

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

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Technical & Scientific Computing II (4820-1028)
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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

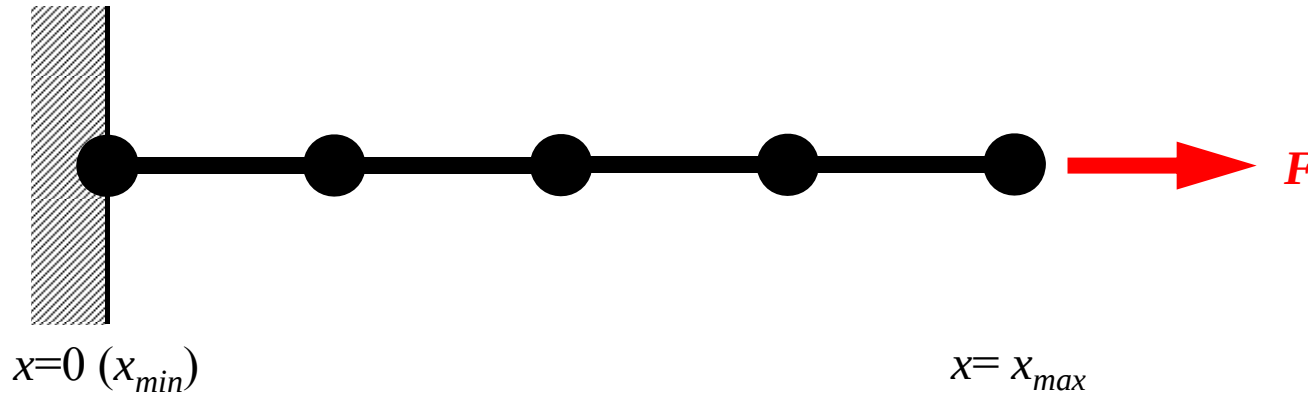
- 1D Static Linear Elastic Problems
- Galerkin Method
- Linear Element
- Preconditioned Conjugate Gradient Method

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.)
 - $x=0$: $u=0$ (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

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

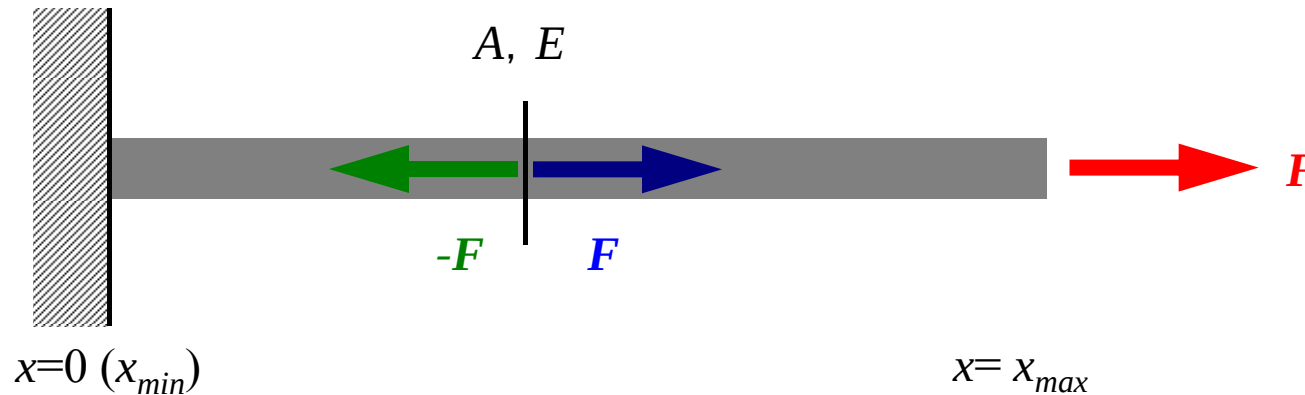
- calc. strain

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

- 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 = ε) $u = 2.5 @ x = x_{max}$

1D Linear Element (1/4)

一次元線形要素

- 1D Linear Element

- Length = L

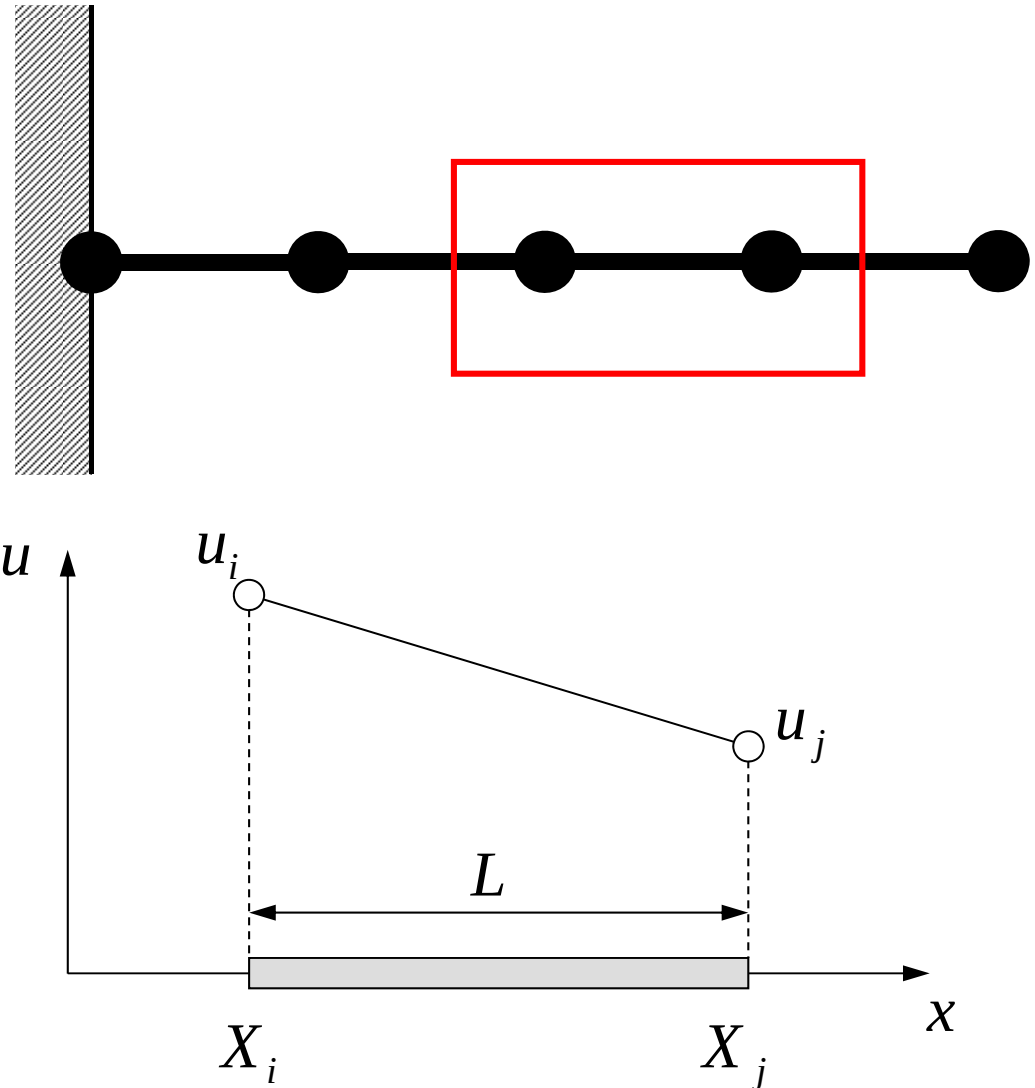
- Node (Vertex)
- Element

- u_i Displacement at i

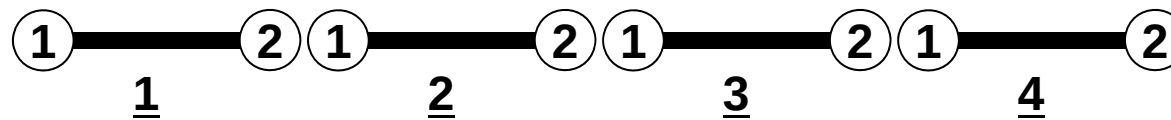
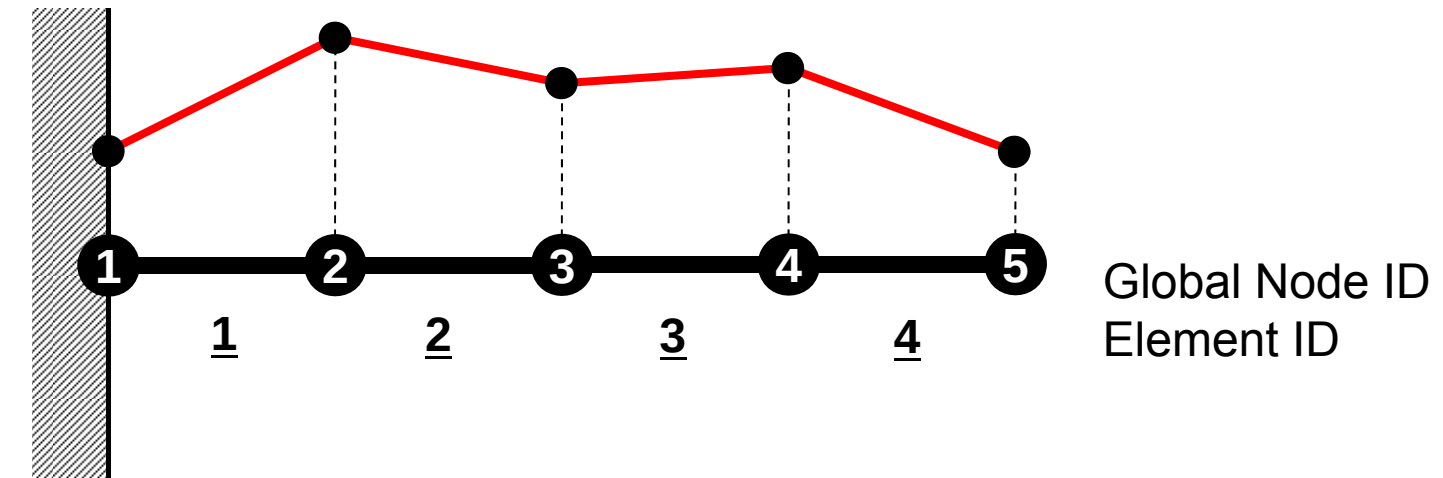
- u_j Displacement at j

- Displacement u on each element is linear function of x (Piecewise Linear):

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



Piecewise Linear



Local Node ID
for each elem.

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

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

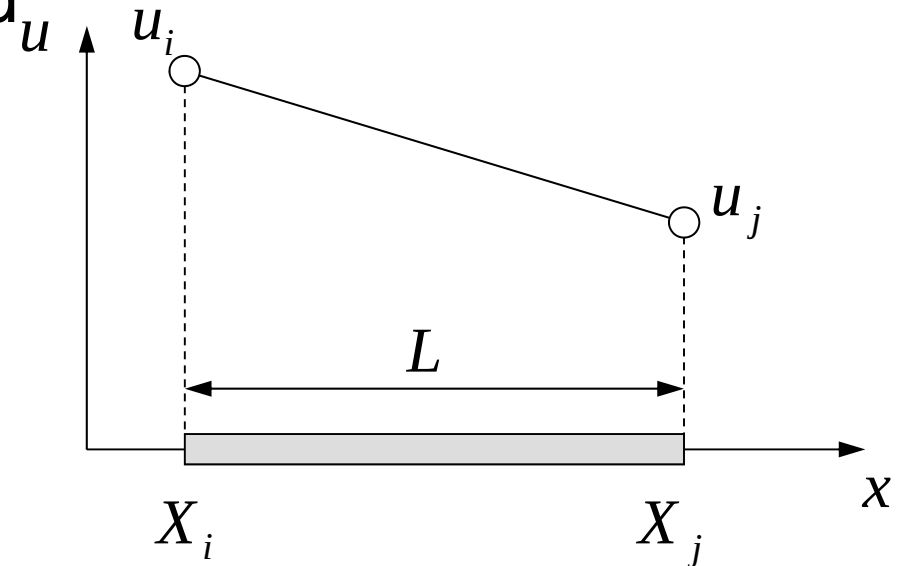
- Coef's are calculated based on info. at each node

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

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

- 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 :

