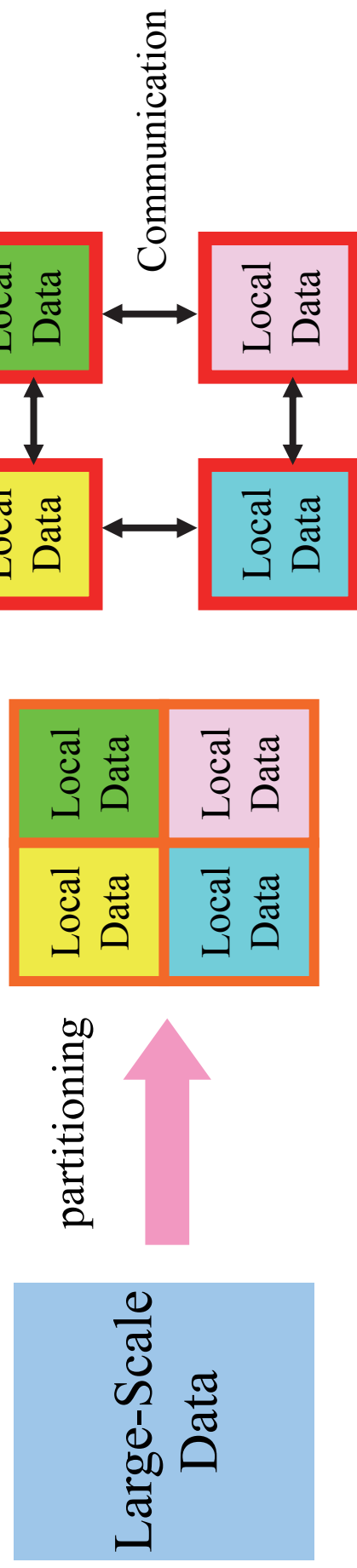


Heterogeneous

**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.

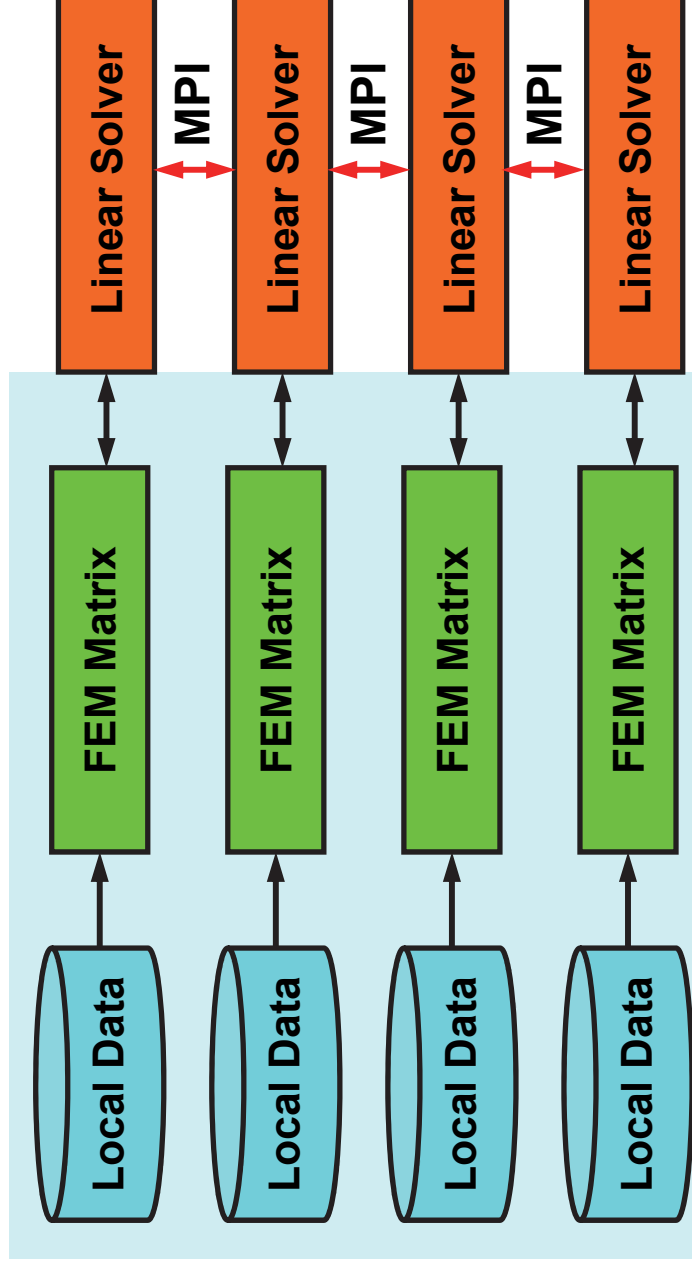
# Operations in Parallel FEM

## 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

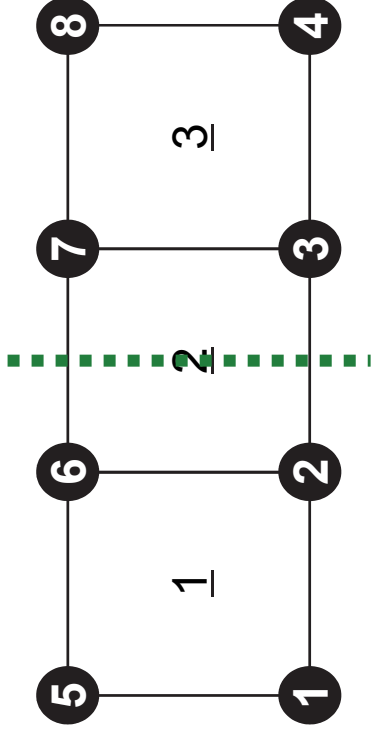


# Parallel FEM Procedures

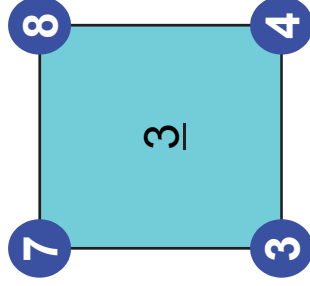
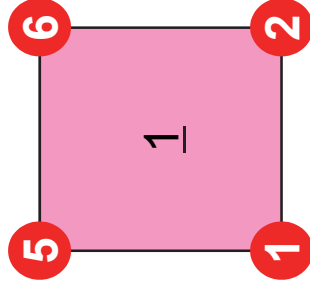
- Design on “Local Data Structure” is important
  - for SPMD-type operations in the previous page
- Matrix Generation
- Preconditioned Iterative Solvers for Linear Equations

# Bi-Linear Square Elements

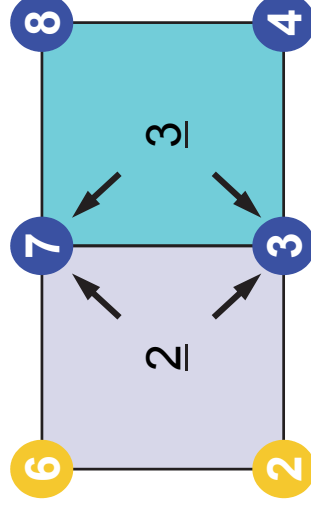
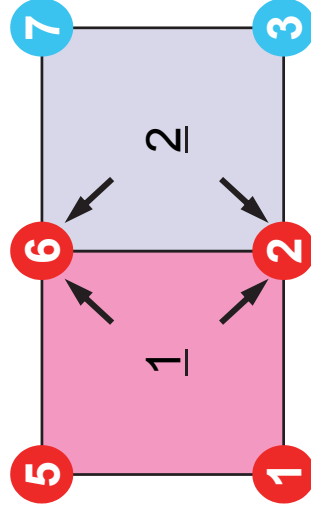
Values are defined on each node



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.



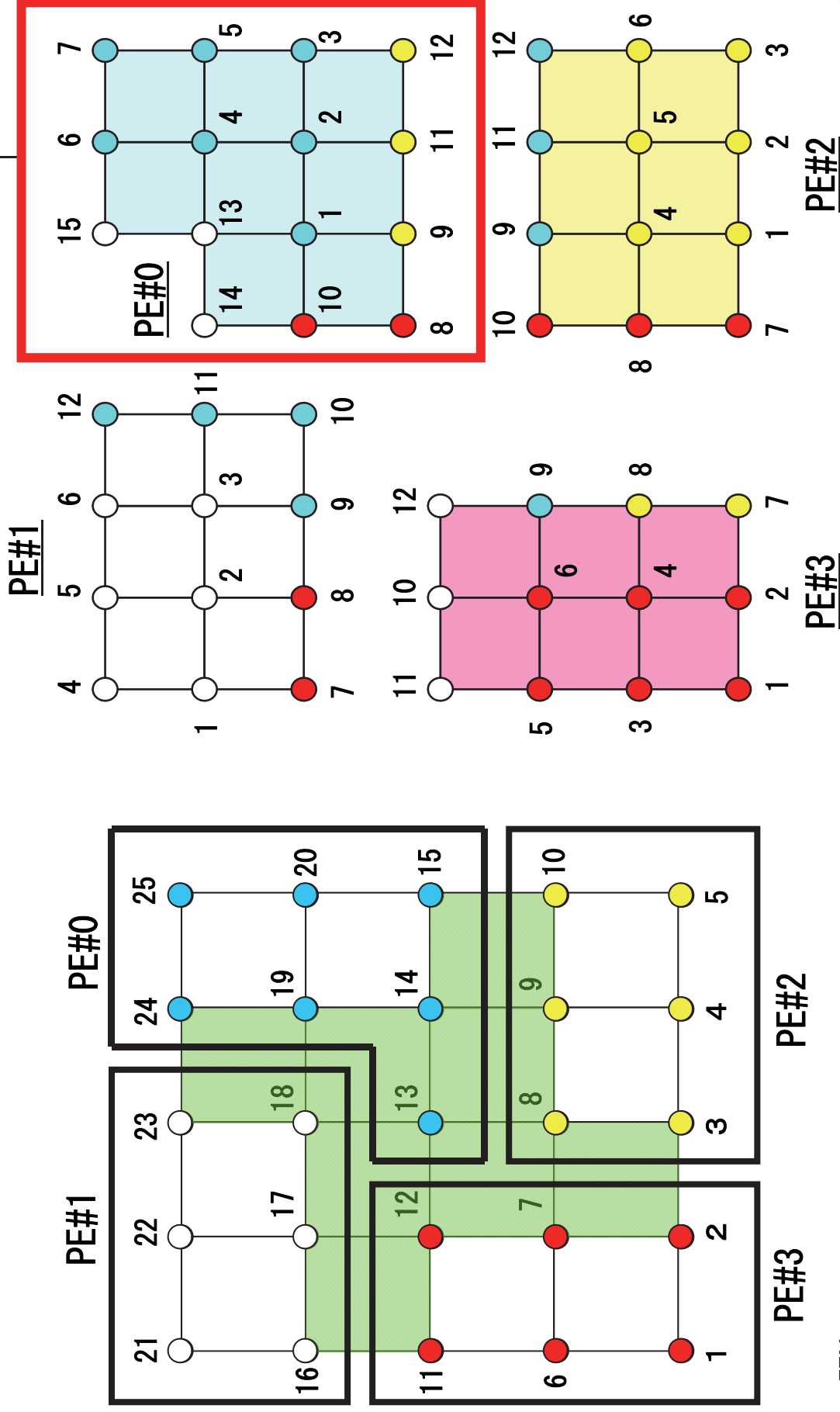


# Local Data of Parallel FEM

- **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



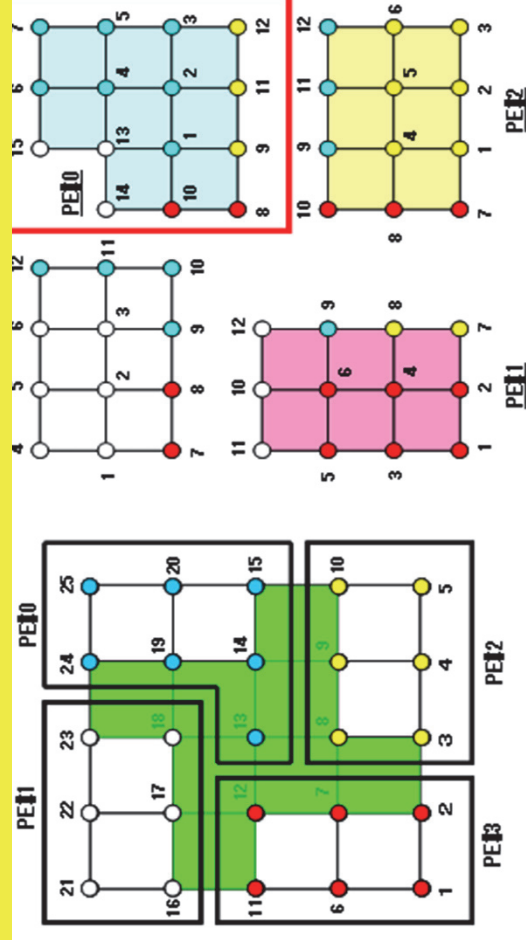
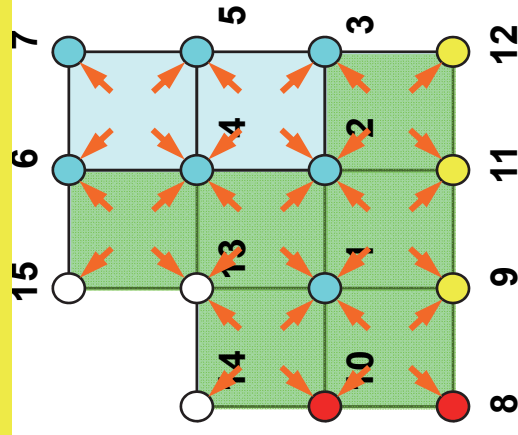
# Node-based Partitioning

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.

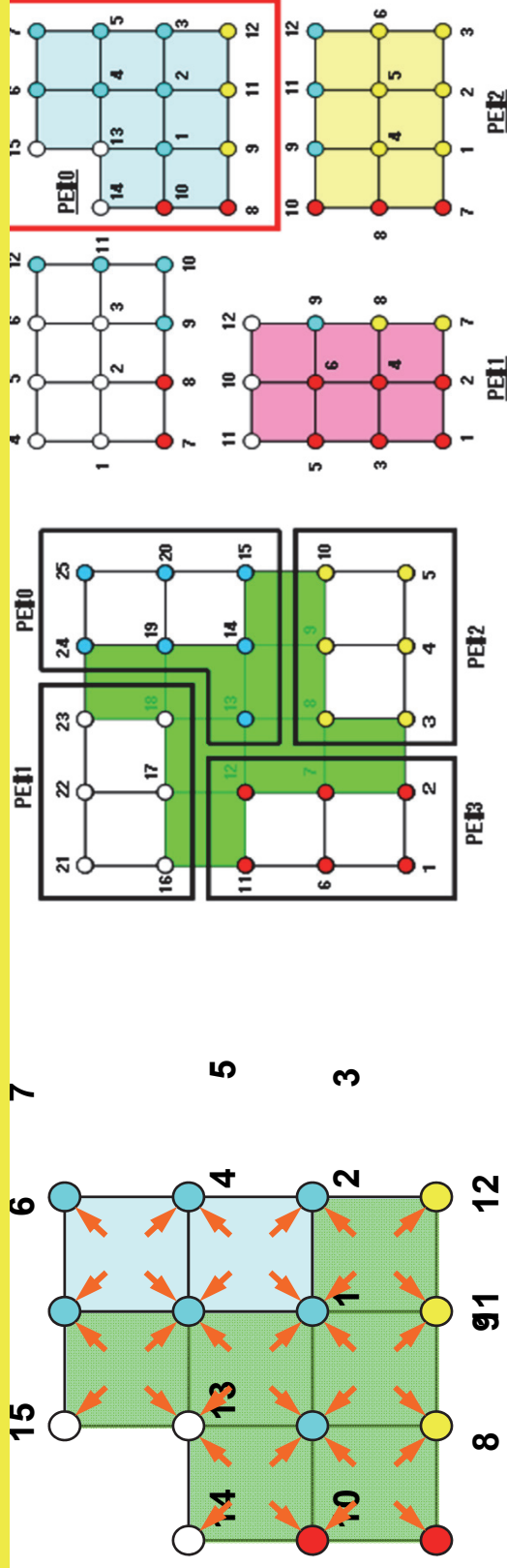
- Info of External Nodes are required for completely local element-based operations on each processor.