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

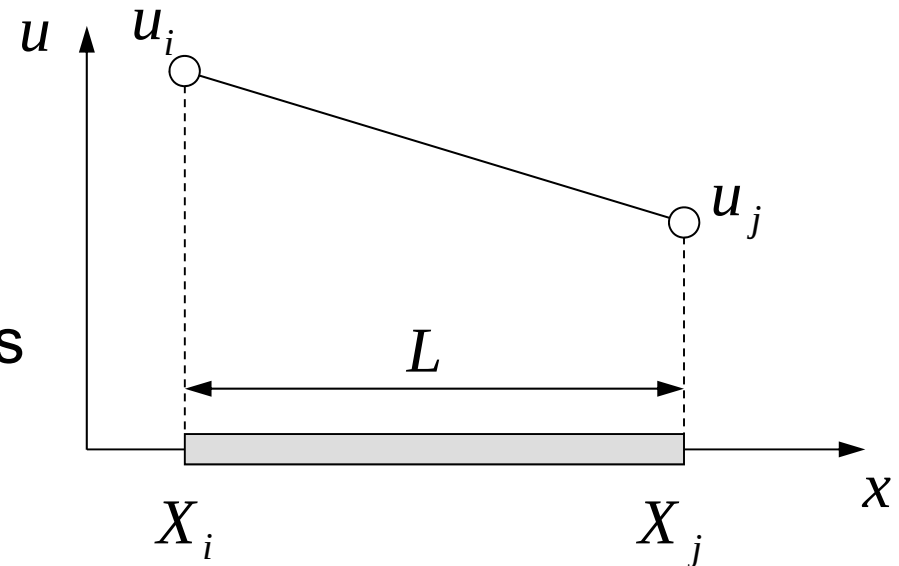
N_i, N_j

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

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

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

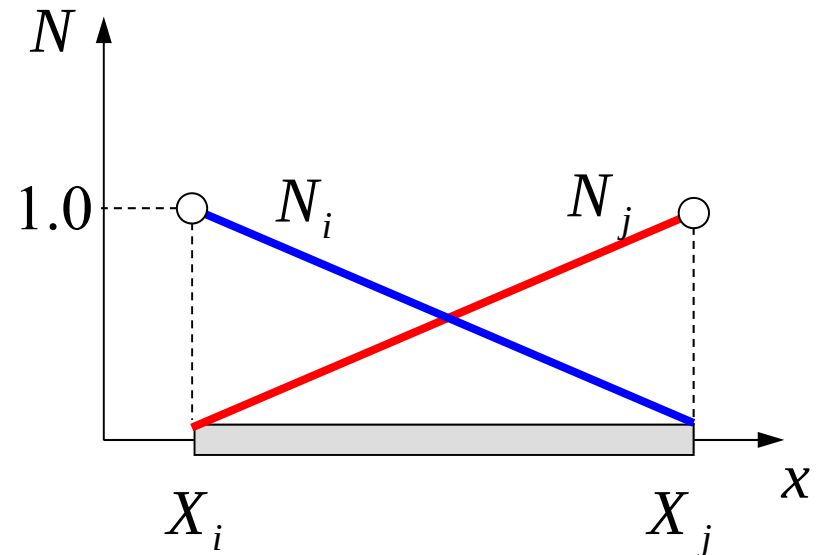
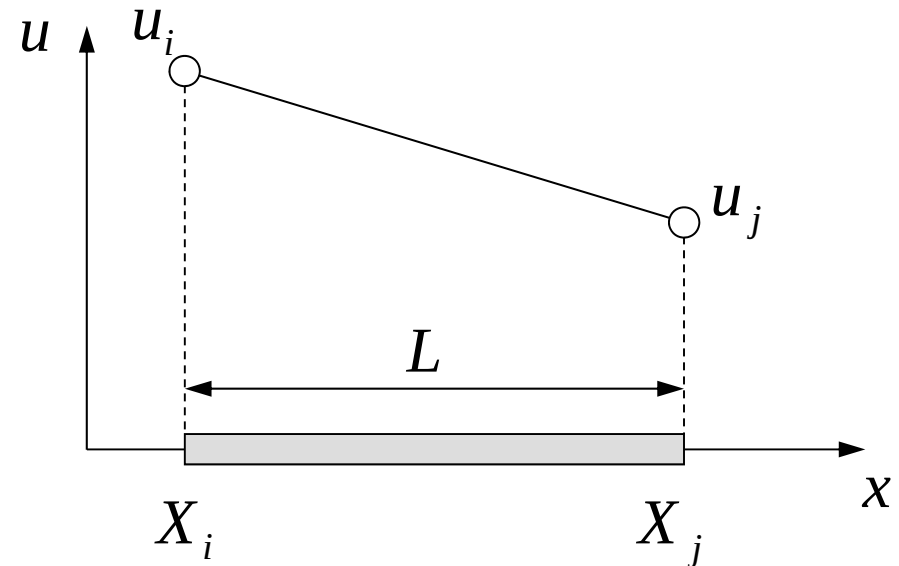
Ψ_i Trial/Test Function (known function of position, defined in domain and at boundary. “Basis” in linear algebra.)

a_i Coefficients (unknown)

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

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

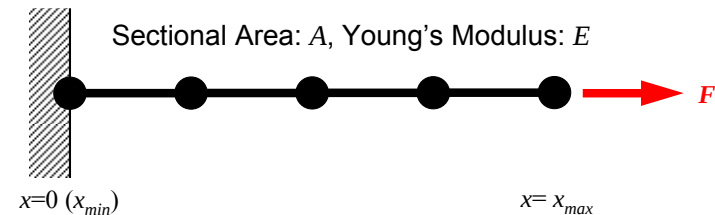
$$N_i = \left(\frac{X_j - x}{L} \right), \quad N_j = \left(\frac{x - X_i}{L} \right)$$



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), ϕ : Displacement at Each Node

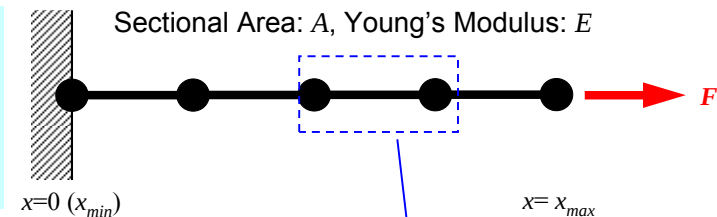
- Following integral equation is obtained at each element by Galerkin method, where $[N]$'s are also weighting functions:

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

Galerkin Method (2/4)

- Green's Theorem (1D)

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



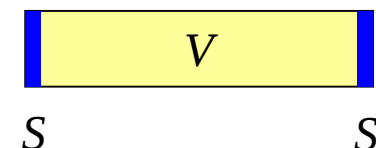
- Apply this to the 1st part of eqn with 2nd-order diff.:

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

- Consider the following terms:

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

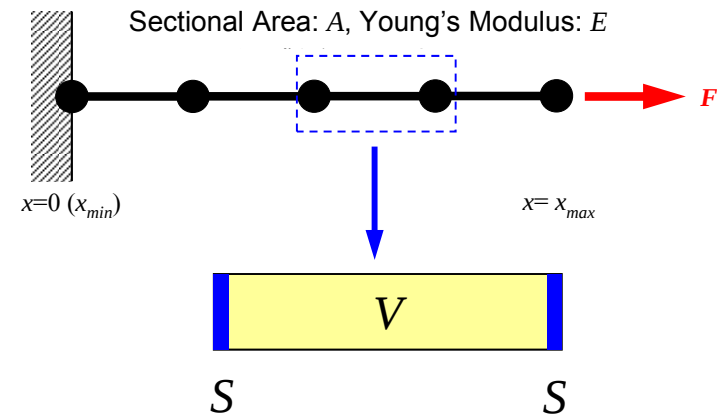
Stress on Surfaces
of Each Element



Galerkin Method (3/4)

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

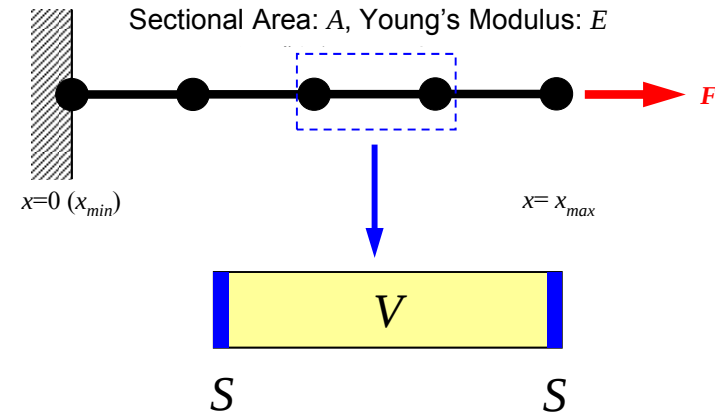
$$-\int_V E \left(\frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV \cdot \{\phi\} + \int_S \bar{\sigma} [N]^T dS + \int_V X [N]^T dV = 0$$



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

Galerkin Method (4/4)

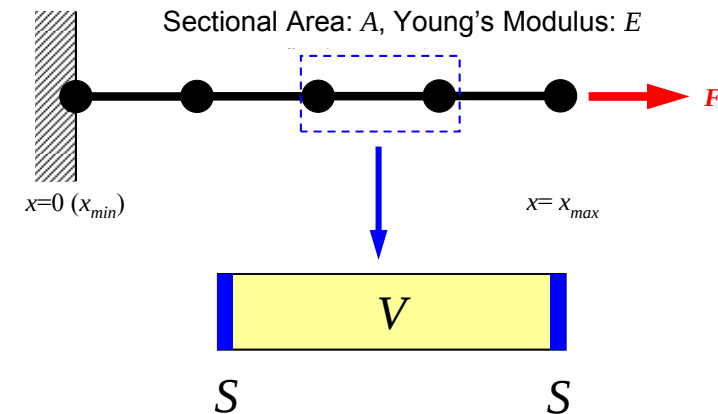
$$\begin{aligned}
 & - \int_V E \left(\frac{d[N]^T}{dx} \frac{d[N]}{dx} \right) dV \cdot \{\phi\} \\
 & + \int_S \bar{\sigma} [N]^T dS + \int_V X [N]^T dV = 0
 \end{aligned}$$



- 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)



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

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

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: $[k]$

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

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

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

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

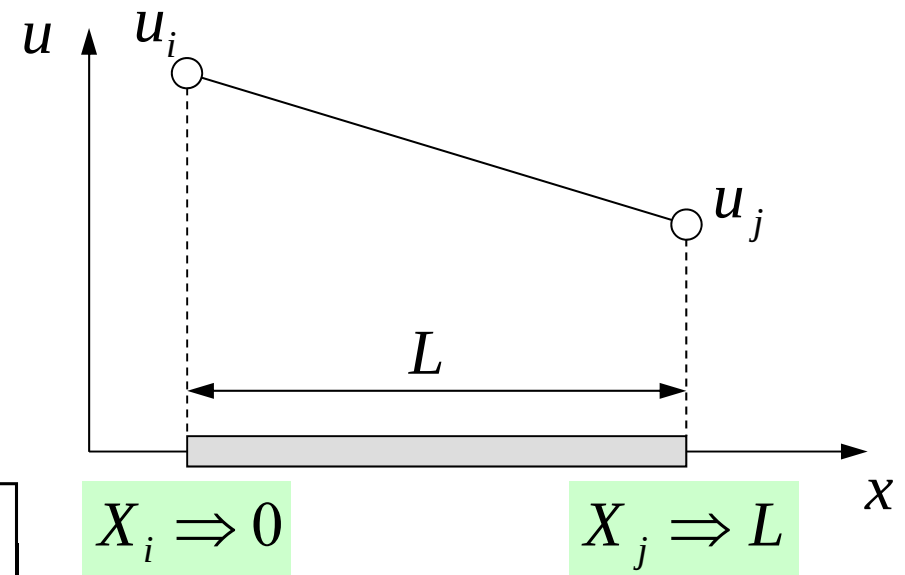
2x1 matrix

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



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

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)

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

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

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

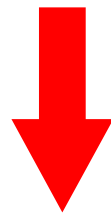


when surface force acts on only this surface.

Global Equations

- Accumulate Element Equations:

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



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

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

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

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
```

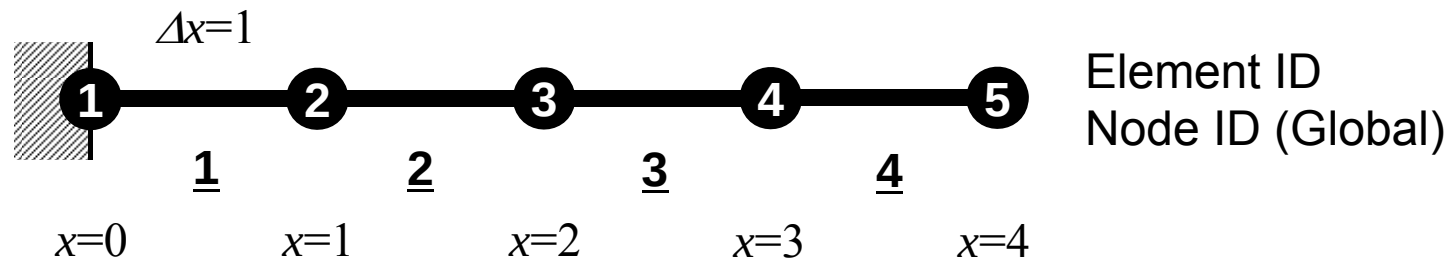
Control Data input.dat

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

NE (Number of Elements)
 Δx (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)
```

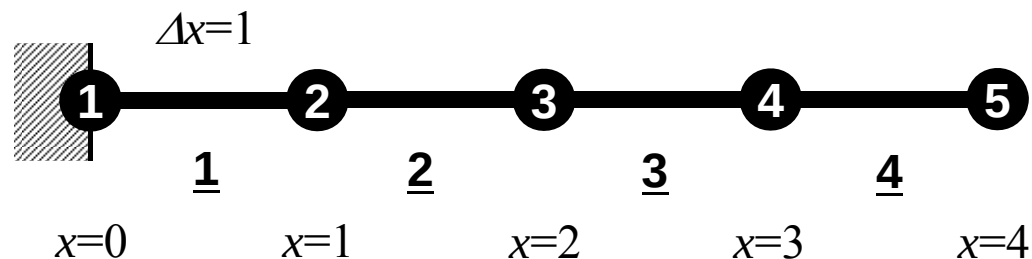
```
1      0.000000E+00
2      1.000000E+00
3      2.000000E+00
4      3.000000E+00
5      4.000000E+00
```

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

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

```
### STRESS      at each element (computed, theoretical)
```

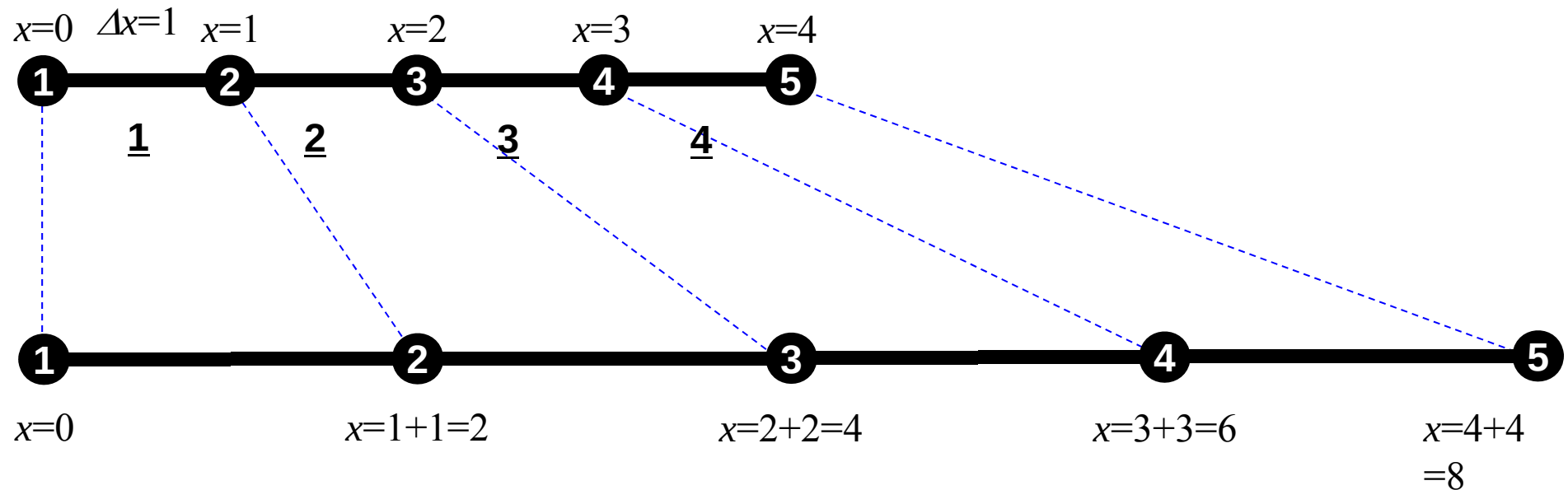
```
1      1.000000E+00      1.000000E+00
2      1.000000E+00      1.000000E+00
3      1.000000E+00      1.000000E+00
4      1.000000E+00      1.000000E+00
```