# We do not need communication during matrix assemble !!

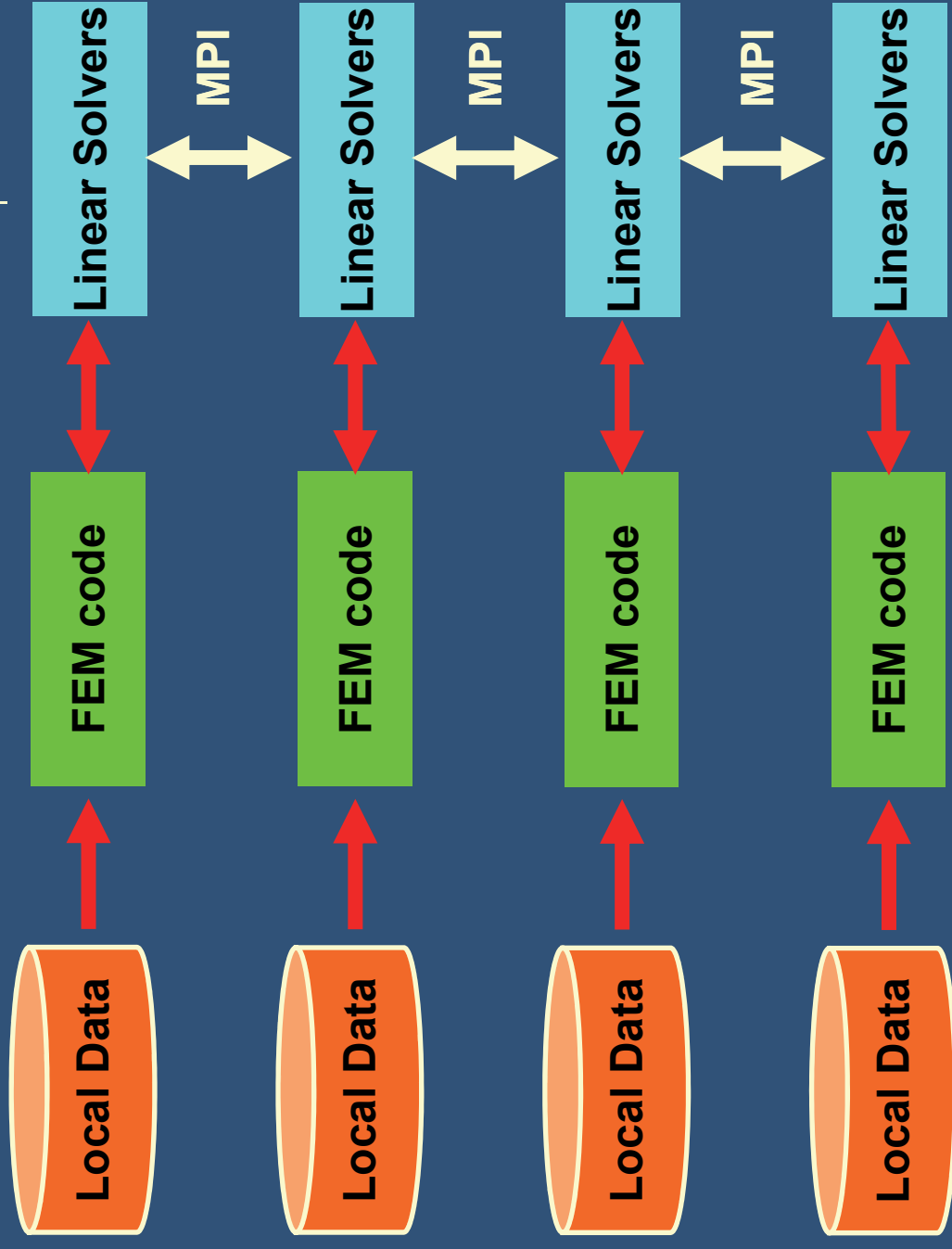
- Elements which include Internal Nodes
- External Nodes included in the Elements in overlapped region among partitions.

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



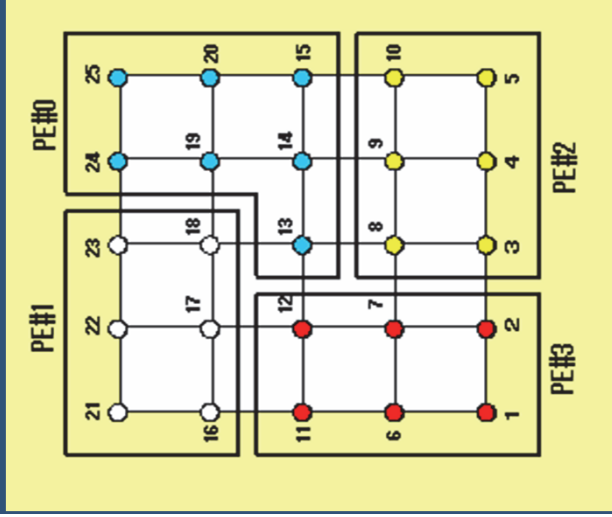
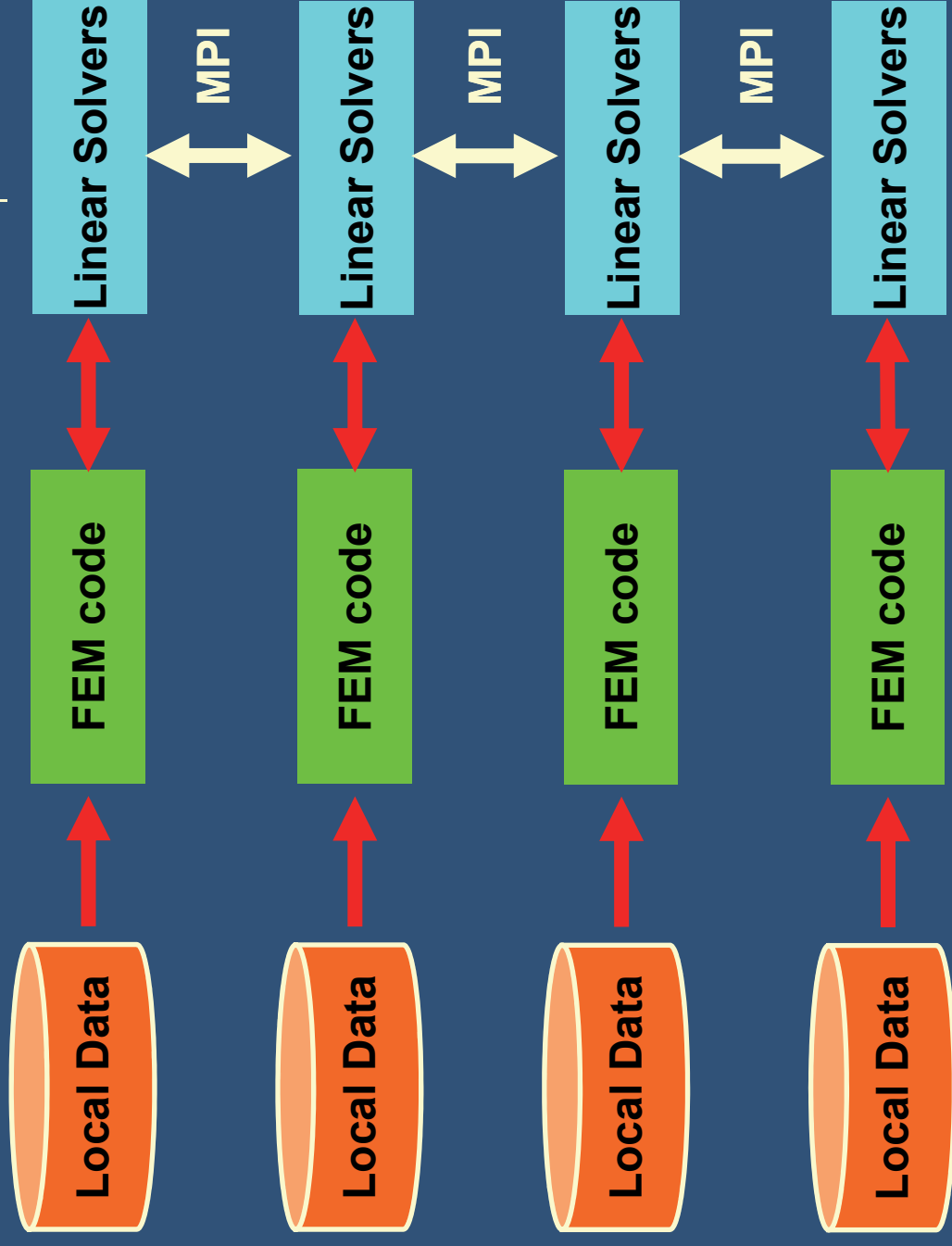
# Parallel Computing in FEM

## SPMD: Single-Program Multiple-Data



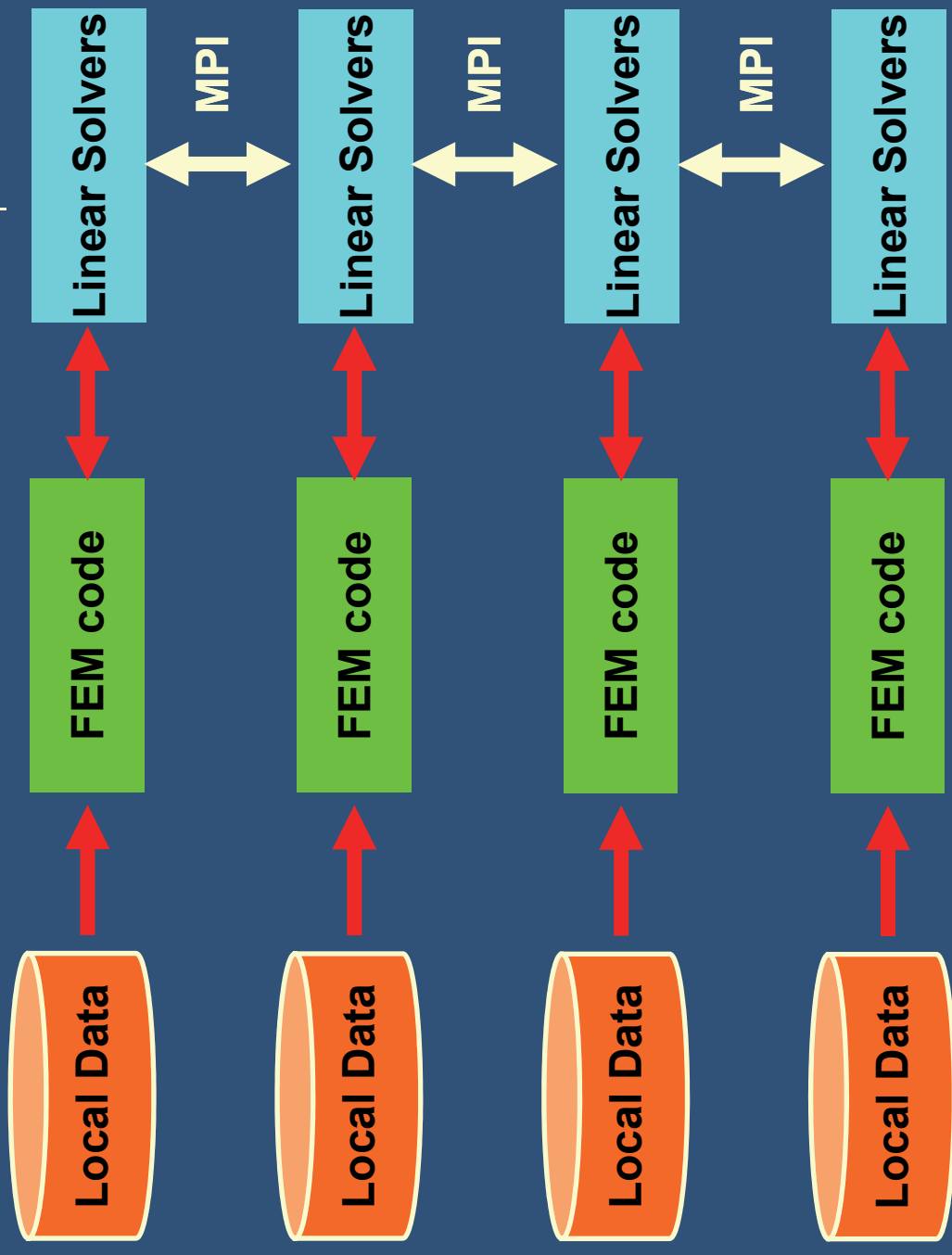
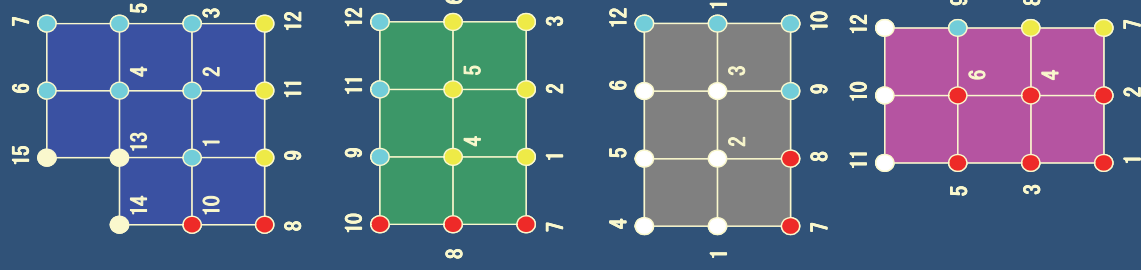
# Parallel Computing in FEM