Element ID
Node ID (Global)

Strain=1.00 (100%)

Length of each element is doubled compared to initial condition

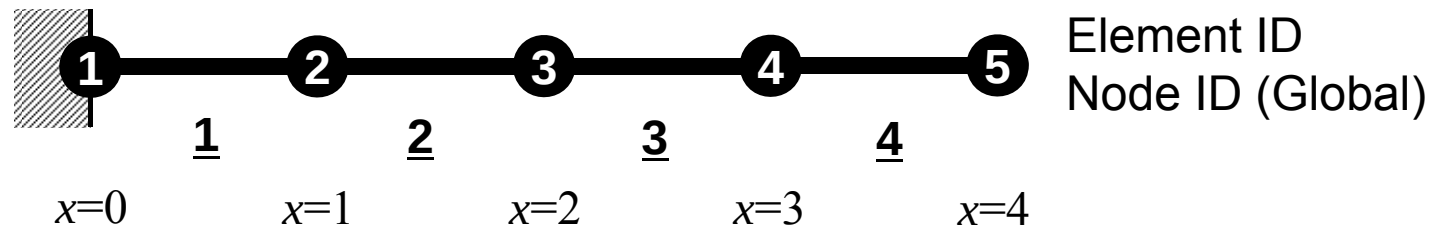


DISPLACEMENT at each node (computed)

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:

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

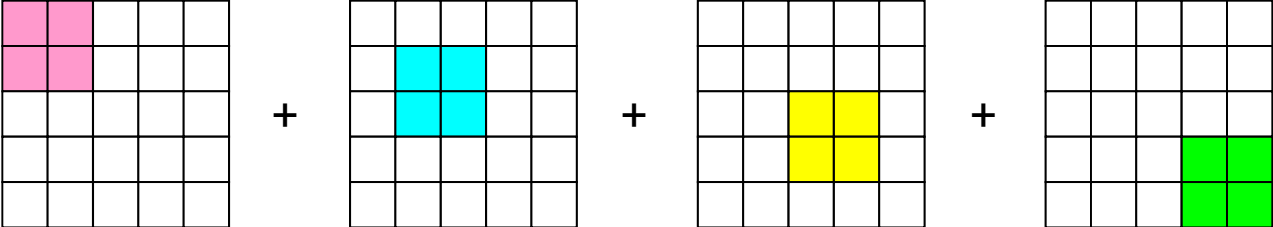
$X=0$ in this case

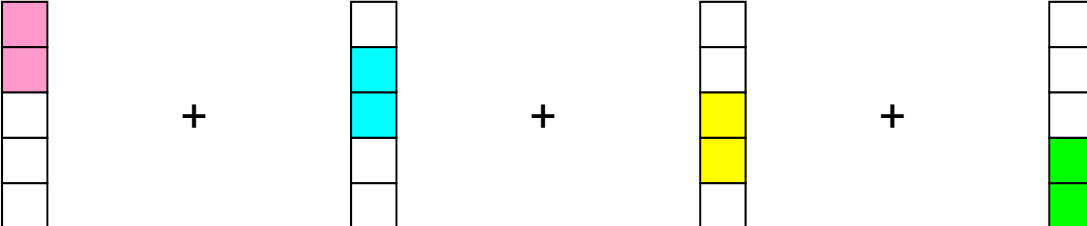
- As for Element-4:

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

Element Eqn's/Accumulation (2/3)

- Element-by-Element Accumulation:

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


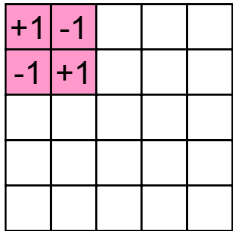
$$\{F\} = \sum_{e=1}^4 \{f\}^{(e)} =$$


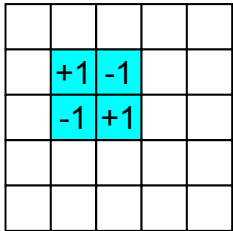
Element-by-Element Operation

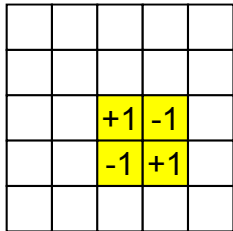
very flexible if each element has different material property, size, etc.

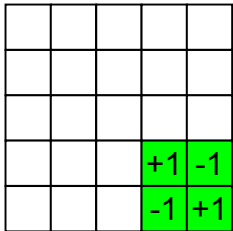
$$[k]^{(e)} = \frac{E^{(e)} A^{(e)}}{L^{(e)}} \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix}$$

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


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

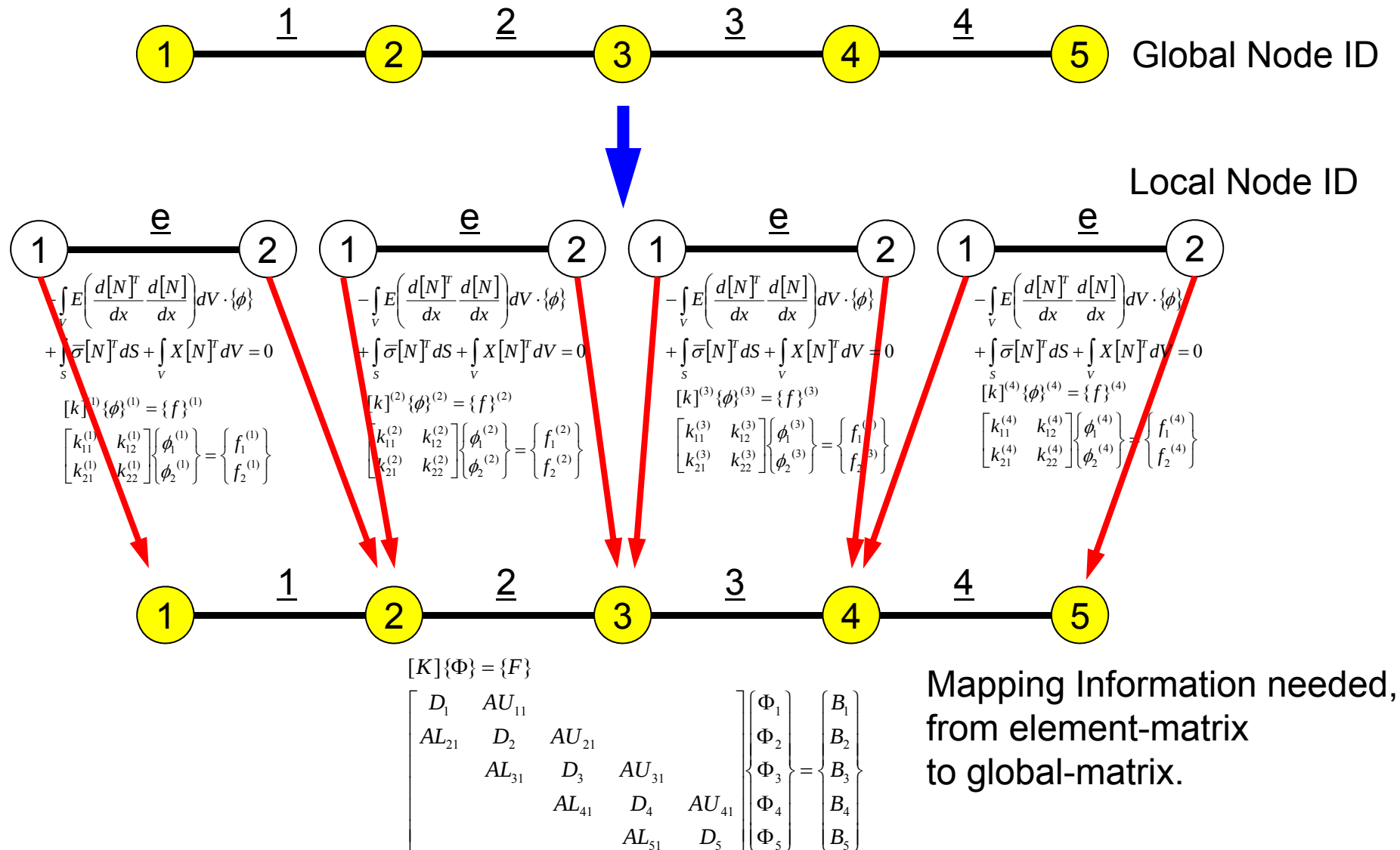

 $\times \frac{E^{(2)} A^{(2)}}{L^{(2)}}$


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


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

+

Element/Global Operations



- 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 $\mathbf{Ax}=\mathbf{b}$ 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, α_i : coefficient
 - Solution $\{x\}$ minimizes $\{x-y\}^T[A]\{x-y\}$, where $\{y\}$ is exact solution.

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

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

α_i : Scalar

Preconditioning for Iterative Solvers

- Convergence rate of iterative solvers strongly depends on the spectral properties (eigenvalue distribution) of the coefficient matrix $\mathbf{A}$.
 - It is preferable that distribution is small, and eigenvalues are (close to) 1 $\rightarrow$ identity matrix
- A preconditioner $\mathbf{M}$ transforms the linear system into one with more favorable spectral properties
 - In "ill-conditioned" problems, "condition number" (ratio of max/min eigenvalue if $\mathbf{A}$ is symmetric) is large.
 - $\mathbf{M}$ transforms original equation $\mathbf{Ax}=\mathbf{b}$ into $\mathbf{A'x}=\mathbf{b'}$ where $\mathbf{A'}=\mathbf{M}^{-1}\mathbf{A}$, $\mathbf{b'}=\mathbf{M}^{-1}\mathbf{b}$
 - Therefore if $\mathbf{M}^{-1}\sim\mathbf{A}^{-1}$, this is the best preconditioner (a.k.a. Gaussian Elimination)

Preconditioned CG Solver

```

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

```

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 $[M]z^{(i-1)} = r^{(i-1)}$** 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

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

- 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
N	I	-	# Unknowns
NPLU	I	-	# Non-Zero Off-Diagonal Components
Diag(:)	R	N	Diagonal Components
U(:)	R	N	Unknown Vector
Rhs(:)	R	N	RHS Vector
Index(:)	I	0:N N+1	Off-Diagonal Components (Number of Non-Zero Off-Diagonals at Each ROW)
Item(:)	I	NPLU	Off-Diagonal Components (Corresponding Column ID)
AMat(:)	R	NPLU	Off-Diagonal Components (Value)

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

Mat-Vec. Multiplication for Sparse Matrix

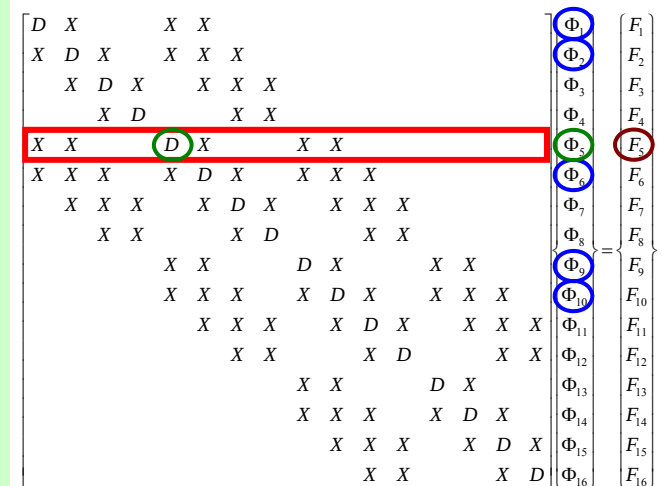
Compressed Row Storage (CRS)

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 ⊙	2.4 ①,0	3.2 ④,1		
1	3.6 ①	4.3 ⊙,2	2.5 ③,3	3.7 ⑤,4	9.1 ⑦,5
2	5.7 ②	1.5 ④,6	3.1 ⑥,7		
3	9.8 ③	4.1 ①,8	2.5 ④,9	2.7 ⑤,10	
4	11.5 ④	3.1 ⊙,11	9.5 ①,12	10.4 ②,13	4.3 ⑥,14
5	12.4 ⑤	6.5 ②,15	9.5 ⑥,16		
6	23.1 ⑥	6.4 ①,17	2.5 ②,18	1.4 ⑤,19	13.1 ⑦,20
7	51.3 ⑦	9.5 ①,21	1.3 ②,22	9.6 ③,23	3.1 ⑤,24