## SPMD: Single-Program Multiple-Data



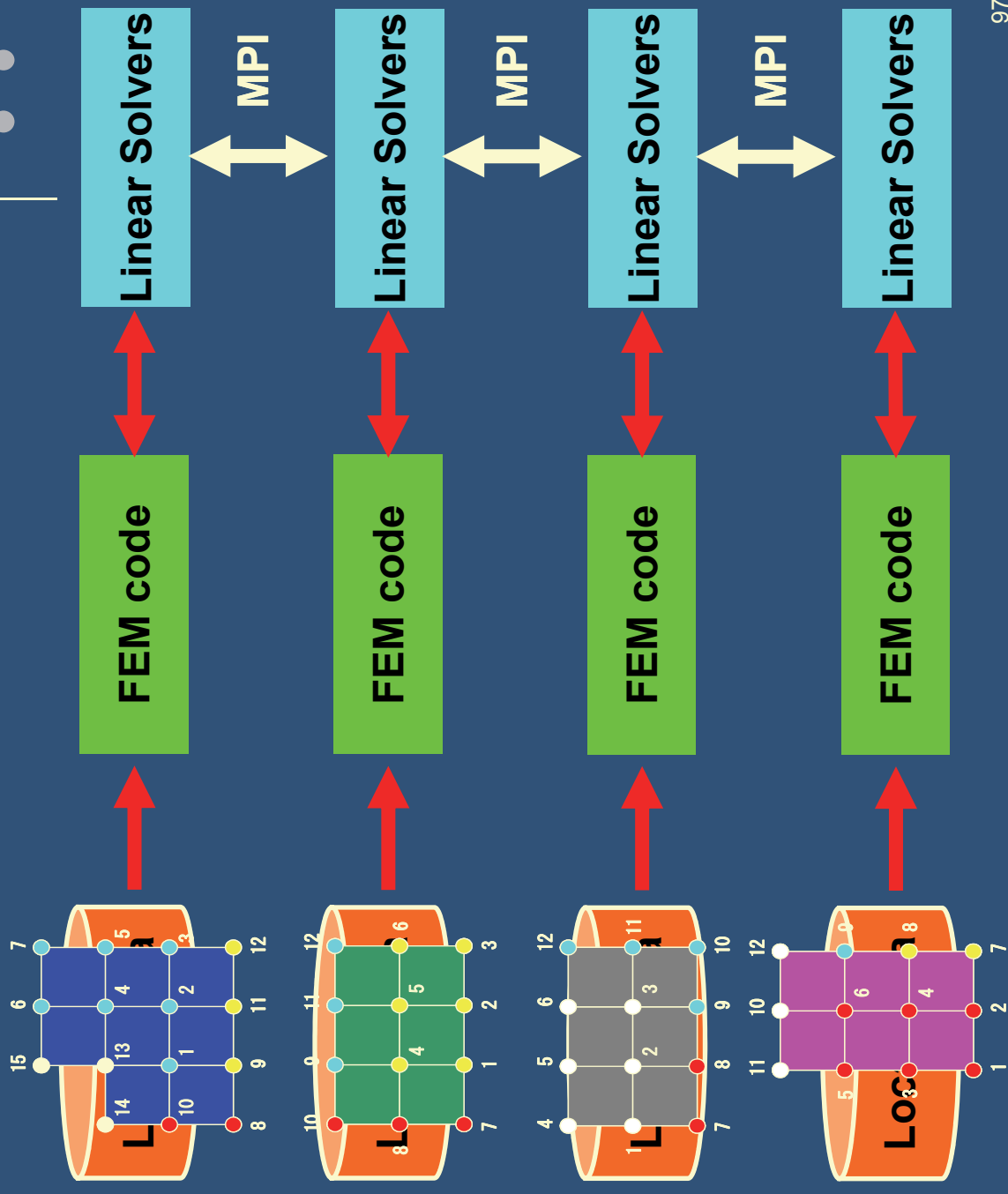
# Parallel Computing in FEM

## SPMD: Single-Program Multiple-Data



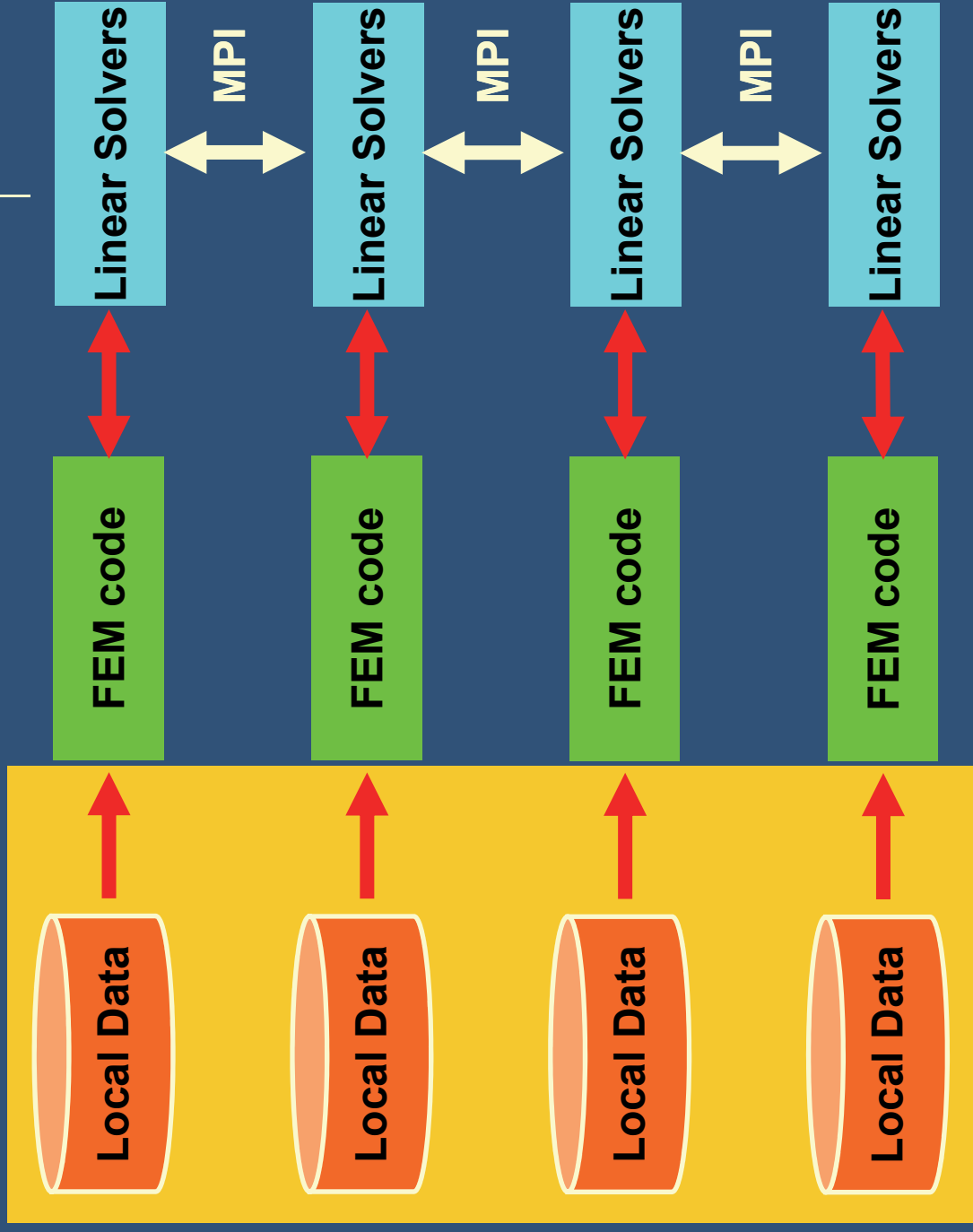
# Parallel Computing in FEM

## SPMD: Single-Program Multiple-Data



# Parallel Computing in FEM

## SPMD: Single-Program Multiple-Data

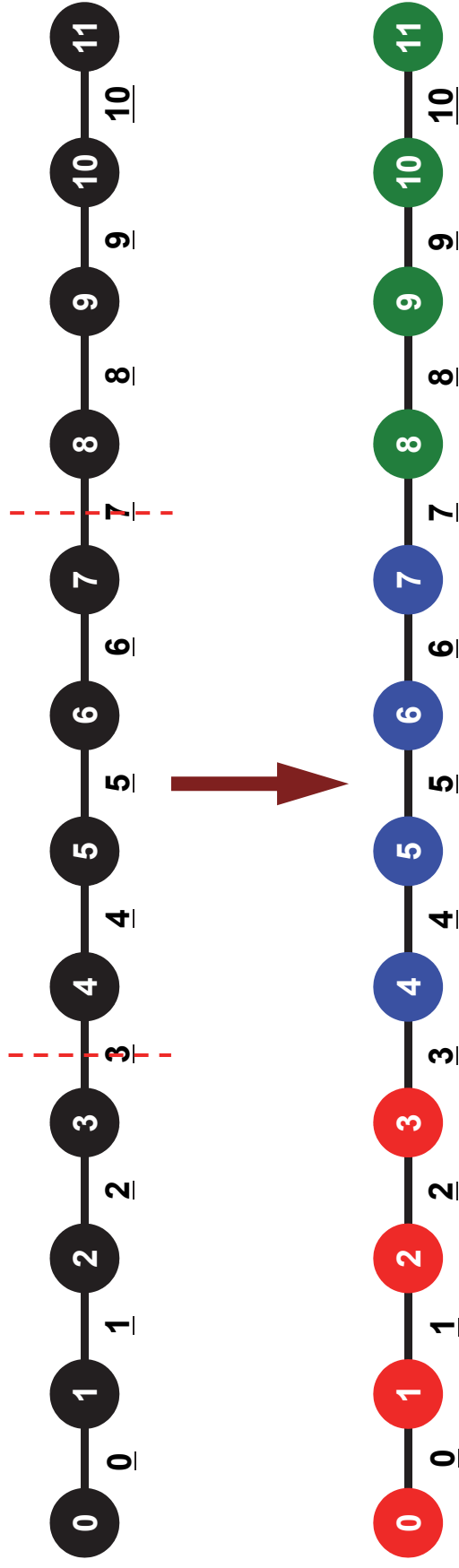


# What is Communications ?

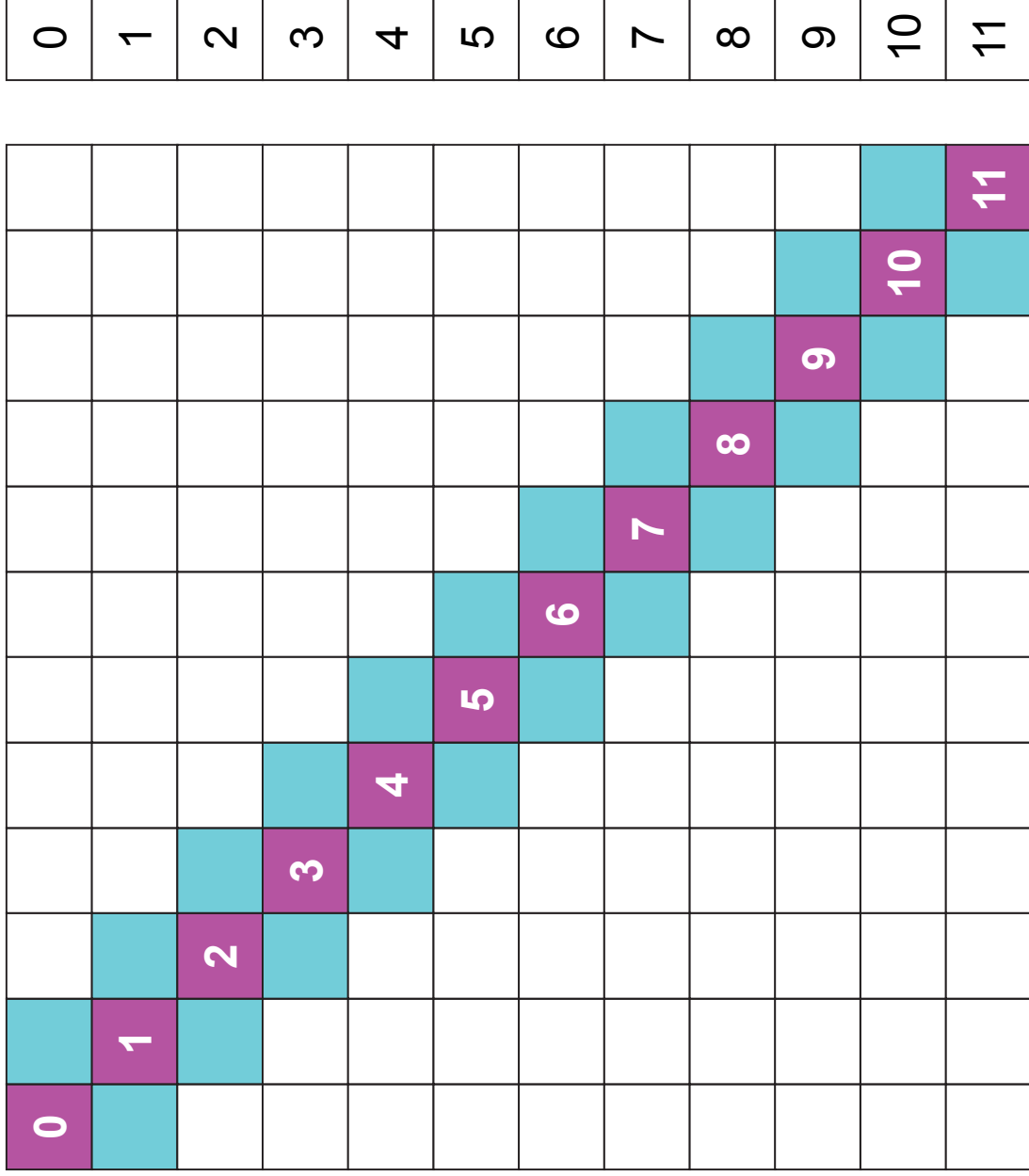


- to get information of “external nodes” from external partitions (local data)
- “Communication tables” contain the information