Diag (i) Diagonal Components (REAL, i=1~N)
Index(i) Number of Non-Zero Off-Diagonals at Each ROW (INT, i=0~N)
Item(k) Off-Diagonal Components (Corresponding Column ID) (INT, k=1, index(N))
AMat (k) Off-Diagonal Components (Value) (REAL, k=1, 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[Item[k]];
    }
}
```

- 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

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
//
//  $d/dx(E dU/dx) + F = 0$ 
//  $U=0@x=0$ 
*/

#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
NE	I		I	# Element
N	I		0	# Node
NPLU	I		0	# Non-Zero Off-Diag. Components
IterMax	I		I	MAX Iteration Number for CG
errno	I		0	ERROR flag
R, Z, Q, P, DD	I		0	Name of Vectors in CG
dX	R		I	Length of Each Element
Resid	R		0	Residual for CG
Eps	R		I	Convergence Criteria for CG
Area	R		I	Sectional Area of Element
F	R		I	Axial Force F at X=Xmax
Young	R		I	Young's Modulus
X1, X2, U1, U2	R		0	Location/Displacement at Local Nodes

Variable/Arrays (2/2)

Name	Type	Size	I/O	Definition
DL, Ck	R		0	Coef's for Element Matrix
Strain, Stress	R		0	Element Strain, Element Stress
X	R	N	0	Location of Each Node
U	R	N	0	Displacement of Each Node
Rhs	R	N	0	RHS Vector
Diag	R	N	0	Diagonal Components
W	R	[4][N]	0	Work Array for CG
Amat	R	NPLU	0	Off-Diagonal Components (Value)
Index	I	N+1	0	Number of Non-Zero Off-Diagonals at Each ROW
Item	I	NPLU	0	Off-Diagonal Components (Corresponding Column ID)
Icelnod	I	2*NE	0	Node ID for Each Element
Kmat	R	[2][2]	0	Element Matrix [k]
Emat	R	[2][2]	0	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 %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

1.0 1.0 1.0 1.0

100

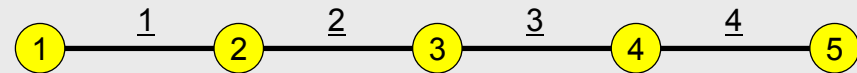
1.e-8

NE (Number of Elements)

Δx (Length of Each Elem.: **L**), **F**, **A**, **E**

Number of MAX. Iterations for CG Solver

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 %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));
```

```

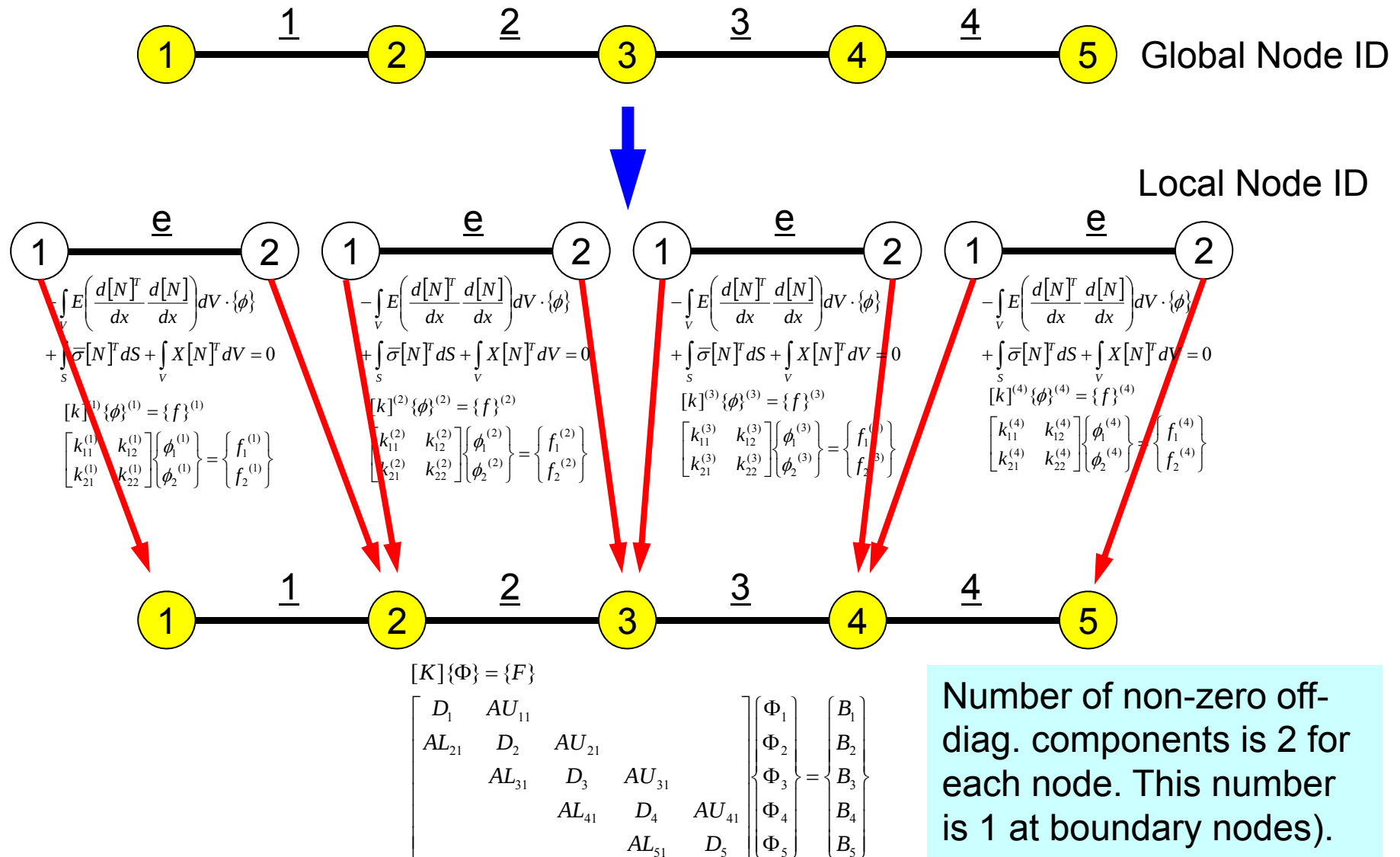
Rhs = calloc(N, sizeof(double));
Index= calloc(N+1, sizeof(int));
Item = calloc(2*N-2, sizeof(int));

```

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

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

Element/Global Operations



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 %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(icel=0; icel<NE; icel++) {
    Icelnod[2*icel] = icel;
    Icelnod[2*icel+1] = icel+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(icel=0; icel<NE; icel++) {
    Icelnod[2*icel] = icel;
    Icelnod[2*icel+1] = icel+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;
    }
}

```

```

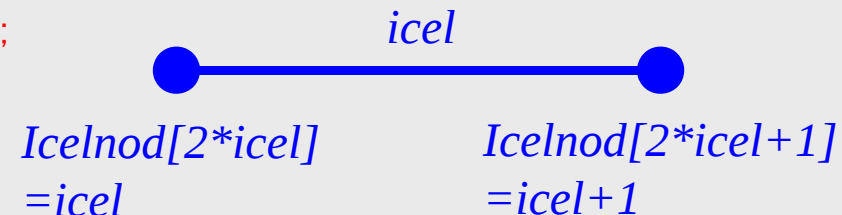
for(i=0; i<N; i++) U[i] = 0.0;
for(i=0; i<N; i++) Diag[i] = 0.0;
for(i=0; i<N; i++) Rhs[i] = 0.0;
for(k=0; k<2*N-2; k++) AMat[k] = 0.0;
for(i=0; i<N; i++) X[i] = i*dX;
for(icel=0; icel<NE; icel++) {
    Icelnod[2*icel] = icel;
    Icelnod[2*icel+1] = icel+1;
}

```

```

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(icel=0; icel<NE; icel++) {
    Icelnod[2*icel] = icel;
    Icelnod[2*icel+1] = icel+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:

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

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

$(\text{Index}[i])^{\text{th}} \sim (\text{Index}[i+1])^{\text{th}}$:

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 == N-1) {
        Item[jS] = i-1;
    } else {
        Item[jS] = i-1;
        Item[jS+1] = i+1;
    }
}

```

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

$(\text{Index}[i])^{\text{th}} \sim (\text{Index}[i+1])^{\text{th}}$:
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);

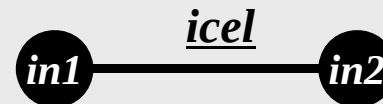
    Ck= Area*Young/DL;
    Emat[0][0]= Ck*Kmat[0][0];
    Emat[0][1]= Ck*Kmat[0][1];
    Emat[1][0]= Ck*Kmat[1][0];
    Emat[1][1]= Ck*Kmat[1][1];

    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];
}

```



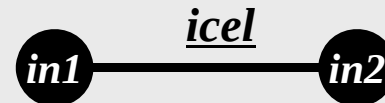
Program: 1d.c (5/7)

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];

```

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

```

    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);

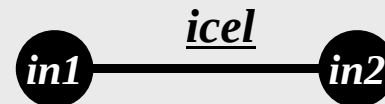
    Ck= Area*Young/DL;
    Emat[0][0]= Ck*Kmat[0][0];
    Emat[0][1]= Ck*Kmat[0][1];
    Emat[1][0]= Ck*Kmat[1][0];
    Emat[1][1]= Ck*Kmat[1][1];

    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];
}

```



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

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);

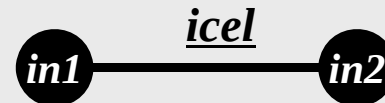
    Ck= Area*Young/DL;
    Emat[0][0]= Ck*Kmat[0][0];
    Emat[0][1]= Ck*Kmat[0][1];
    Emat[1][0]= Ck*Kmat[1][0];
    Emat[1][1]= Ck*Kmat[1][1];

    Diag[in1]= Diag[in1] + Emat[0][0];
    Diag[in2]= Diag[in2] + Emat[1][1];

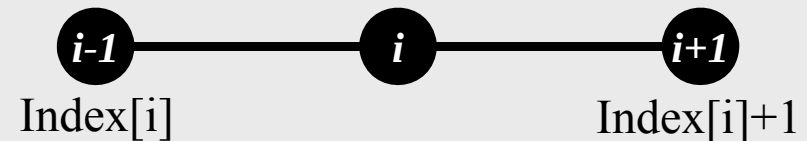
    if (icel==0) {k1=Index[in1];
    } else {k1=Index[in1]+1;
           k2=Index[in2];

    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



$$[Emat] = [k]^{(e)} = \frac{EA}{L} \begin{bmatrix} +1 & \textcircled{-1} \\ \textcircled{-1} & +1 \end{bmatrix} \begin{matrix} k1 \\ k2 \end{matrix}$$

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 $x=0$

$$u_1 = 0 \text{ (or } u_0 = 0)$$



- 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;

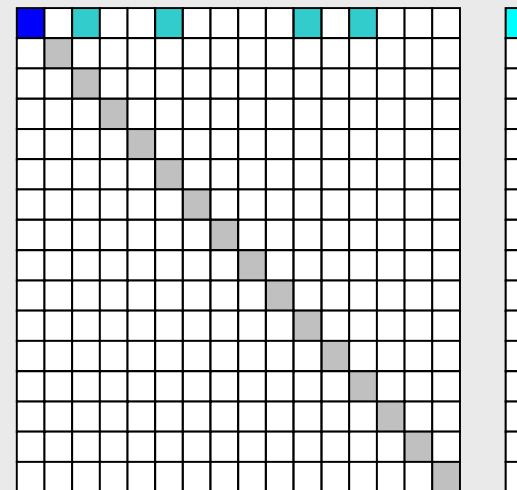
```

$$u_1=0$$

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;

```

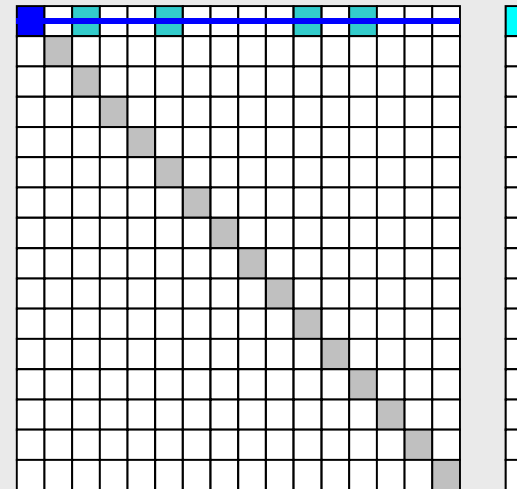
$$u_1=0$$

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;

```

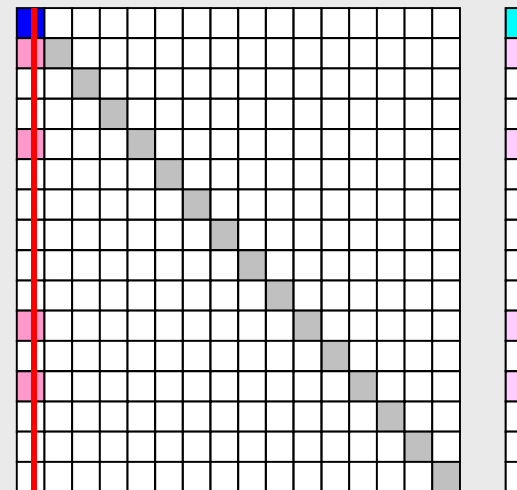
$$u_1=0$$

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;

```

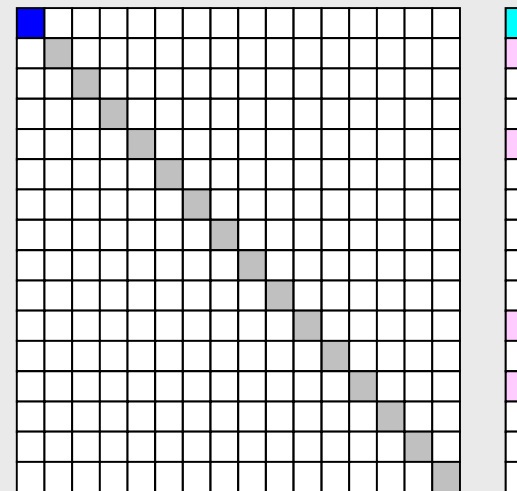
$$u_1=0$$

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;
```

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

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

$$Diag_j u_j + \sum_{k=Index[j], k \neq k_s}^{Index[j+1]} Amat_k u_{Item[k]}$$

$$= Rhs_j - Amat_{k_s} u_{Item[k_s]} = Rhs_j - Amat_{k_s} u_{\min} \quad \text{where } Item[k_s] = 0$$

Program: 1d.c (6/7)

Boundary Conditions

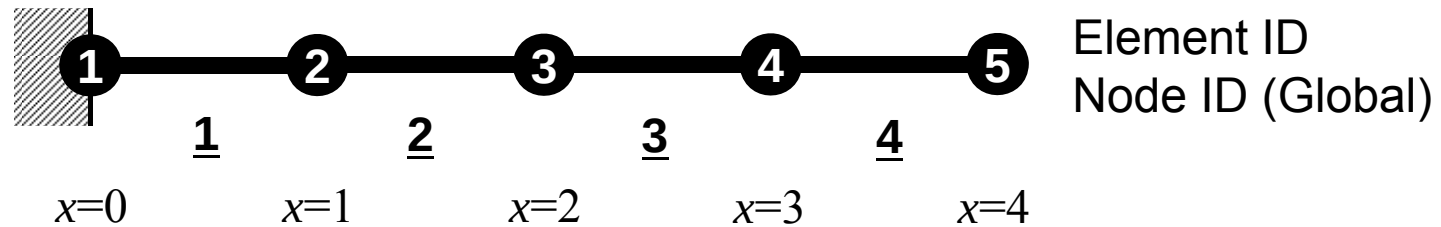
```
/*
// +-----+
// | BOUNDARY conditions |
// +-----+
*/

/* 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  $[M]z^{(i-1)} = r^{(i-1)}$ 
     $\rho_{i-1} = r^{(i-1)} z^{(i-1)}$ 
    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 $[M]z^{(i-1)} = r^{(i-1)}$** 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 (倒数) 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, ...
    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)

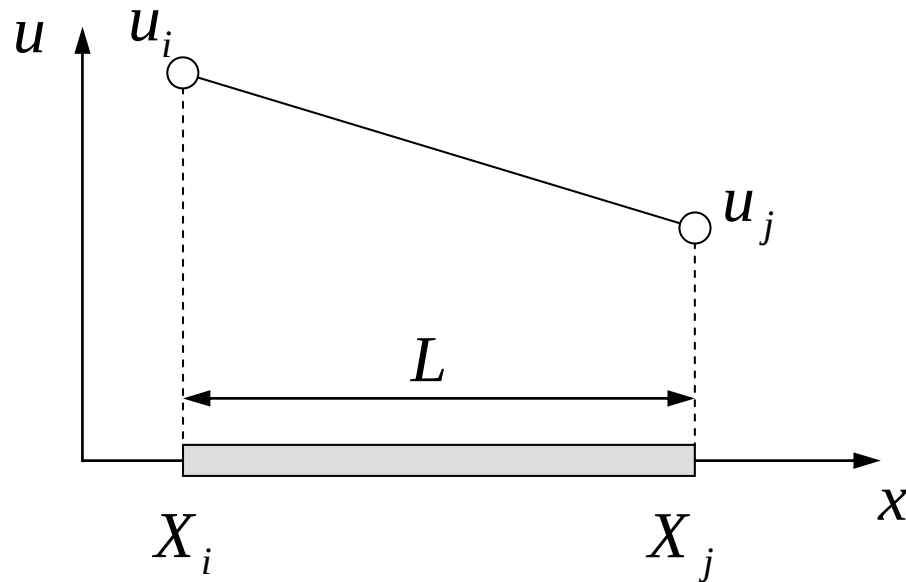
Element Stress