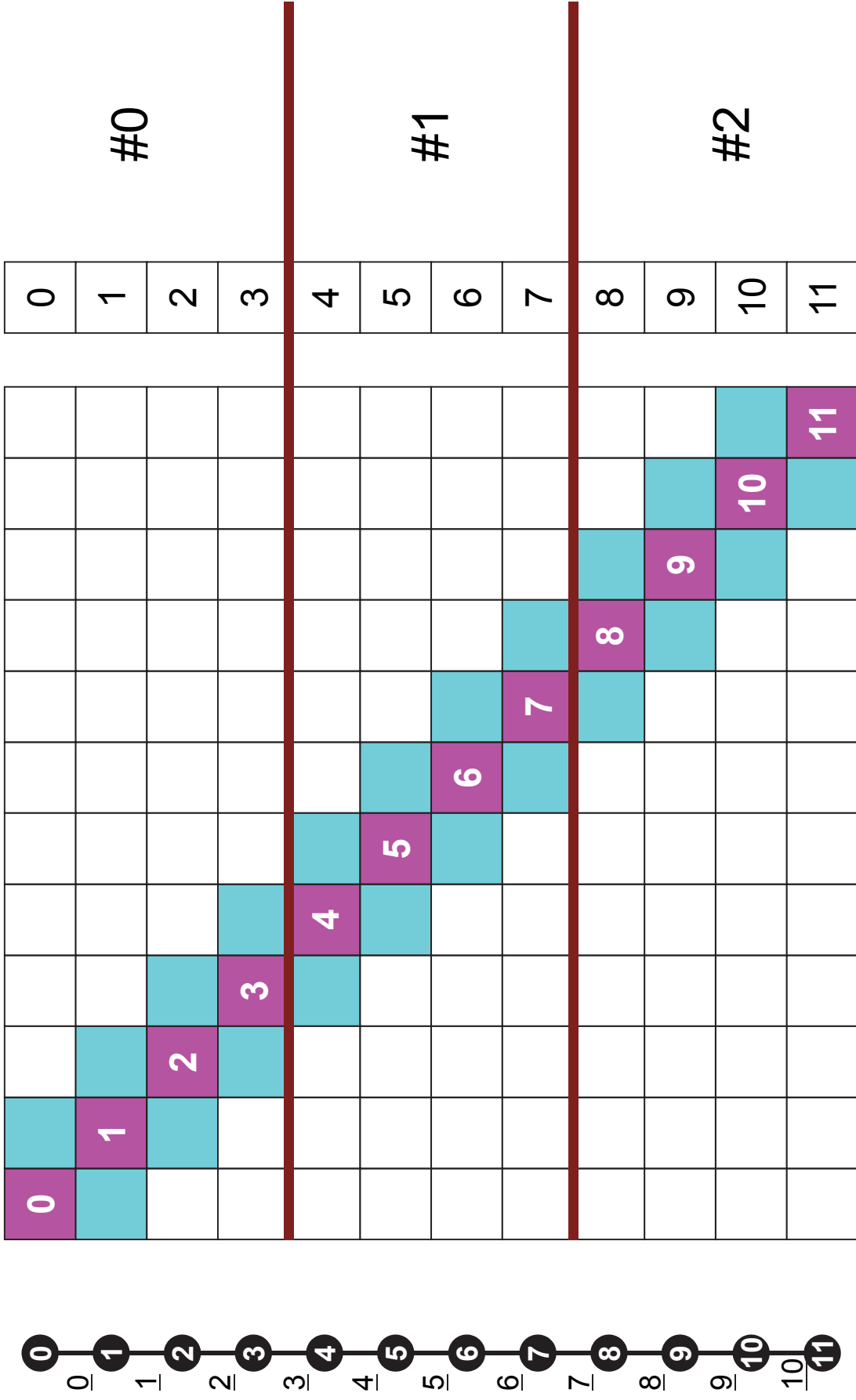
# 1D FEM: 12 nodes/11 elem's/3 domains



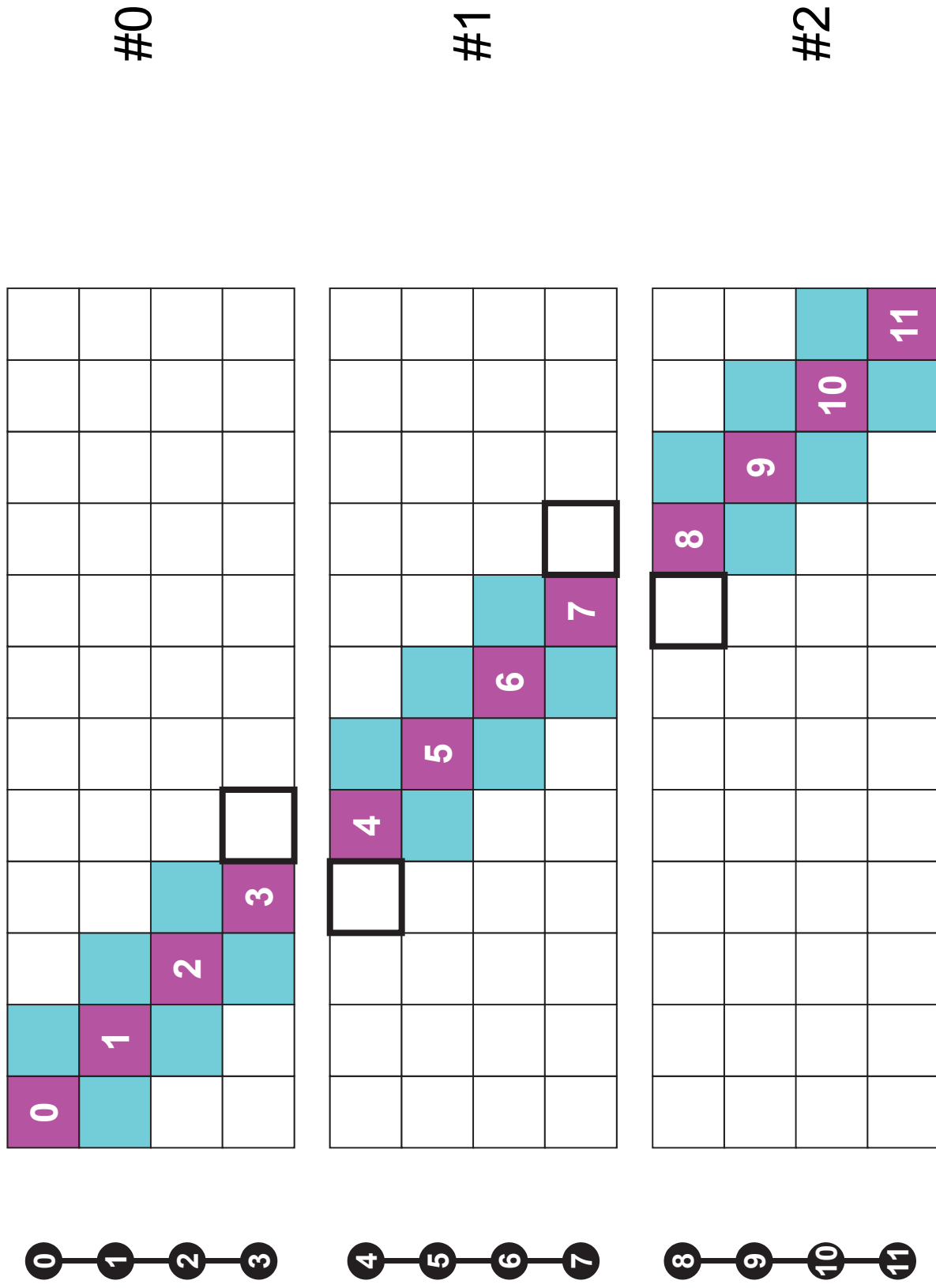
# 1D FEM: 12 nodes/11 elem's/3 domains



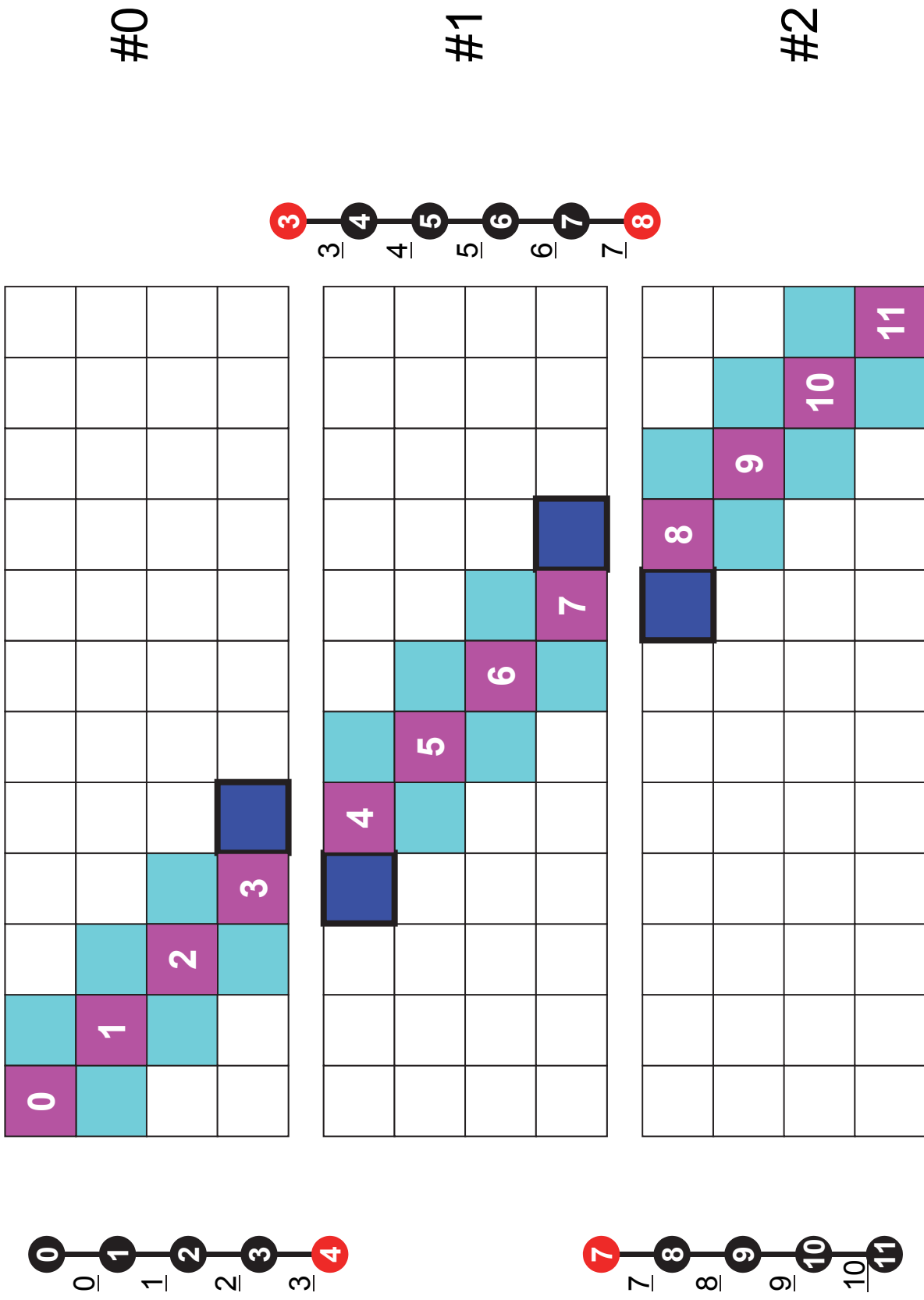
# # “Internal Nodes” should be balanced



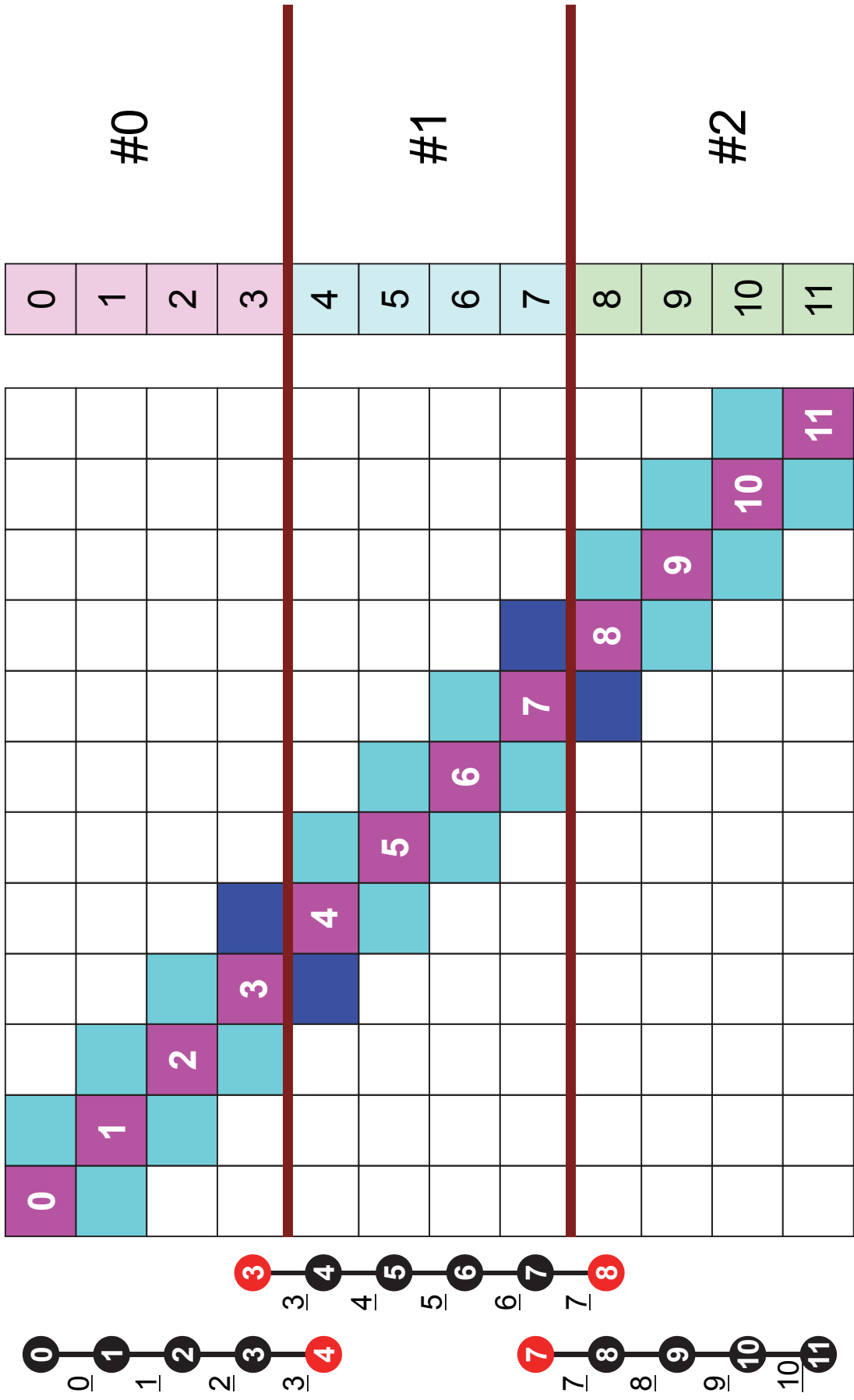
# Matrices are incomplete !



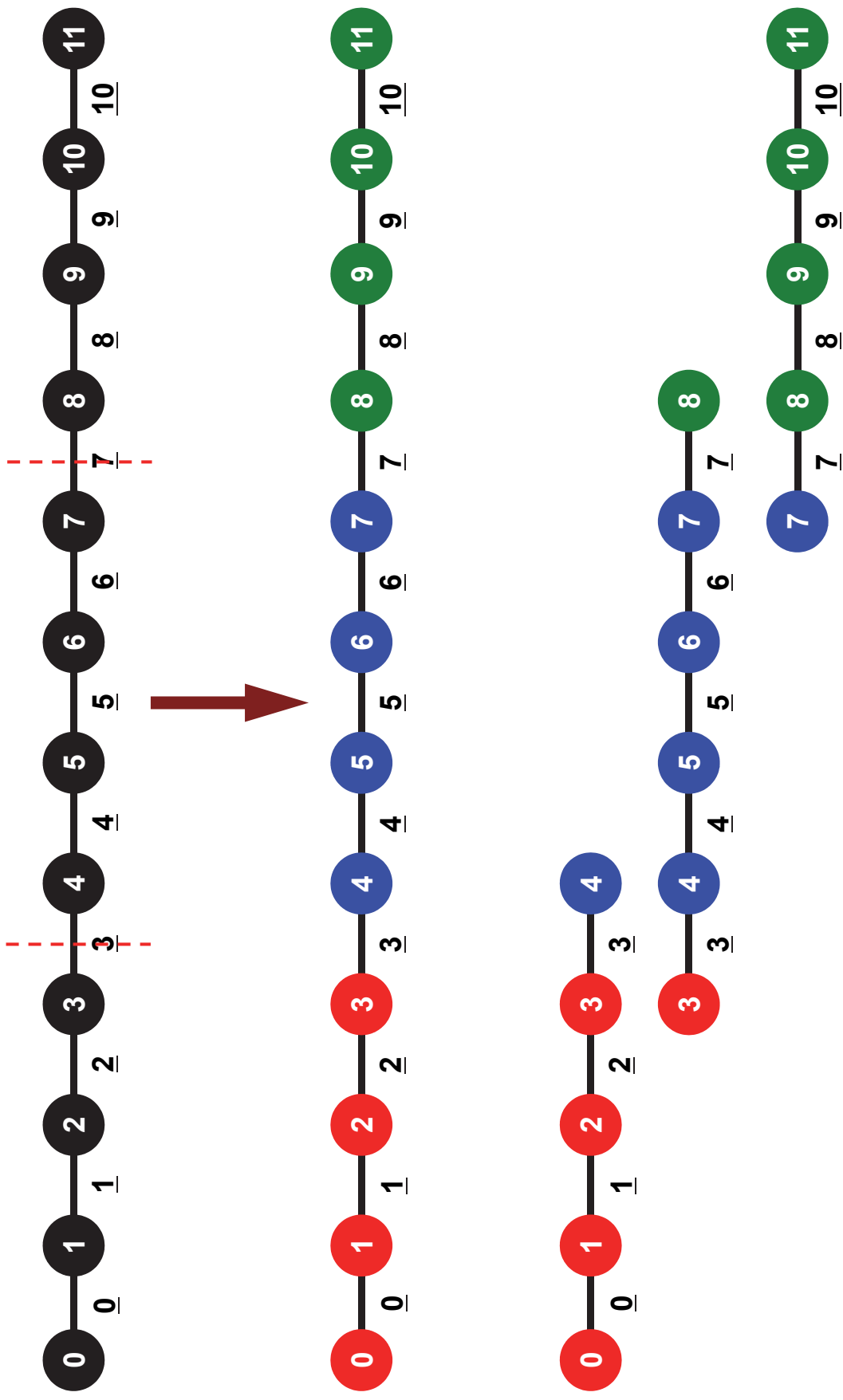
# Connected Elements + External Nodes



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

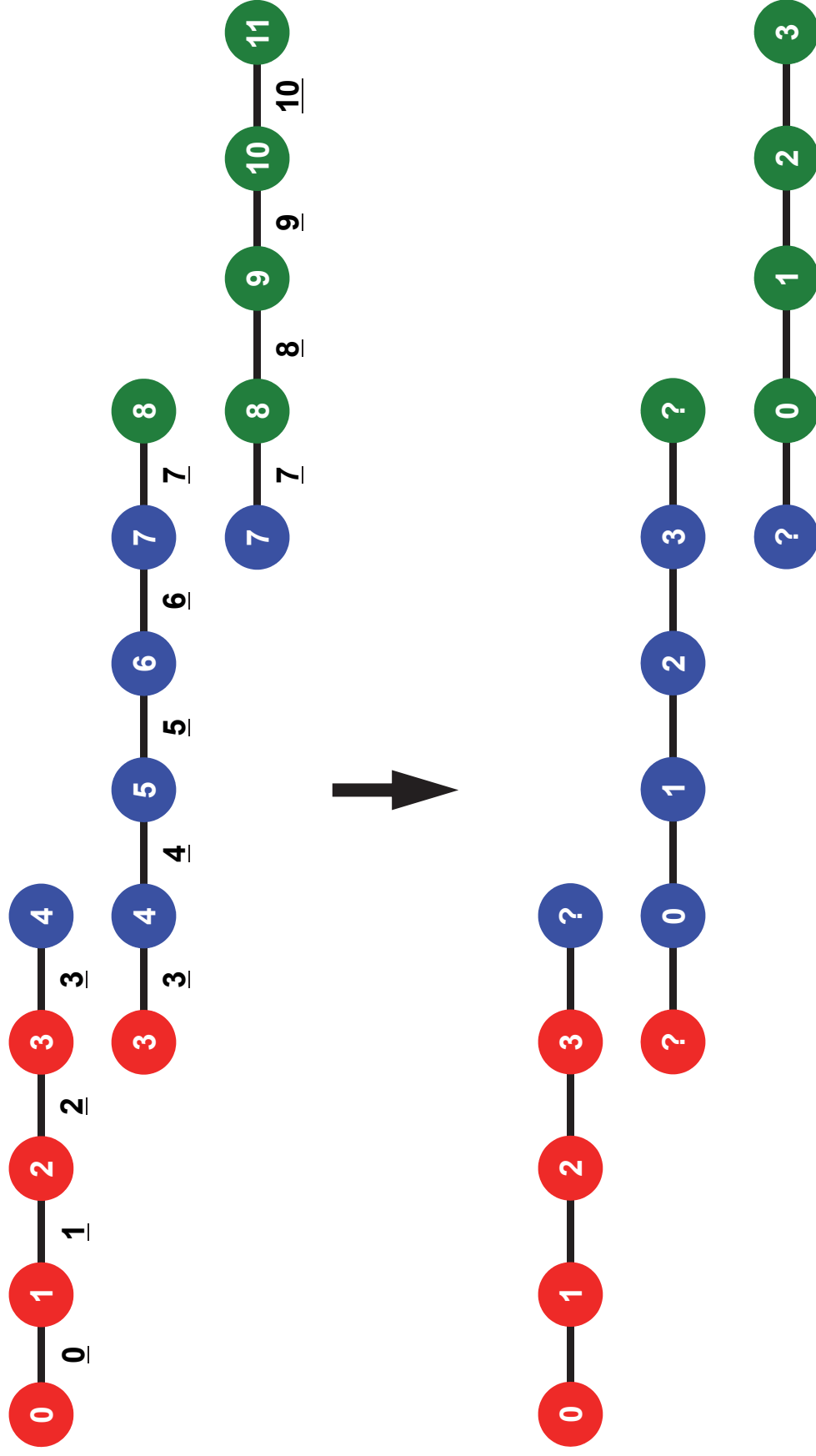


# 1D FEM: 12 nodes/11 elem's/3 domains



# Local Numbering for SPMD

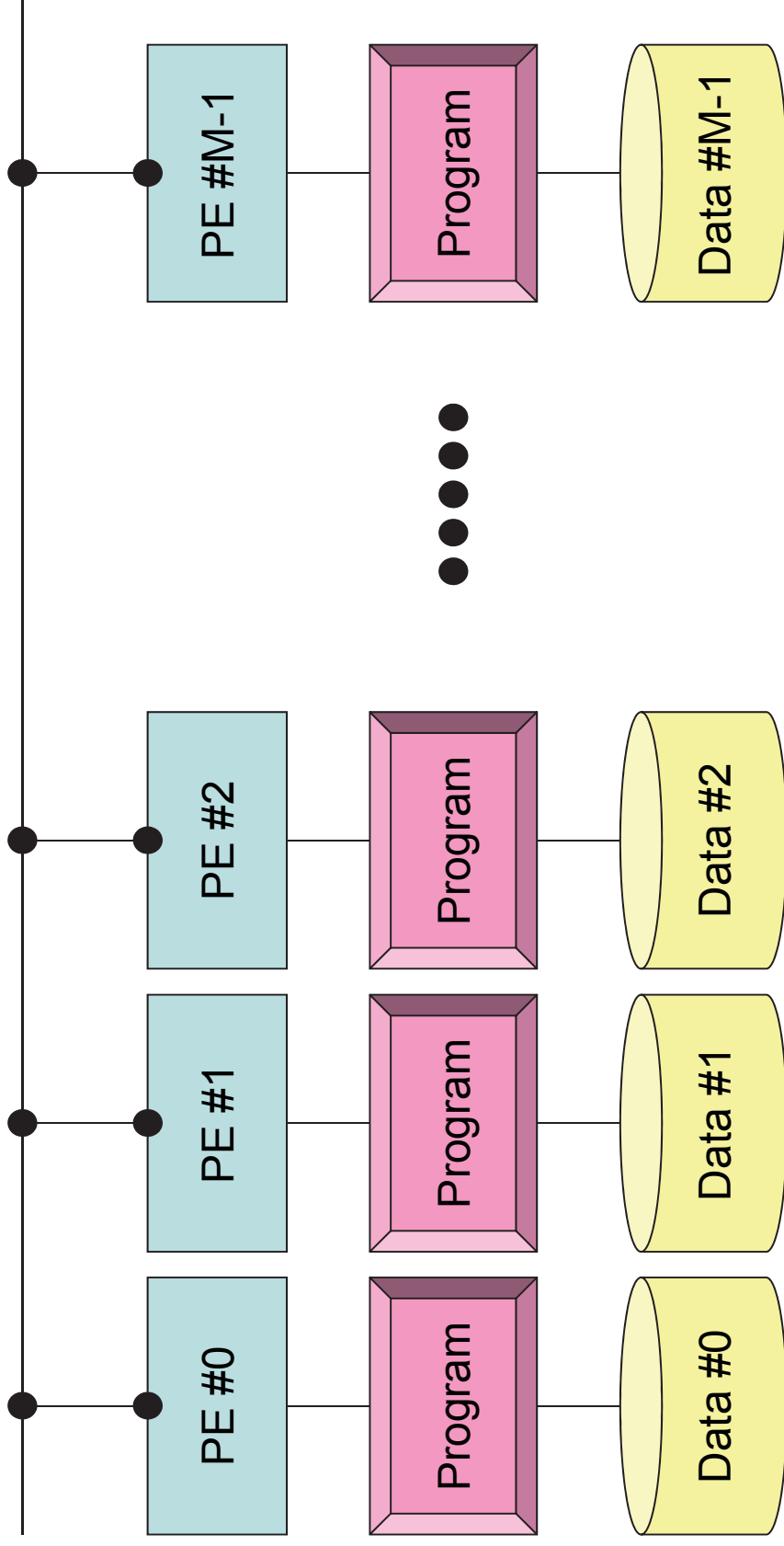
Numbering of internal nodes is 1-N ( $0-N-1$ ), same operations in serial program can be applied. How about numbering of external nodes ?



PE: Processing Element  
Processor, Domain, Process

# SPMD

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

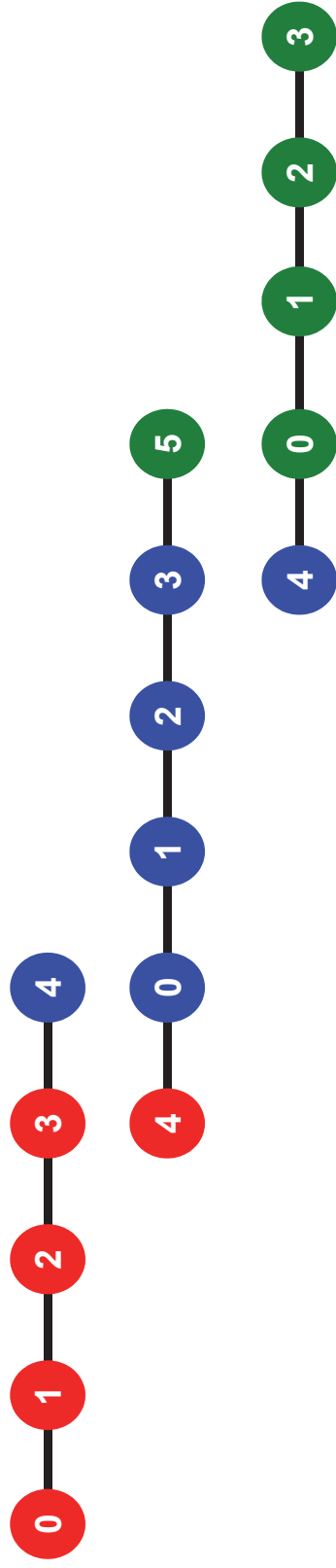


Each process does same operation for different data

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

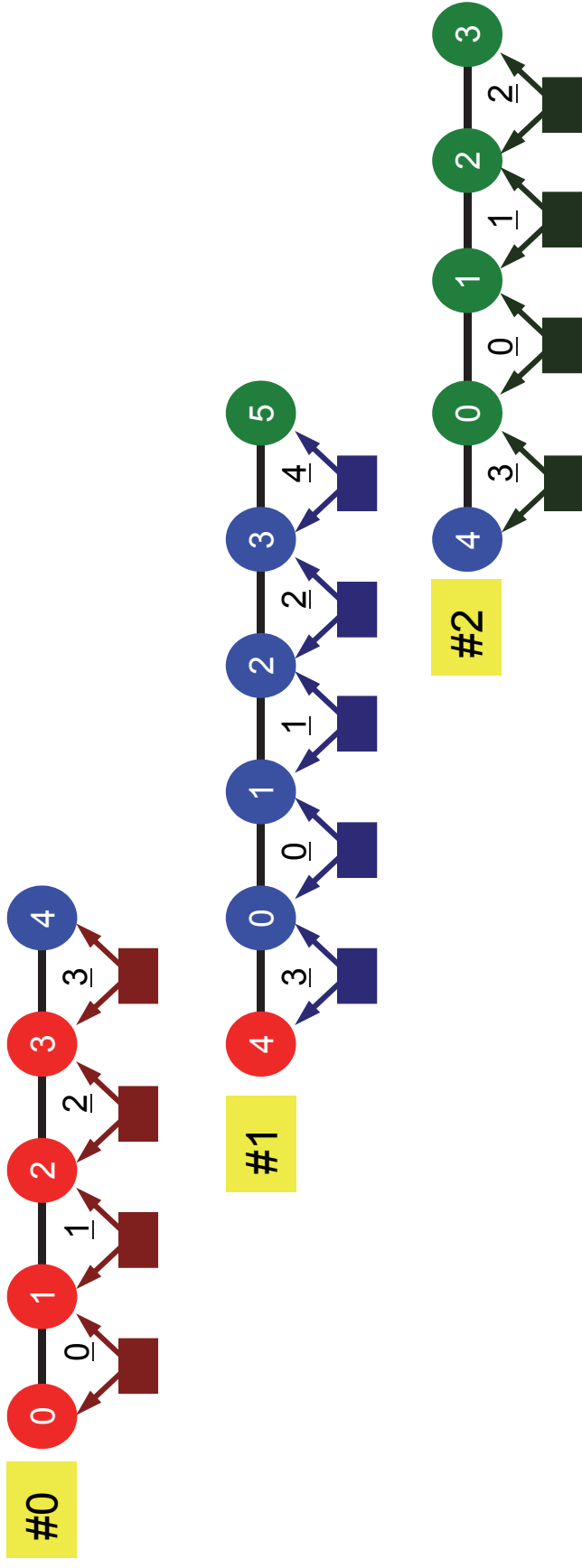
Numbering of external nodes:  $N+1$ ,  $N+2$  ( $N, N+1$ )



# 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

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

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

|    |
|----|
| 0  |
| 1  |
| 2  |
| 3  |
| 4  |
| 5  |
| 6  |
| 7  |
| 8  |
| 9  |
| 10 |
| 11 |