```
/*  
// +-----+  
// | STRESS recovery |  
// +-----+  
*/  
  
printf("\n%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%16.6E\n", icel+1, Sigma, F/Area);  
}
```

Element Stress

Constant for 1D linear element: Constant Strain

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



$$u = N_i u_i + N_j u_j$$

$$\begin{aligned} \varepsilon &= \frac{du}{dx} = \frac{d}{dx} (N_i u_i + N_j u_j) \\ &= \frac{dN_i}{dx} u_i + \frac{dN_j}{dx} u_j \\ &= \left(-\frac{1}{L} \right) u_i + \left(\frac{1}{L} \right) u_j = \boxed{\frac{u_j - u_i}{L}} \end{aligned}$$

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

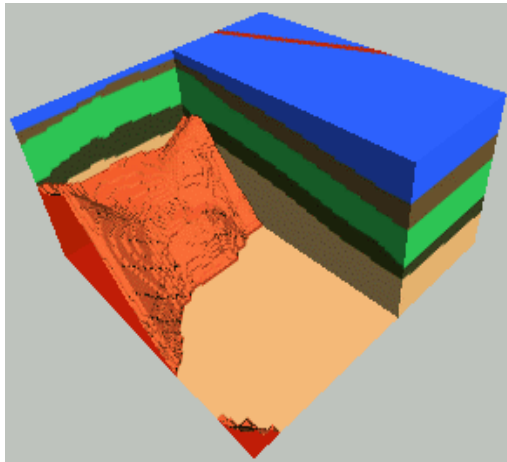
- Faster, Larger & More Complicated
- Scalability
 - Solving N^x scale problem using N^x computational resources during same computation time
 - for large-scale problems: Weak Scaling
 - e.g. CG solver: more iterations needed for larger problems