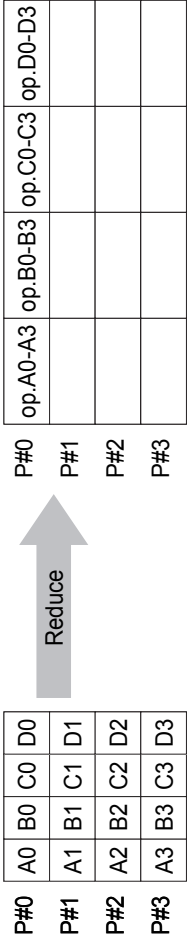
# Dot Products

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;
```

|    |
|----|
| 0  |
| 1  |
| 2  |
| 3  |
| 4  |
| 5  |
| 6  |
| 7  |
| 8  |
| 9  |
| 10 |
| 11 |

# 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
  - count int I number of elements in send/receive buffer
  - datatype MPI\_Datatype I 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

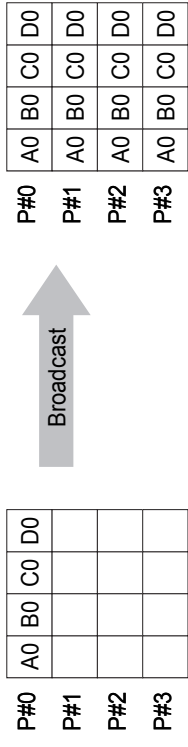
- op MPI\_Op I reduce operation  
MPI\_MAX, MPI\_MIN, MPI\_SUM, MPI\_PROD, MPI\_LAND, MPI\_BAND etc

Users can define operations by MPI\_OP\_CREATE

- root int I rank of root process
- comm MPI\_Comm I communicator

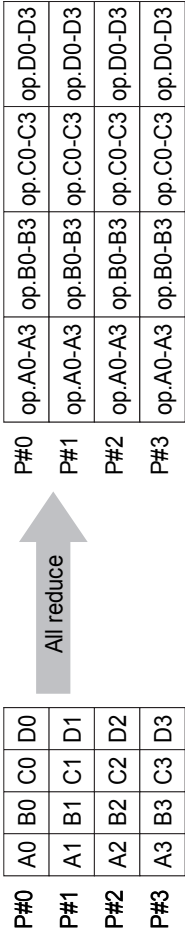


# MPI\_Bcast



- 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/recv buffer
  - datatype      MPI\_Datatype 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      int      I      rank of root process
  - comm      MPI\_Comm I      communicator

# 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/recv buffer
- datatype MPI\_Datatype I data type of elements of send/recv buffer
- op MPI\_Op I reduce operation
- comm MPI\_Comm I communicator

# “op” of MPI\_Reduce/Allreduce

## MPI\_Reduce

`(sendbuf, recvbuf, count, datatype, op, root, comm)`

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

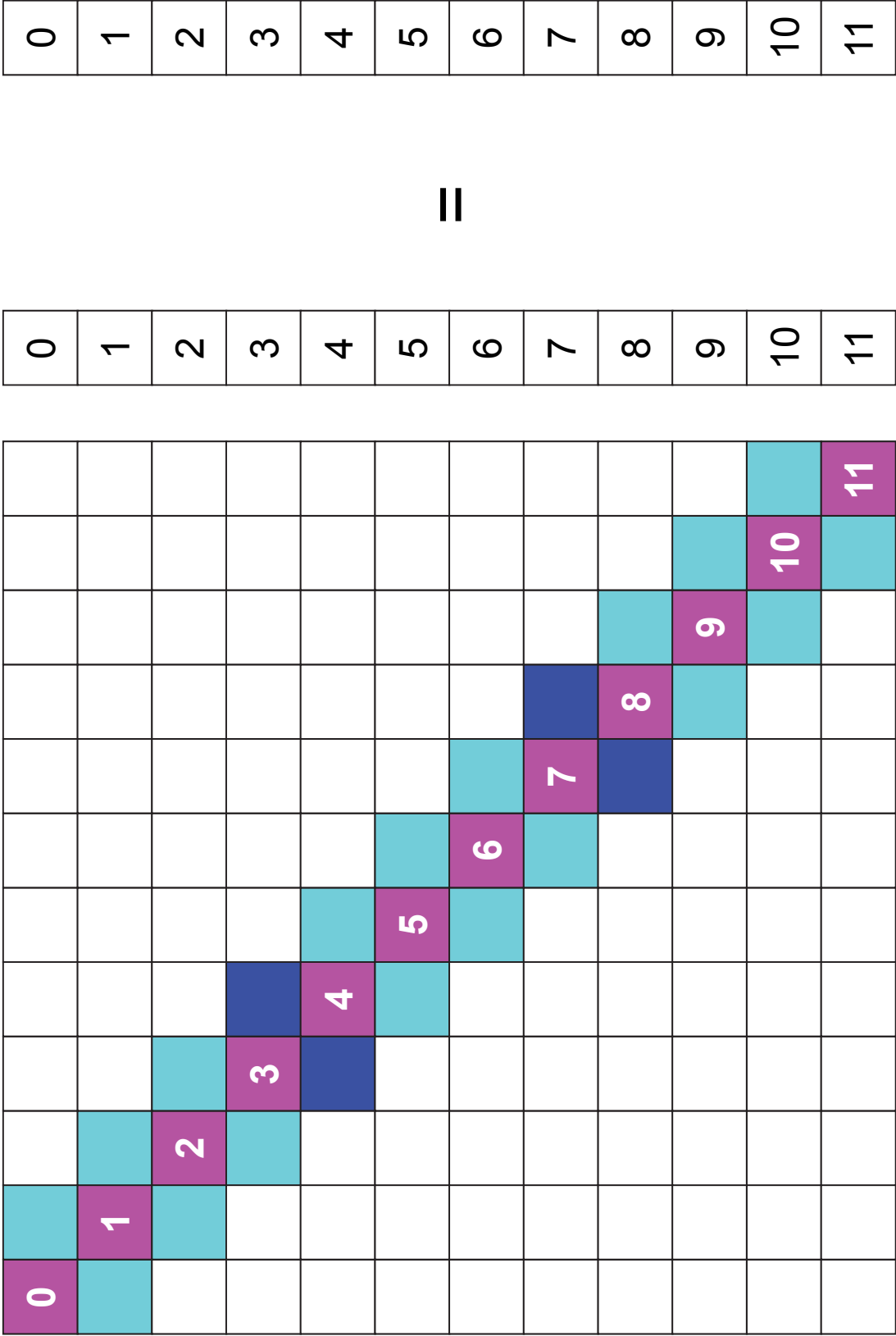
# Matrix-Vector Products

Values at External Points: P-to-P Communication

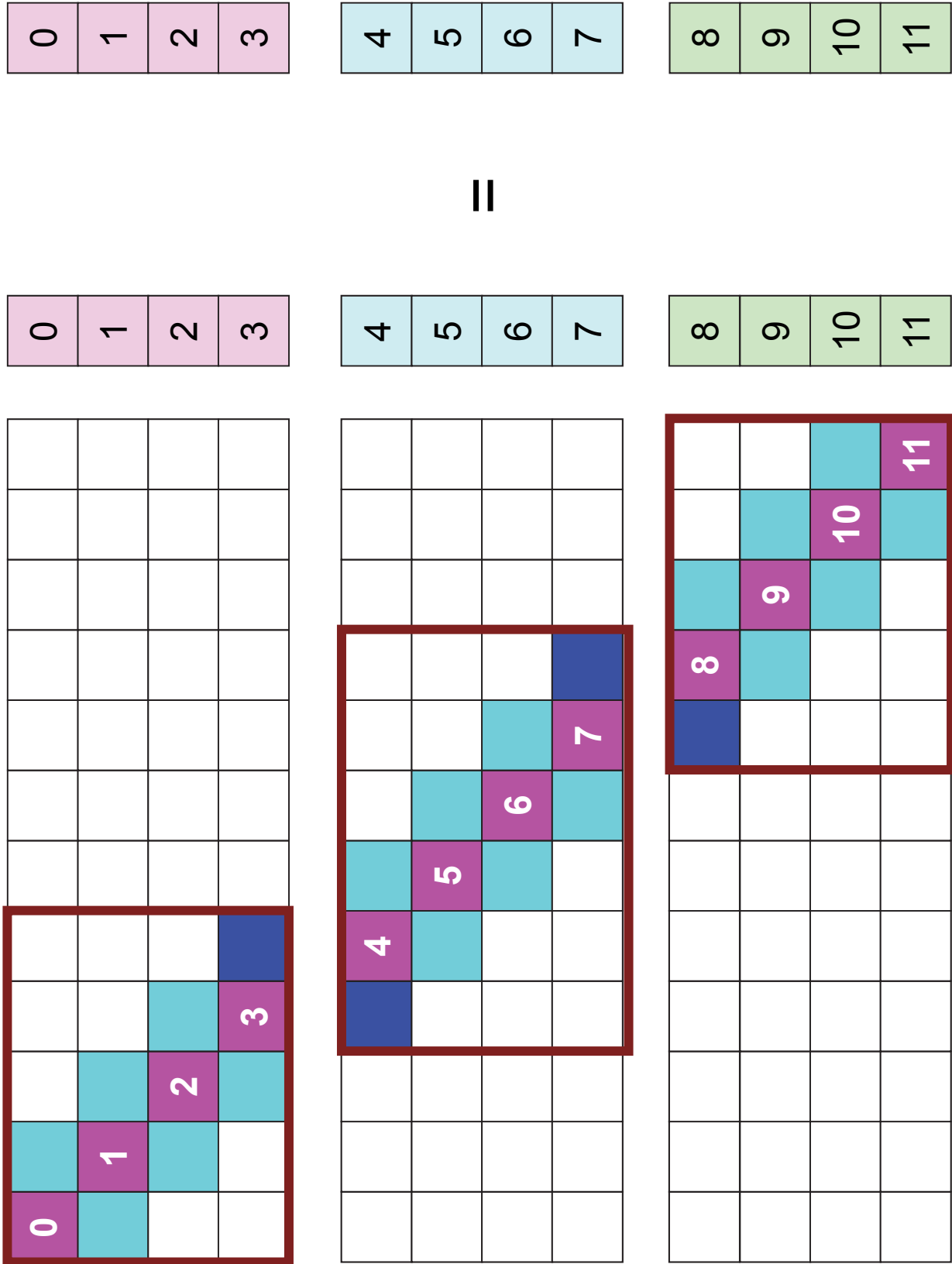
```
/*  
  //-- {q} = [A] {p}  
  */  
  for (i=0; i<N; i++) {  
    W[Q][i] = Diag[i] * W[P][i];  
    for (j=Index[i]; j<Index[i+1]; j++) {  
      W[Q][i] += AMat[j]*W[P][Item[j]];  
    }  
  }  
}
```



# Mat-Vec Products: Local Op. Possible



# Mat-Vec Products: Local Op. Possible



# Mat-Vec Products: Local Op. Possible

|   |   |   |   |