 - Solving a problem using N^x computational resources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

What is Parallel Computing ? (1/2)

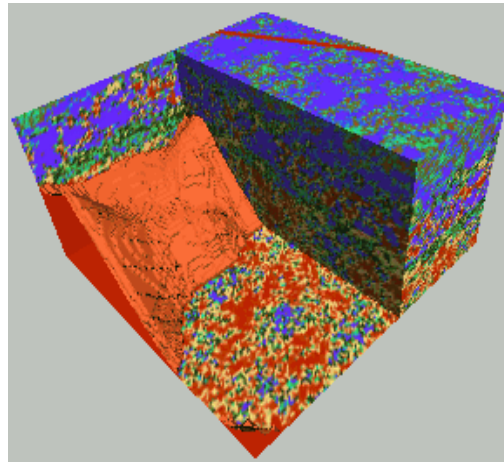
- to solve larger problems faster

Homogeneous/Heterogeneous Porous Media

Lawrence Livermore National Laboratory



Homogeneous

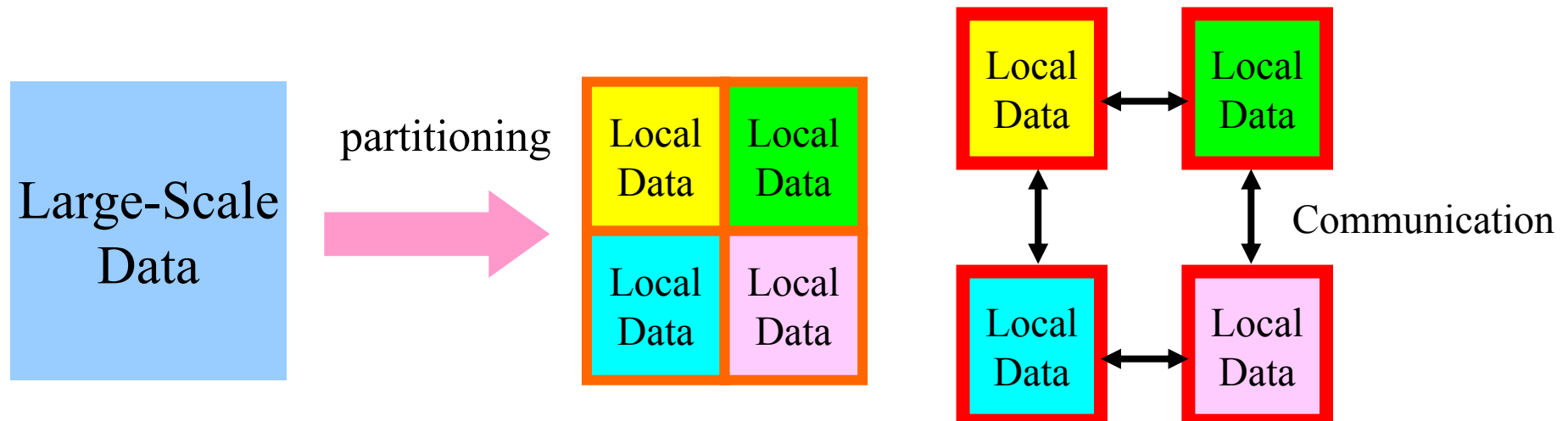


Heterogeneous

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.

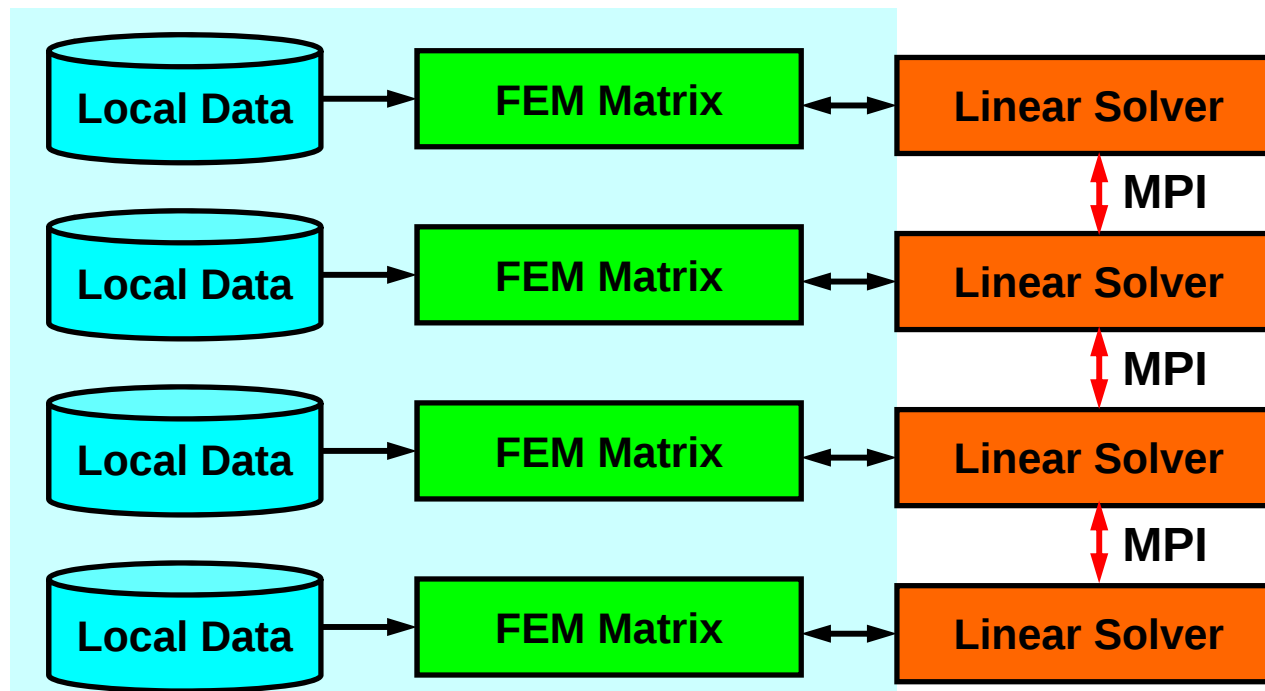
Operations in Parallel FEM

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

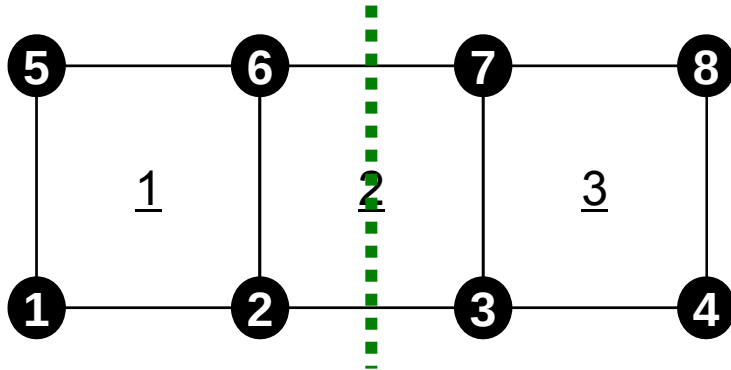


Parallel FEM Procedures

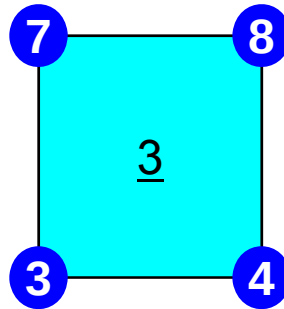
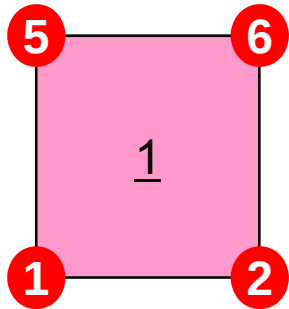
- Design on “Local Data Structure” is important
 - for SPMD-type operations in the previous page
- Matrix Generation
- Preconditioned Iterative Solvers for Linear Equations

Bi-Linear Square Elements

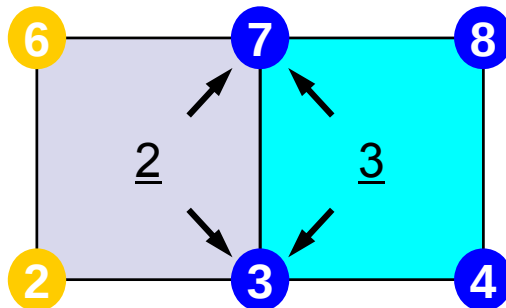
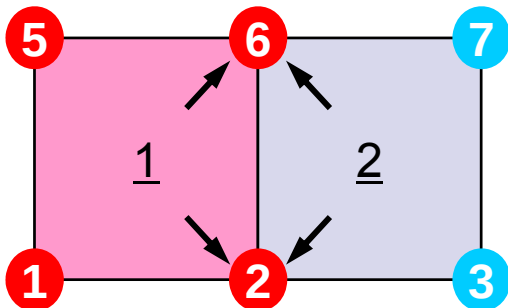
Values are defined on each node



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.

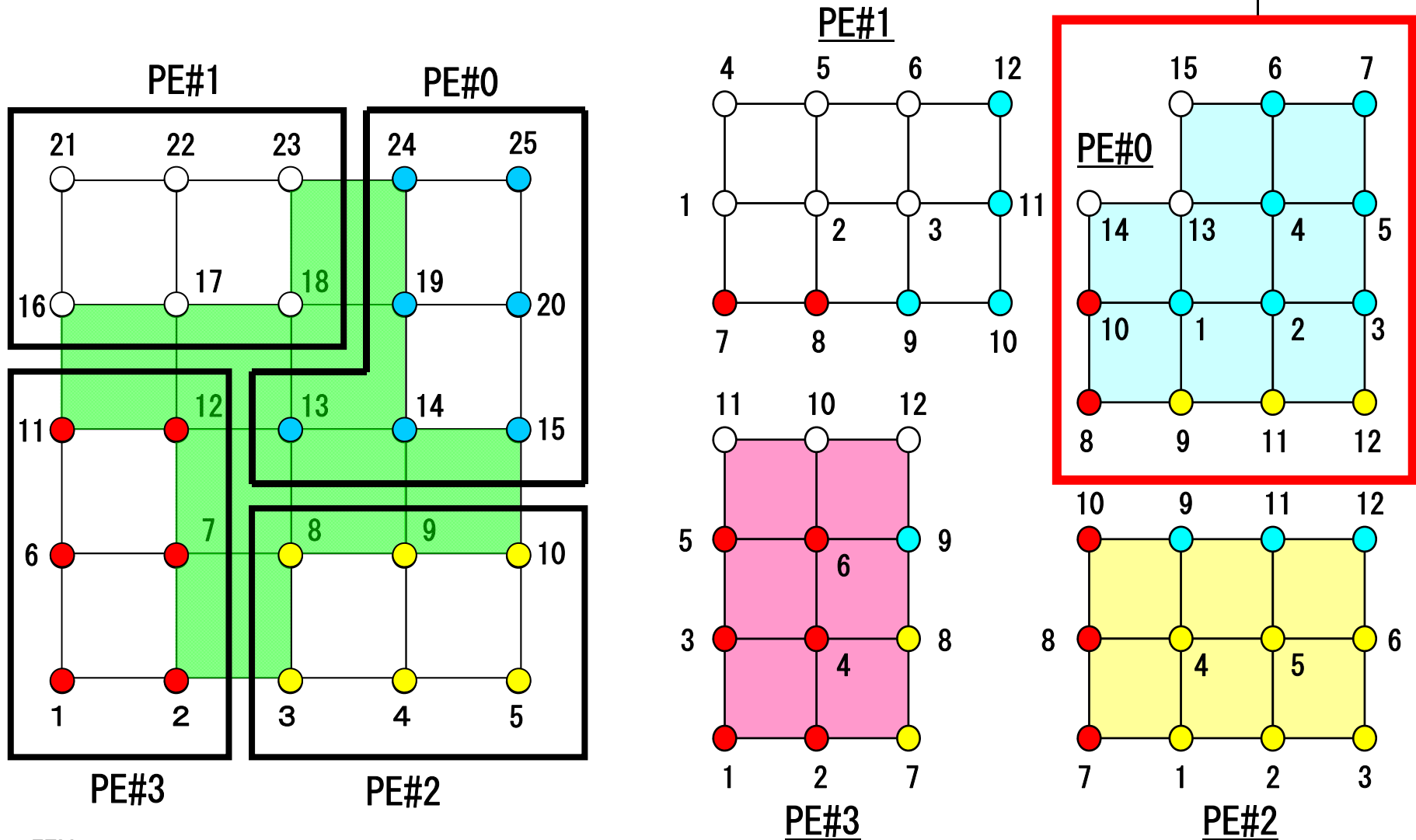


Local Data of Parallel FEM

- **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

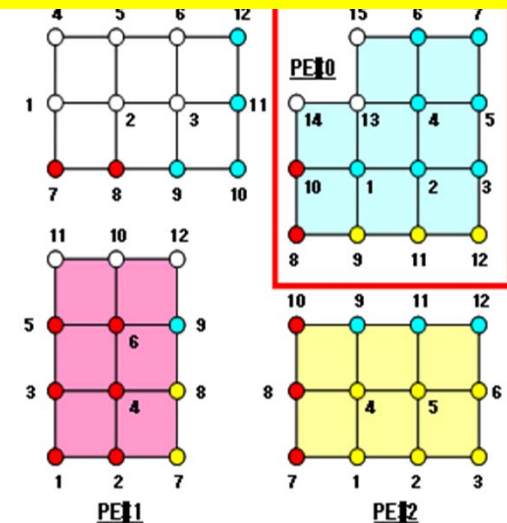
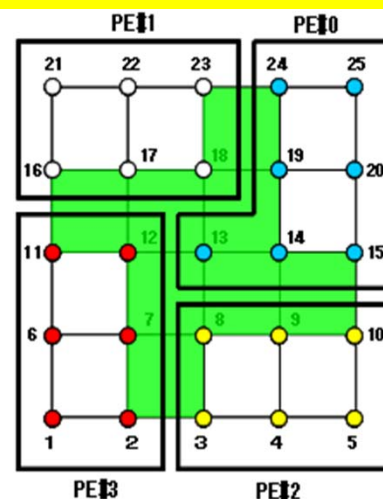
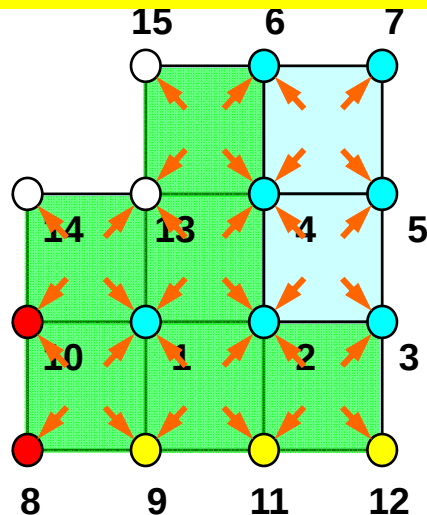


Node-based Partitioning

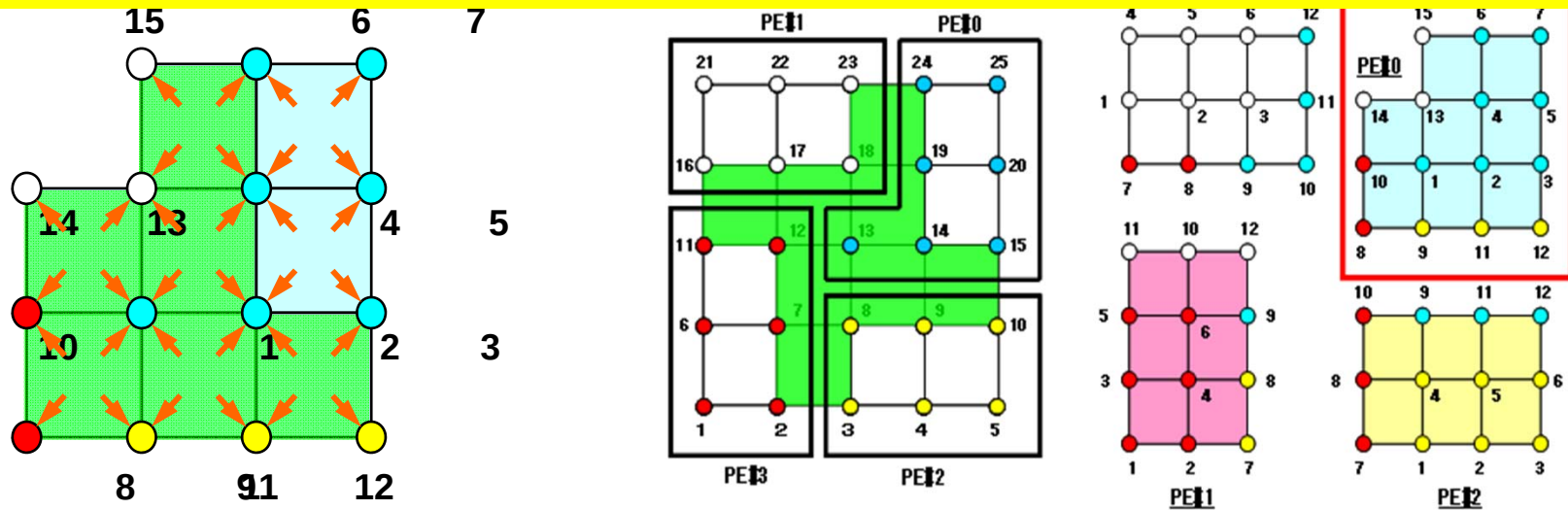
internal nodes - elements - external nodes



- 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.

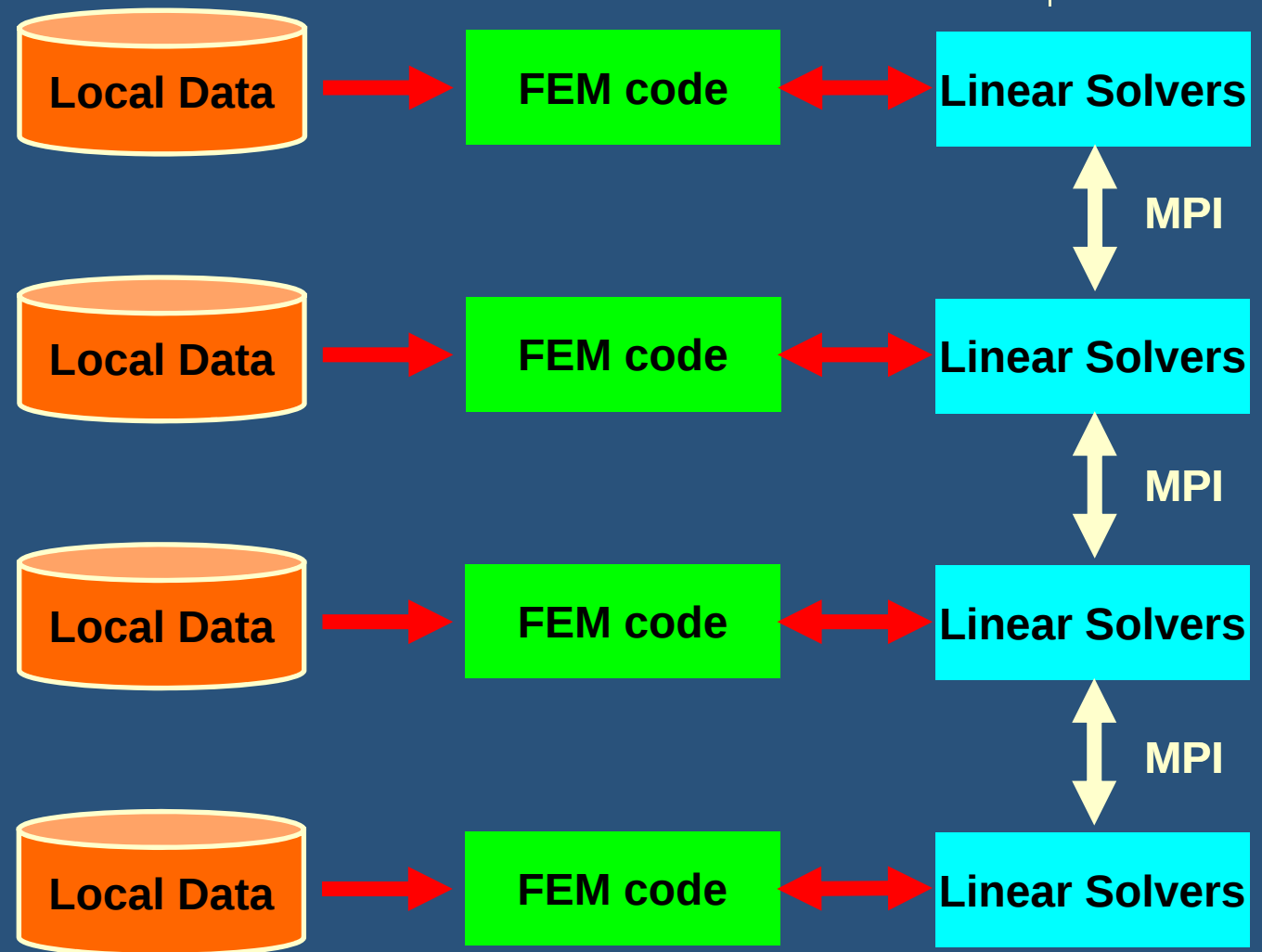


- Info of External Nodes are required for completely local element-based operations on each processor.



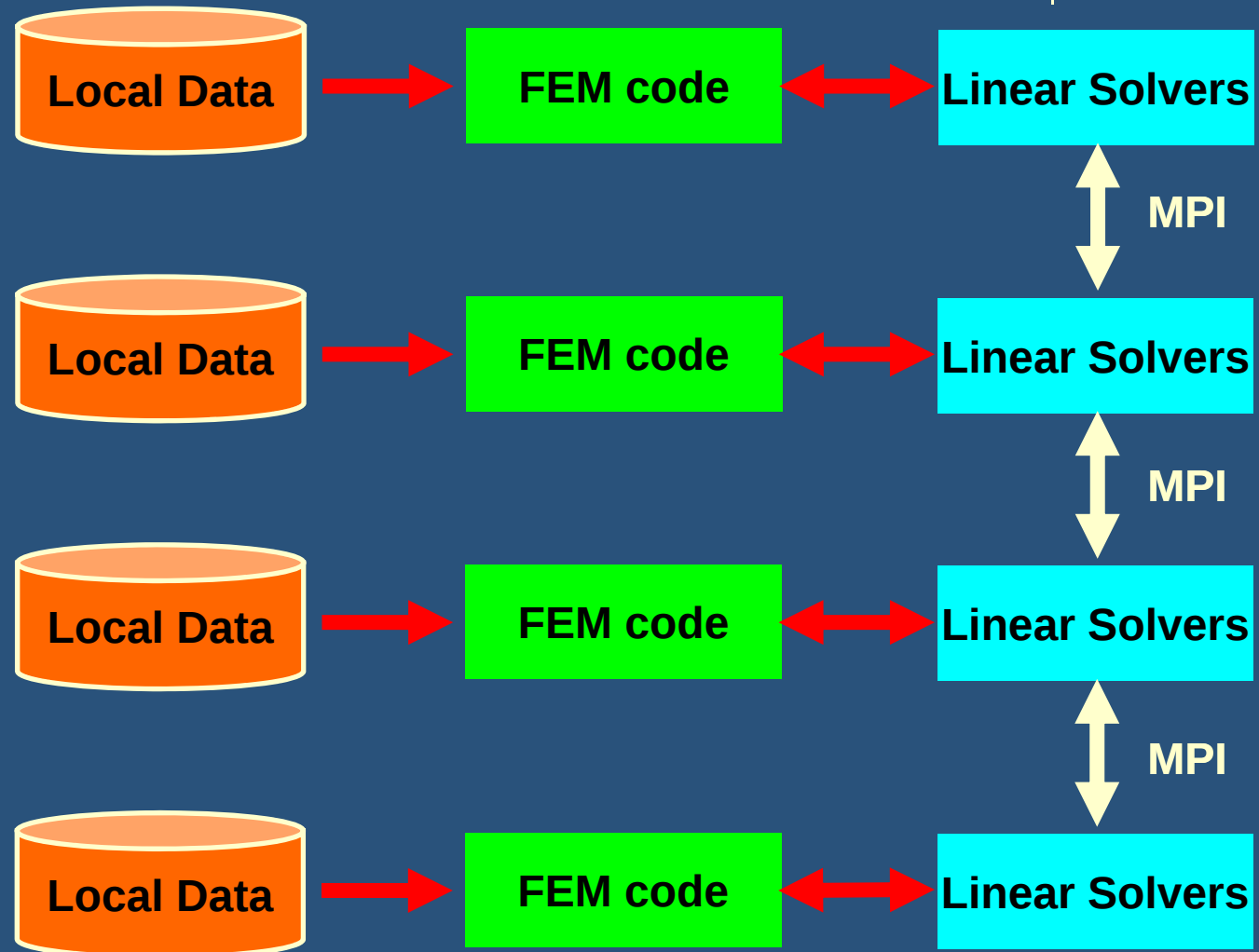
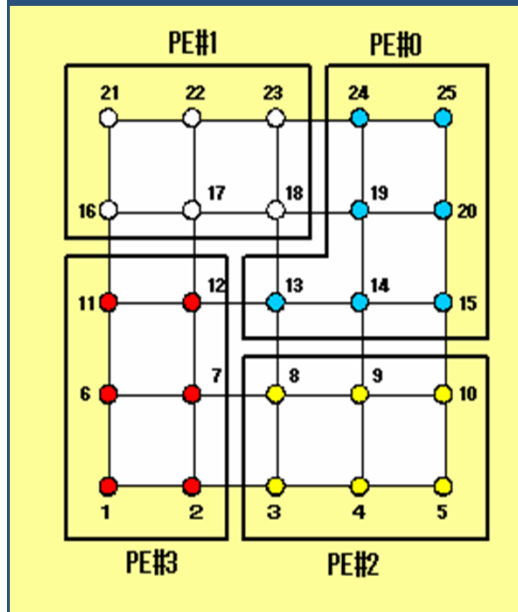
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