|---|---|---|---|
| 0 |   |   |   |
|   | 1 |   |   |
|   |   | 2 |   |
|   |   |   | 3 |

|   |   |   |   |
|---|---|---|---|
| 0 | 1 | 2 | 3 |
|---|---|---|---|

|   |   |   |   |
|---|---|---|---|
| 0 | 1 | 2 | 3 |
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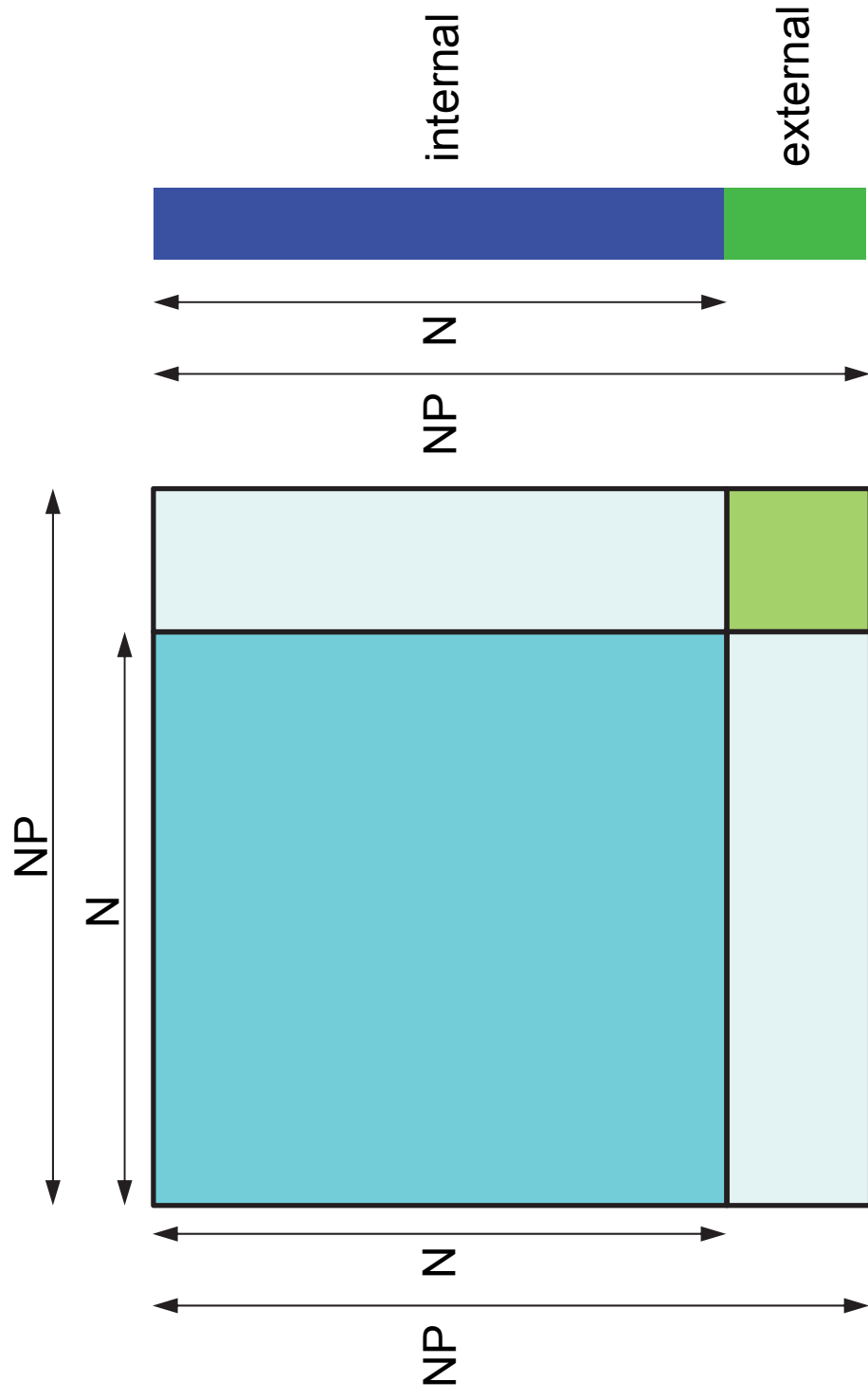
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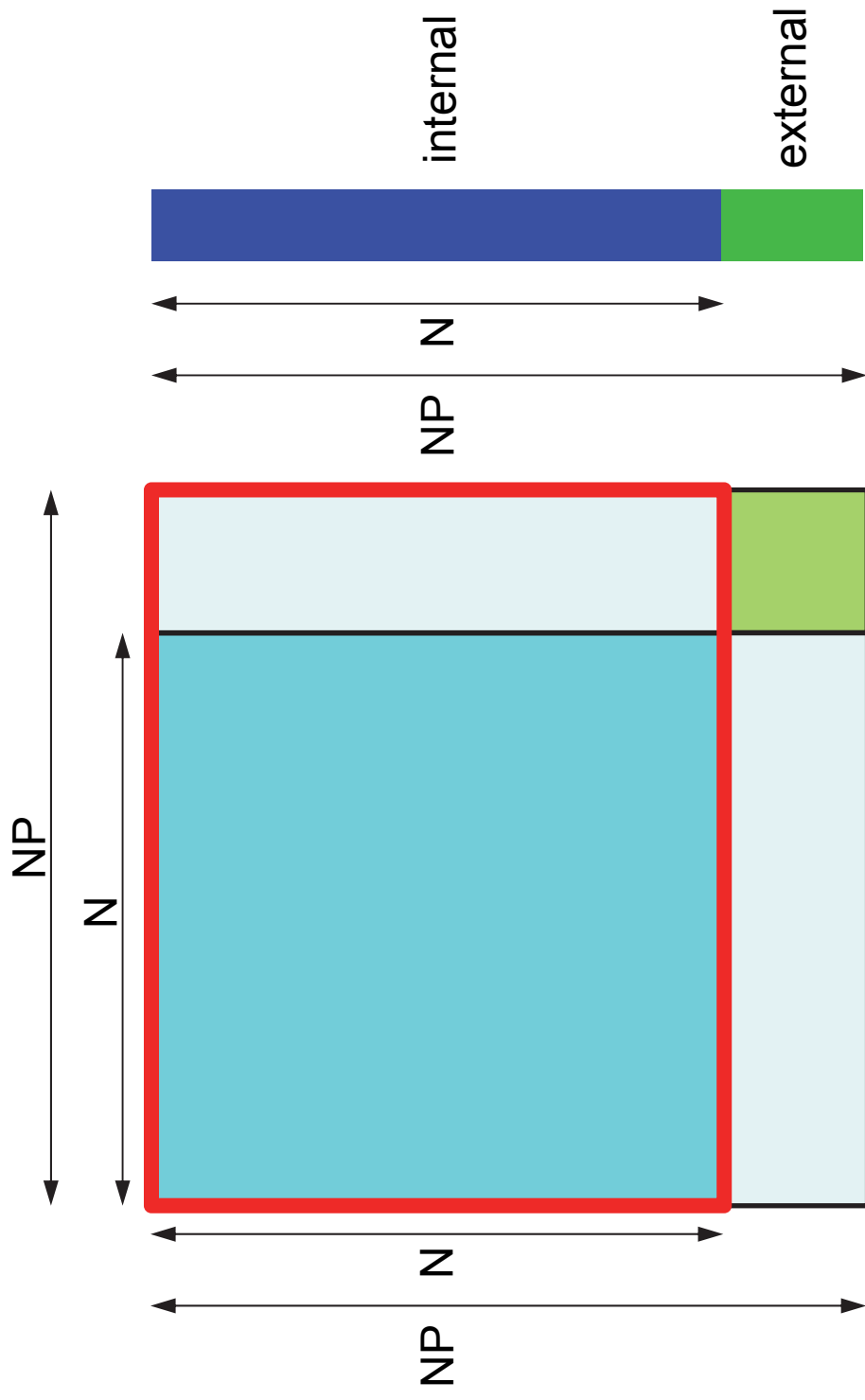
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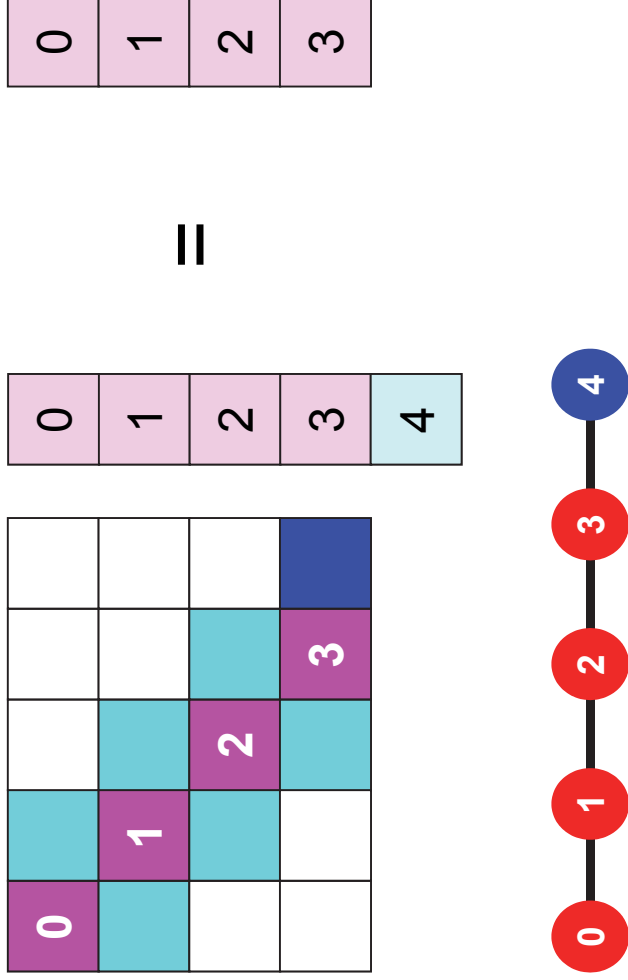
# Local Matrix



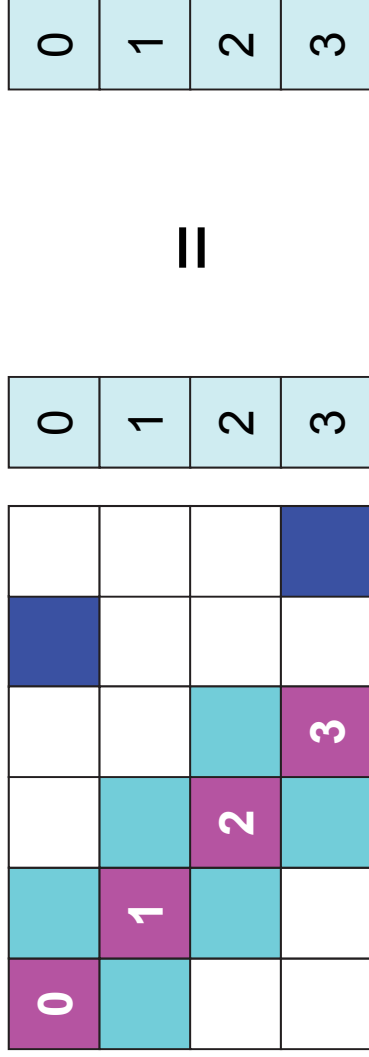
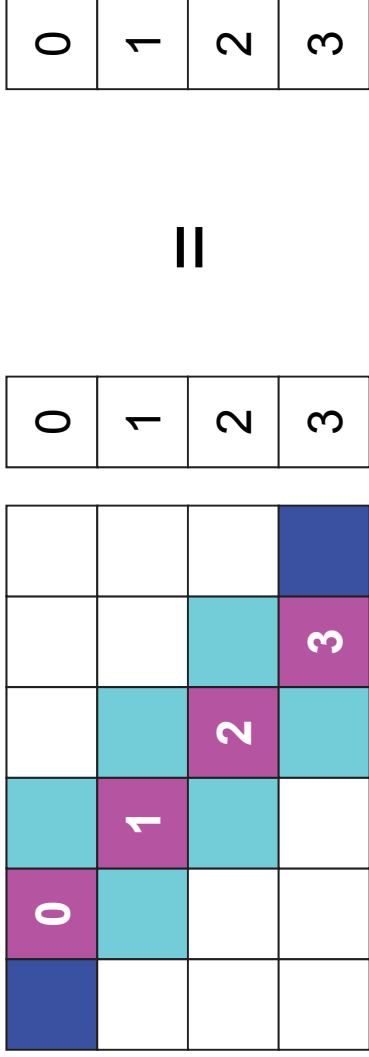
# We really need these parts



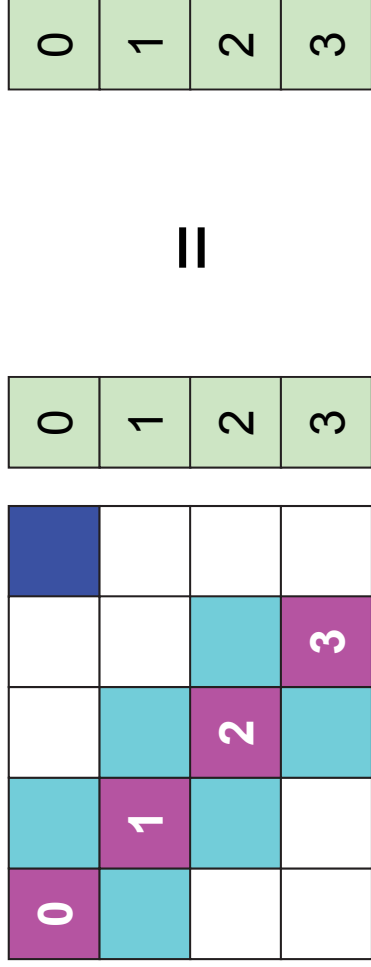
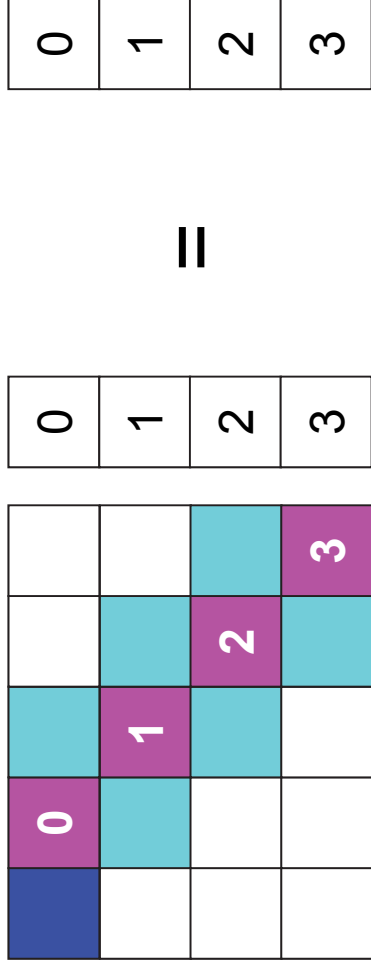
# Mat-Vec Products: Local Op. #0



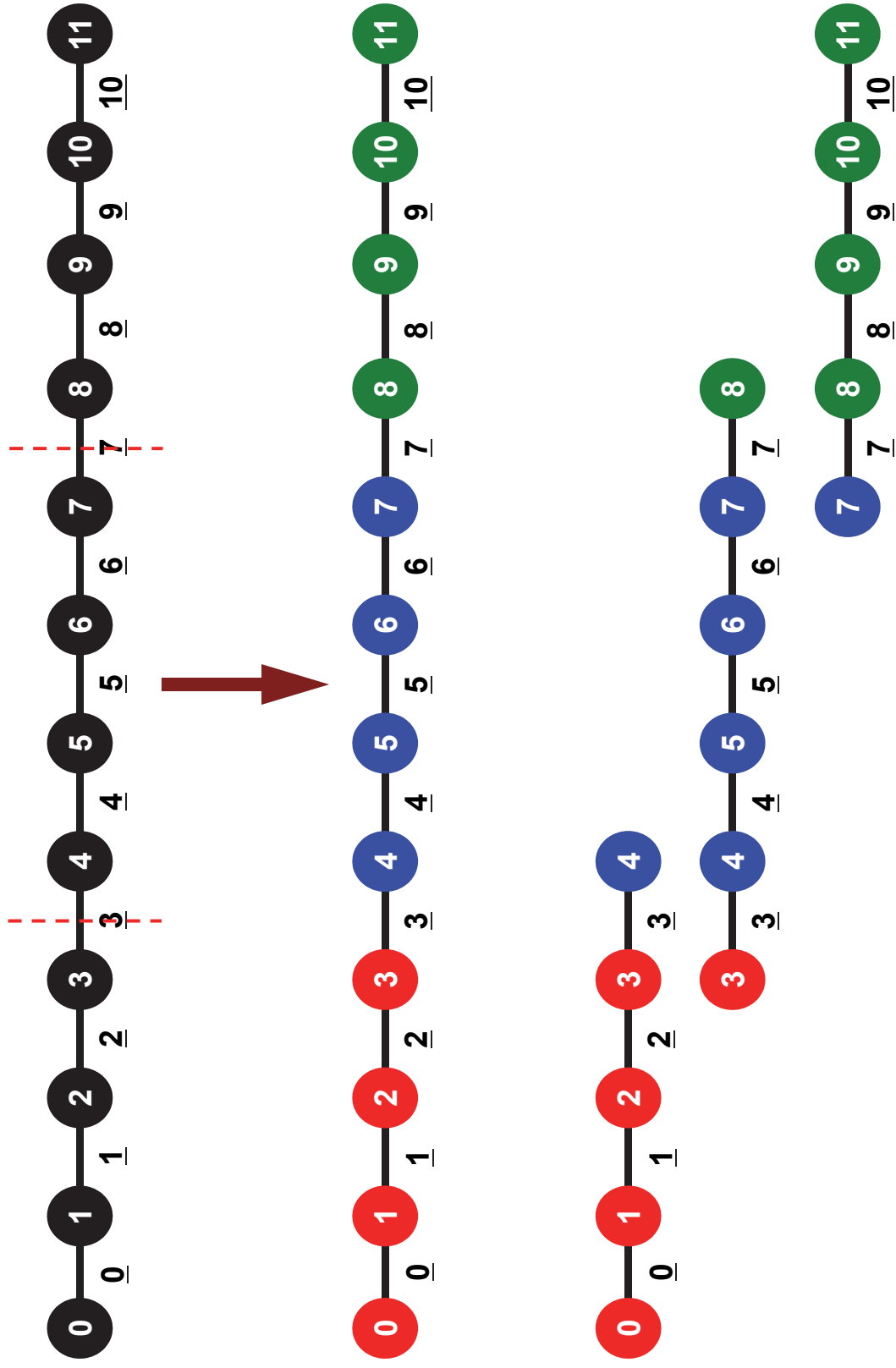
# Mat-Vec Products: Local Op. #1



# Mat-Vec Products: Local Op. #2

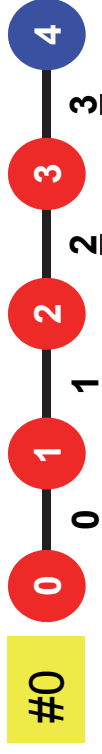


# 1D FEM: 12 nodes/11 elem's/3 domains



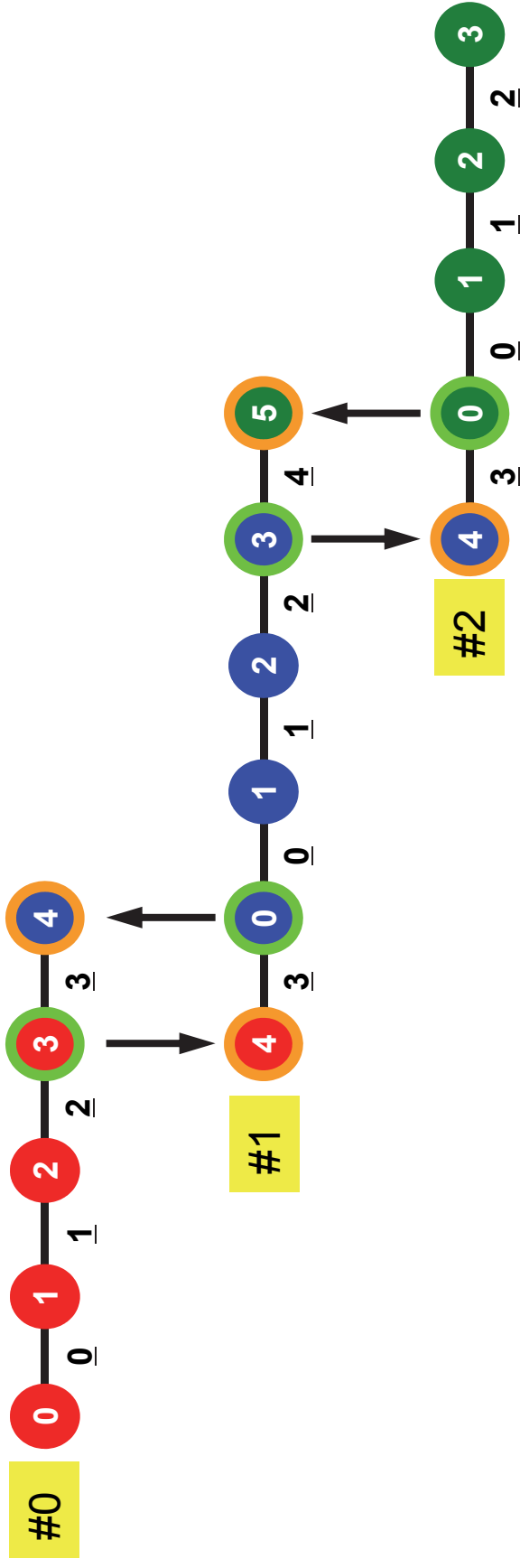
# 1D FEM: 12 nodes/11 elem's/3 domains

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



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

Internal/External Nodes

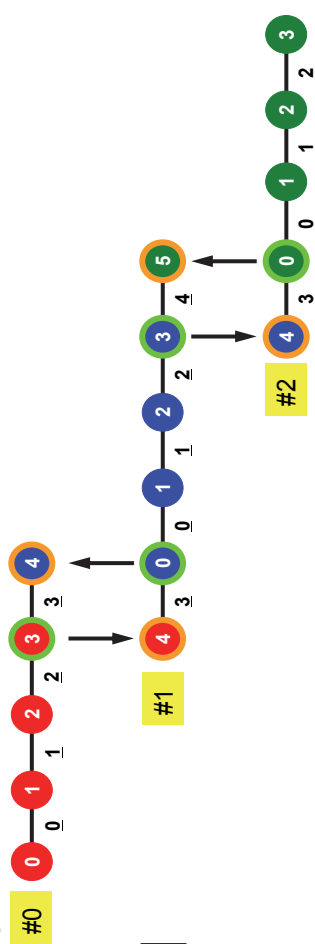


# What is Peer-to-Peer Communication ?

- 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

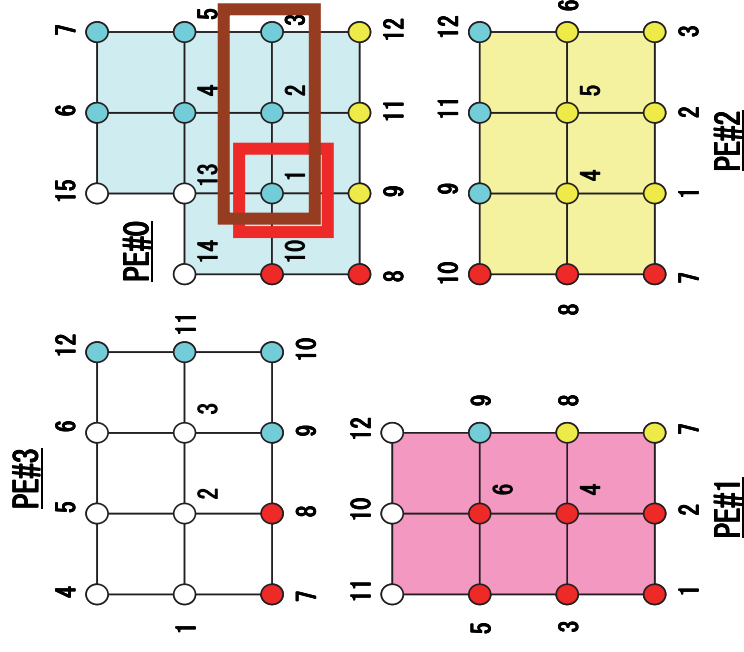
- MPI\_Send, MPI\_Receive
- Communication with limited processes
  - Neighbors
- Application Area
  - FEM, FDM: Localized Method



# 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 number of elements sent to each process
  - datatype I data type of elements of sending buffer
  - dest I rank of destination





# 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),  
communicator

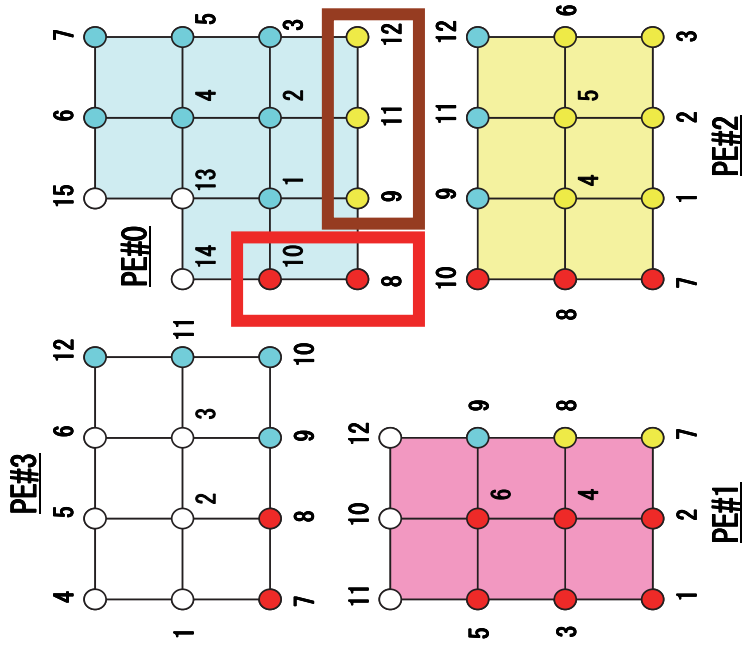
- `comm`            MPI\_Comm    I
- `request`        MPI\_Request    O

**communication request array used in `MPI_Waitall`**

# 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 `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),

communicator

- comm MPI\_Comm I

- request MPI\_Request O **communication request array used in `MPI_Waitall`**

# MPI\_Waitall



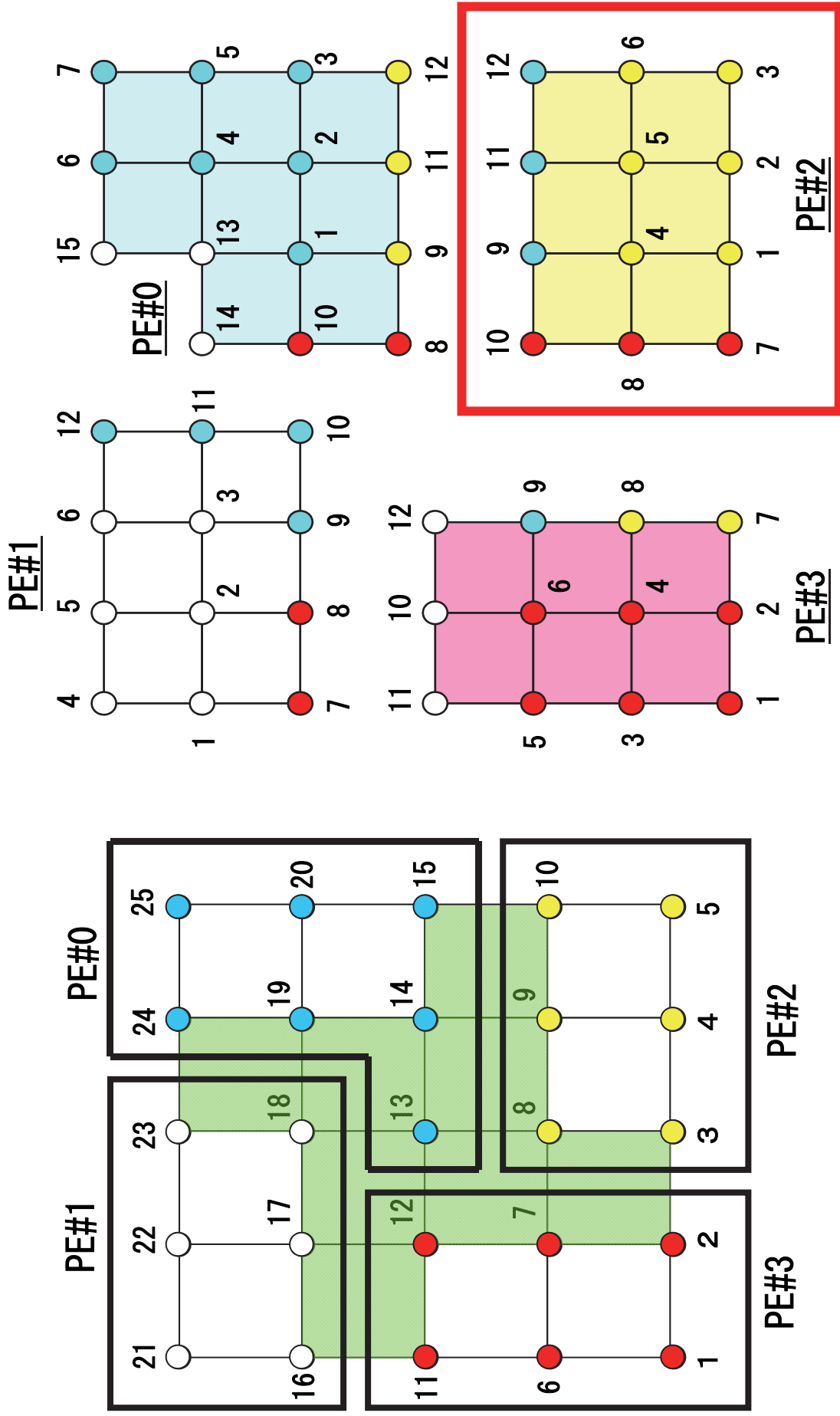
- **MPI\_Waitall** blocks until all comm's, associated with request in the array, complete. It is used for synchronizing MPI\_Isend and MPI\_Irecv in this class.
- At sending phase, contents of sending buffer cannot be modified before calling corresponding **MPI\_Waitall**. At receiving phase, contents 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 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.
- **MPI\_Waitall** (**count**, **request**, **status**)
 

|                  |             |     |                                                                     |
|------------------|-------------|-----|---------------------------------------------------------------------|
| – <u>count</u>   | int         | I   | number of processes to be synchronized                              |
| – <u>request</u> | MPI_Request | I/O | comm. request used in <b><u>MPI_Waitall</u></b> (array size: count) |
| – <u>status</u>  | MPI_Status  | O   | array of status objects                                             |

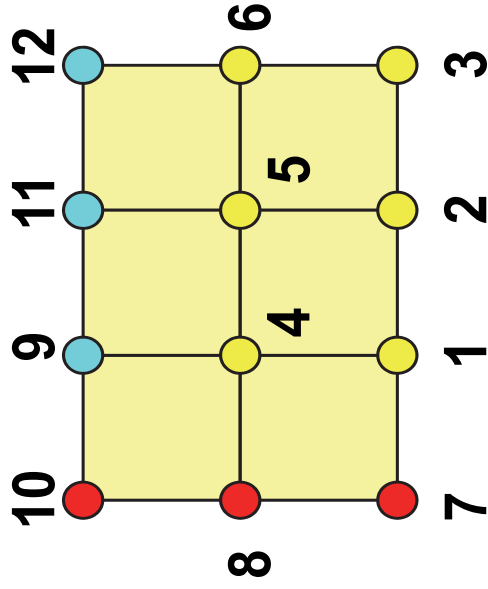
MPI STATUS SIZE: defined in 'mpi.h'

# Node-based Partitioning

## internal nodes - elements - external nodes



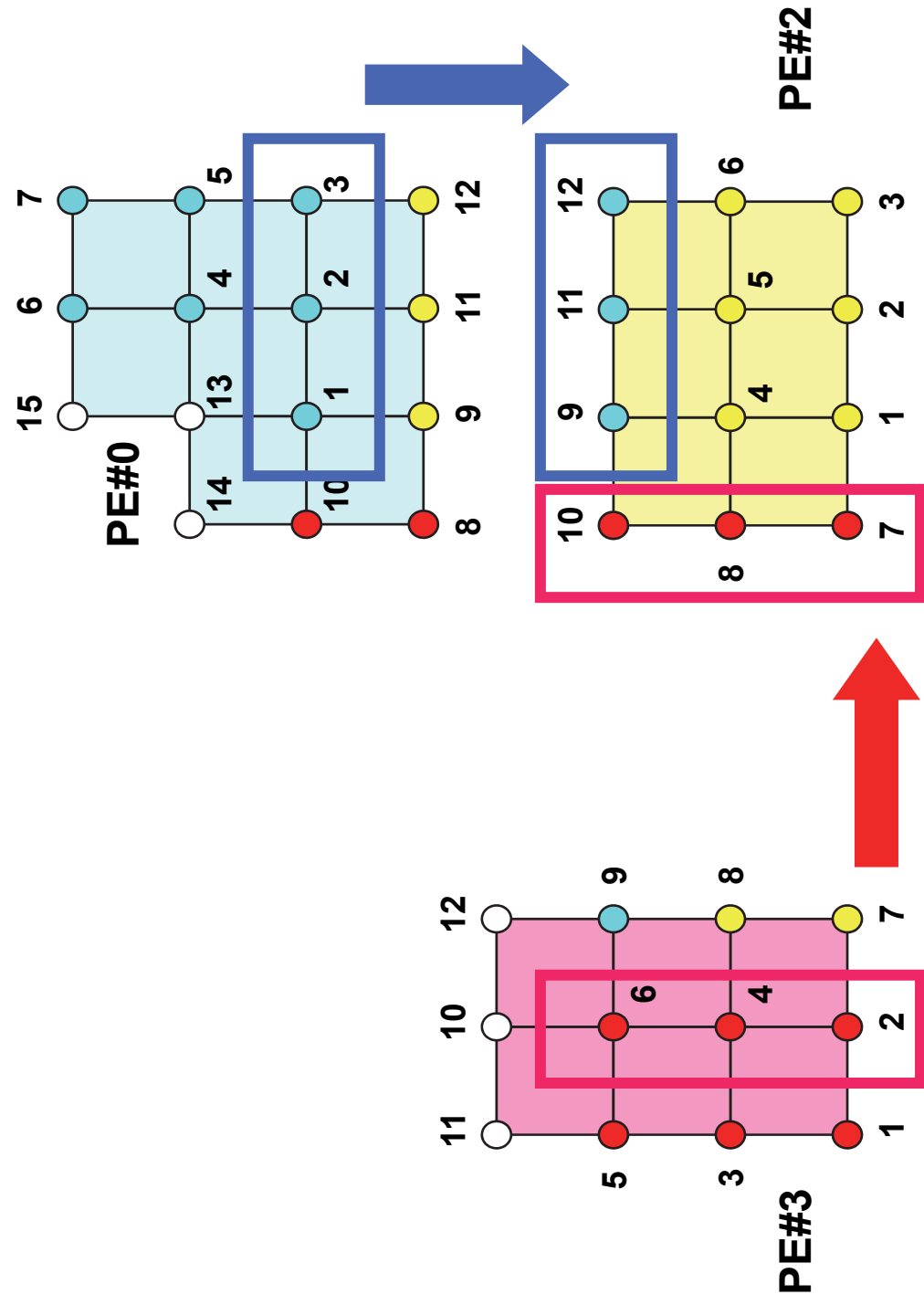
# Description of Distributed Local Data



- 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 ?

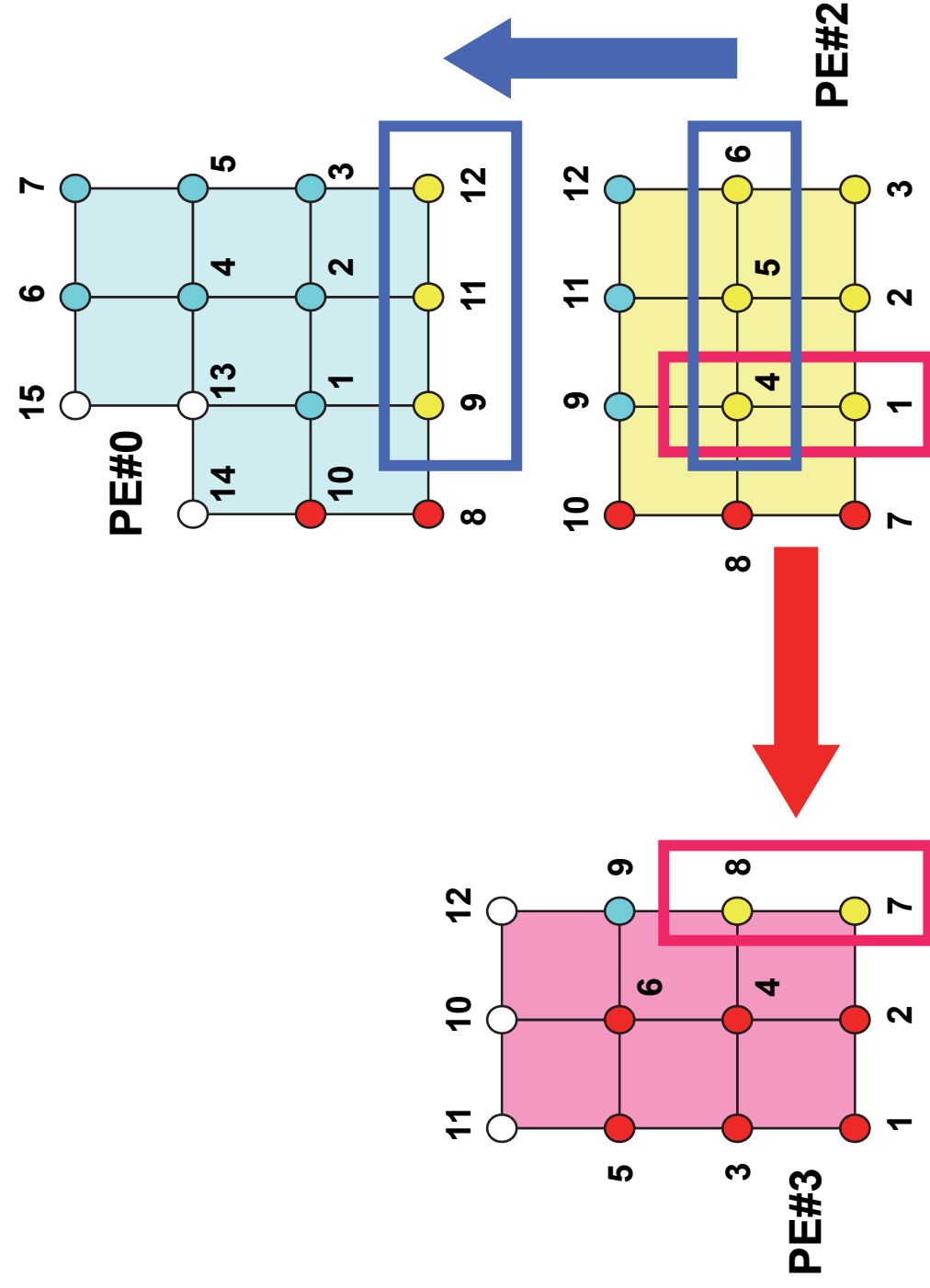
# External Nodes (外点) : RECEIVE

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