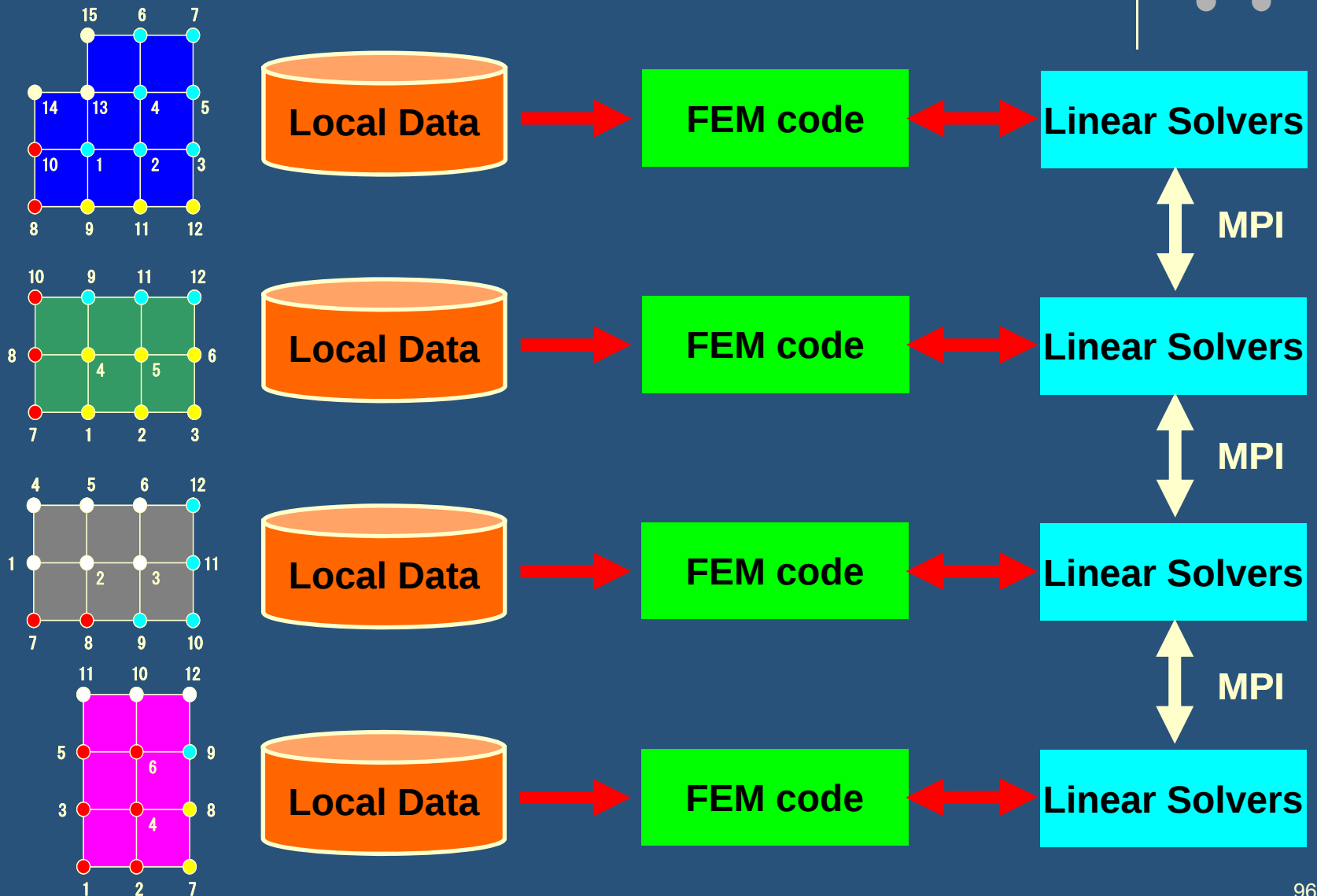
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



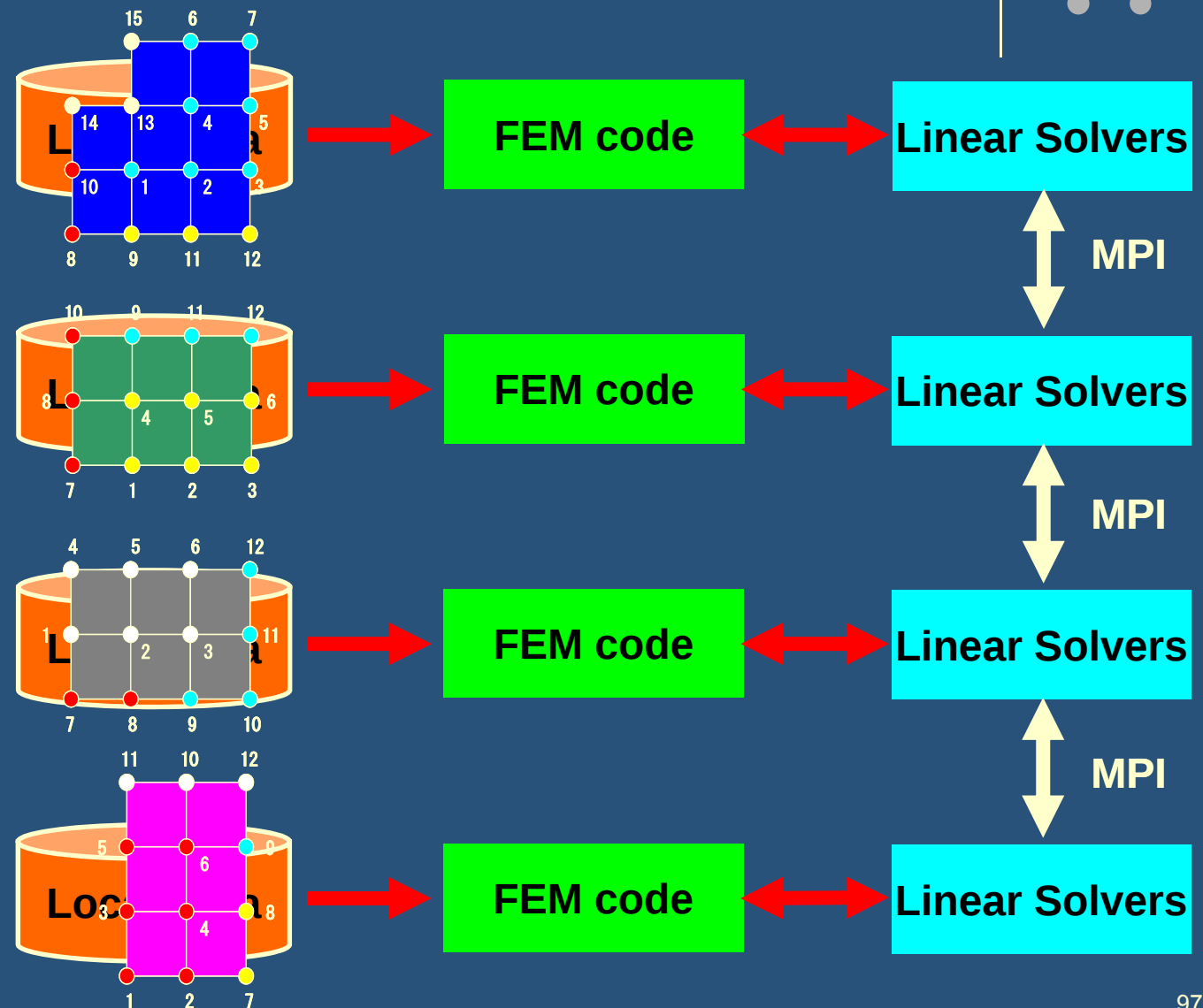
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data



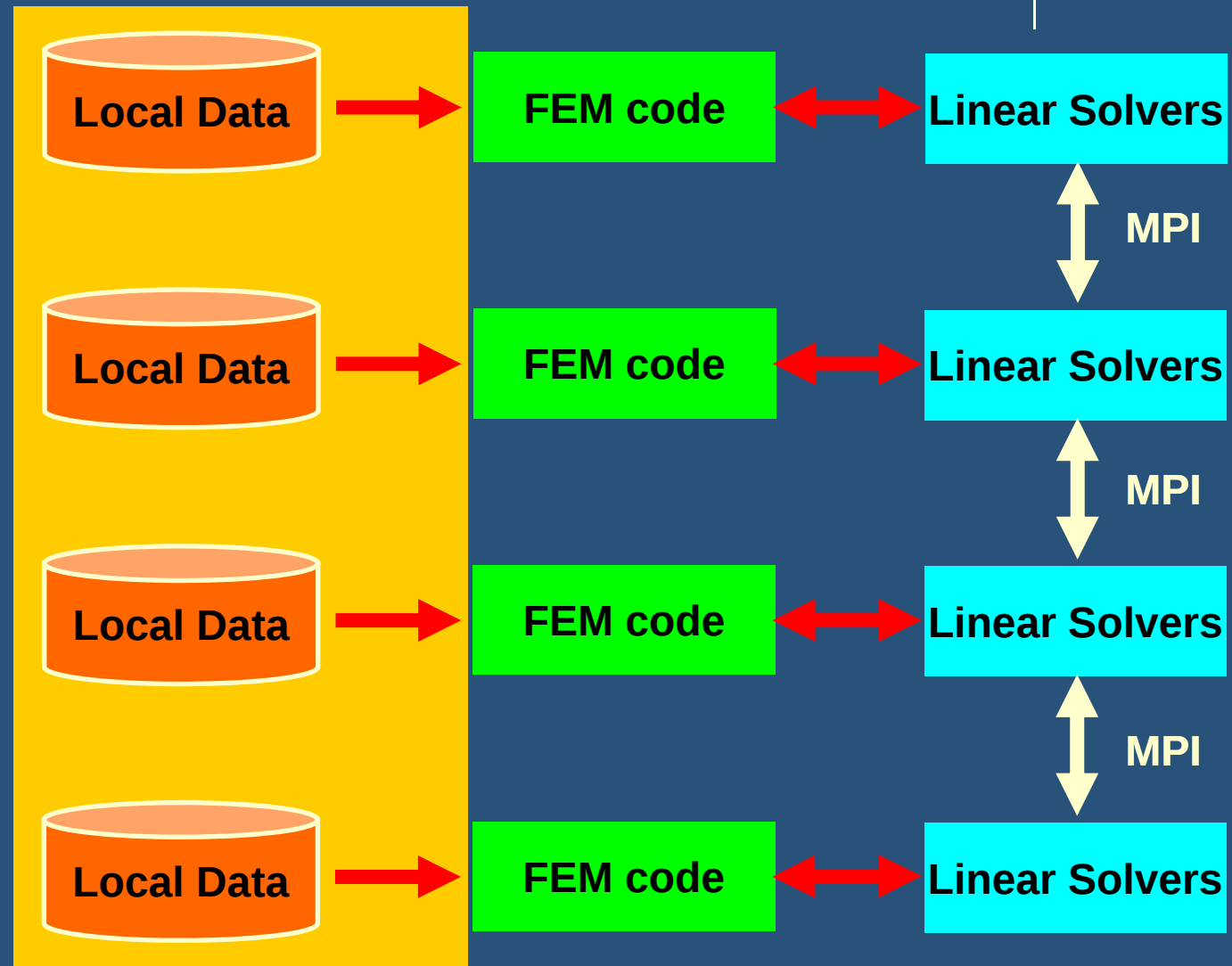
Parallel Computing in FEM

SPMD: Single-Program Multiple-Data

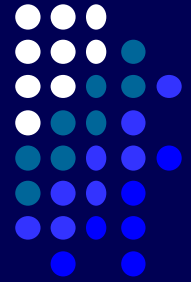


Parallel Computing in FEM

SPMD: Single-Program Multiple-Data

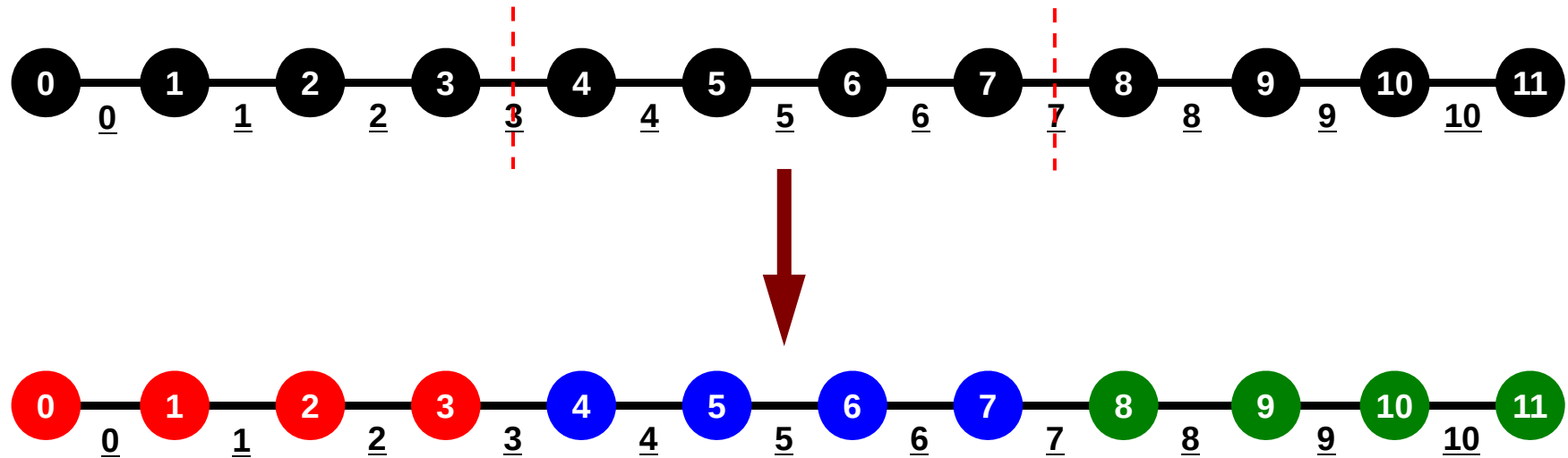


What is Communications ?

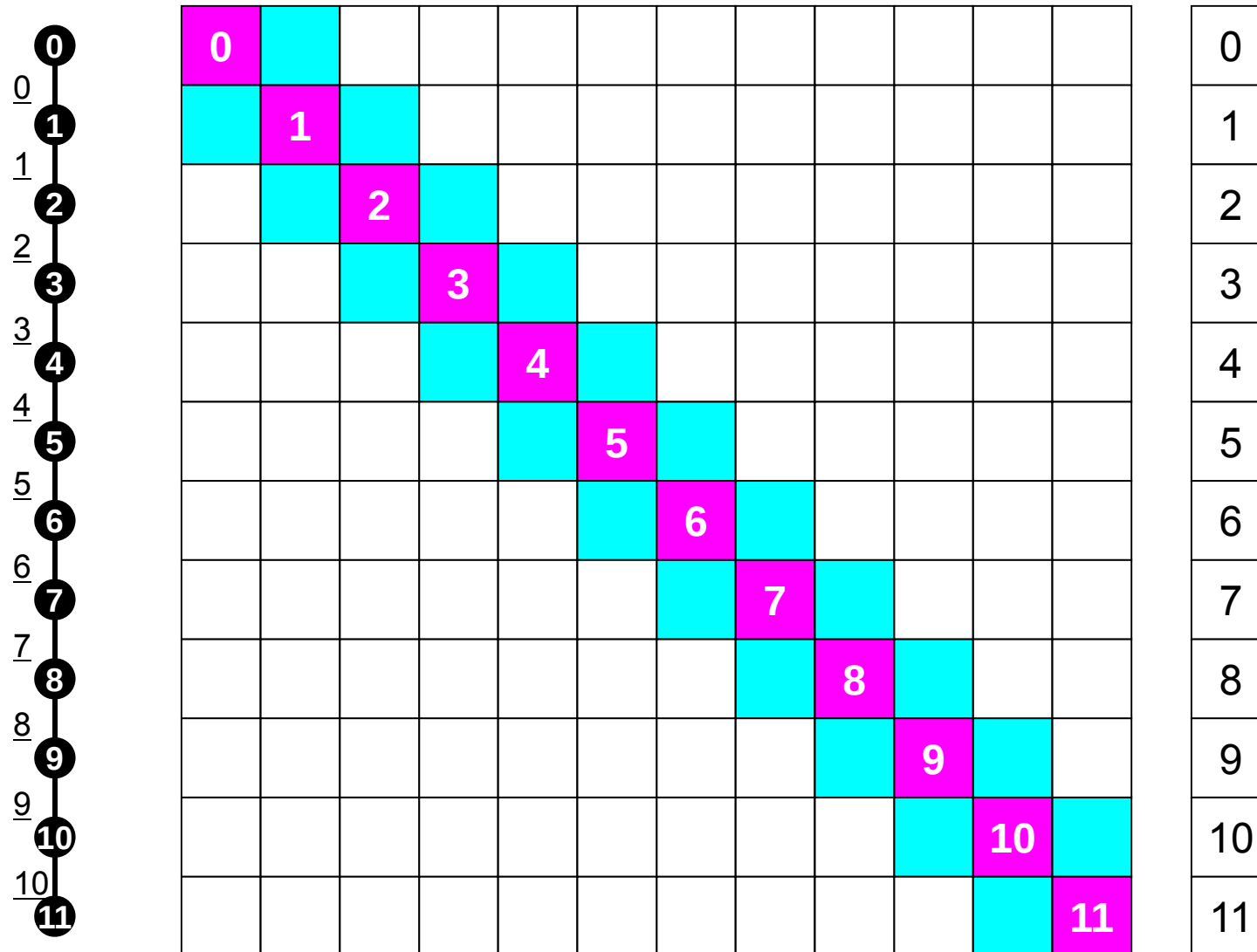


- to get information of “external nodes” from external partitions (local data)
- “Communication tables” contain the information

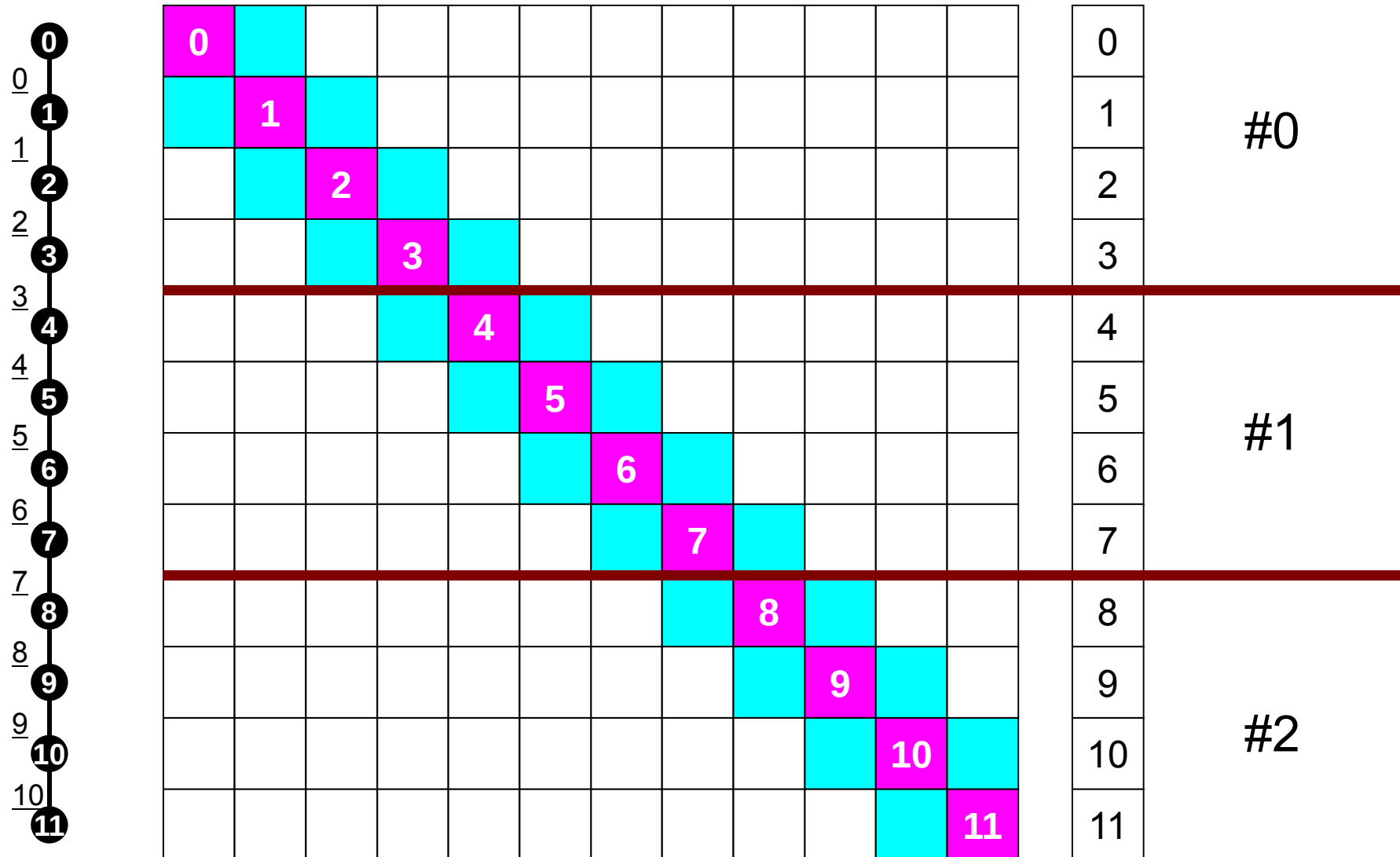
1D FEM: 12 nodes/11 elem's/3 domains



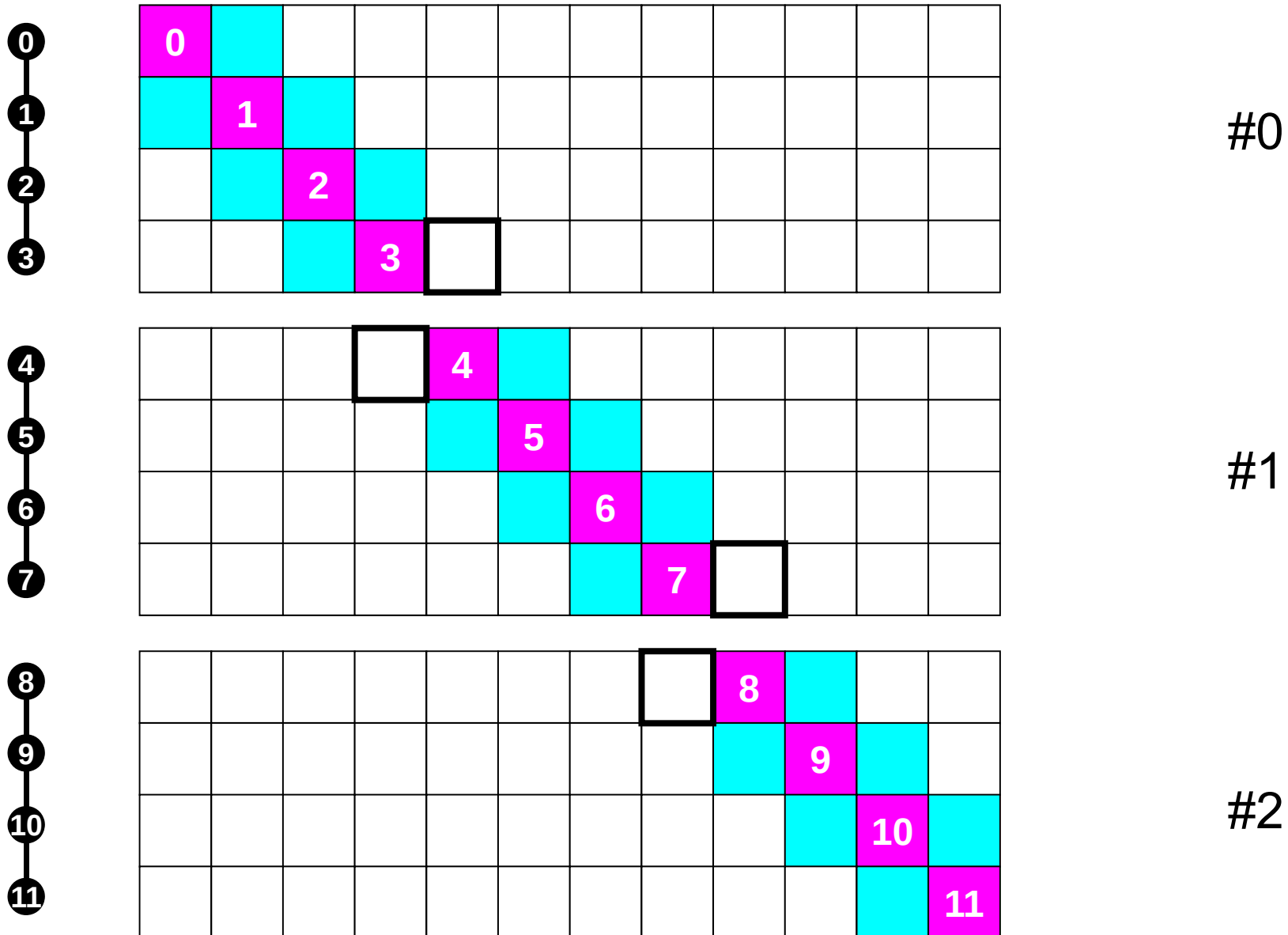
1D FEM: 12 nodes/11 elem's/3 domains



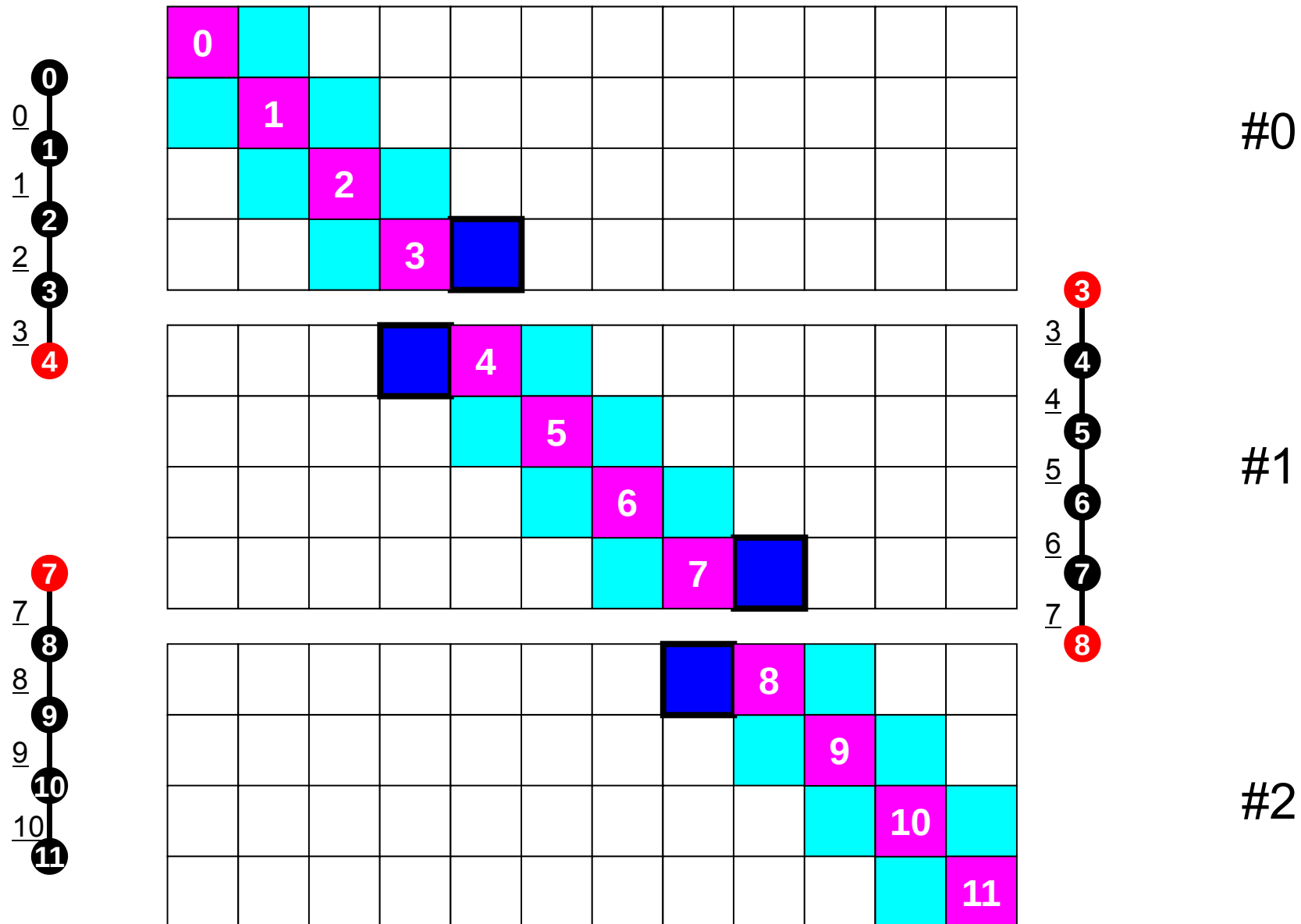
“Internal Nodes” should be balanced



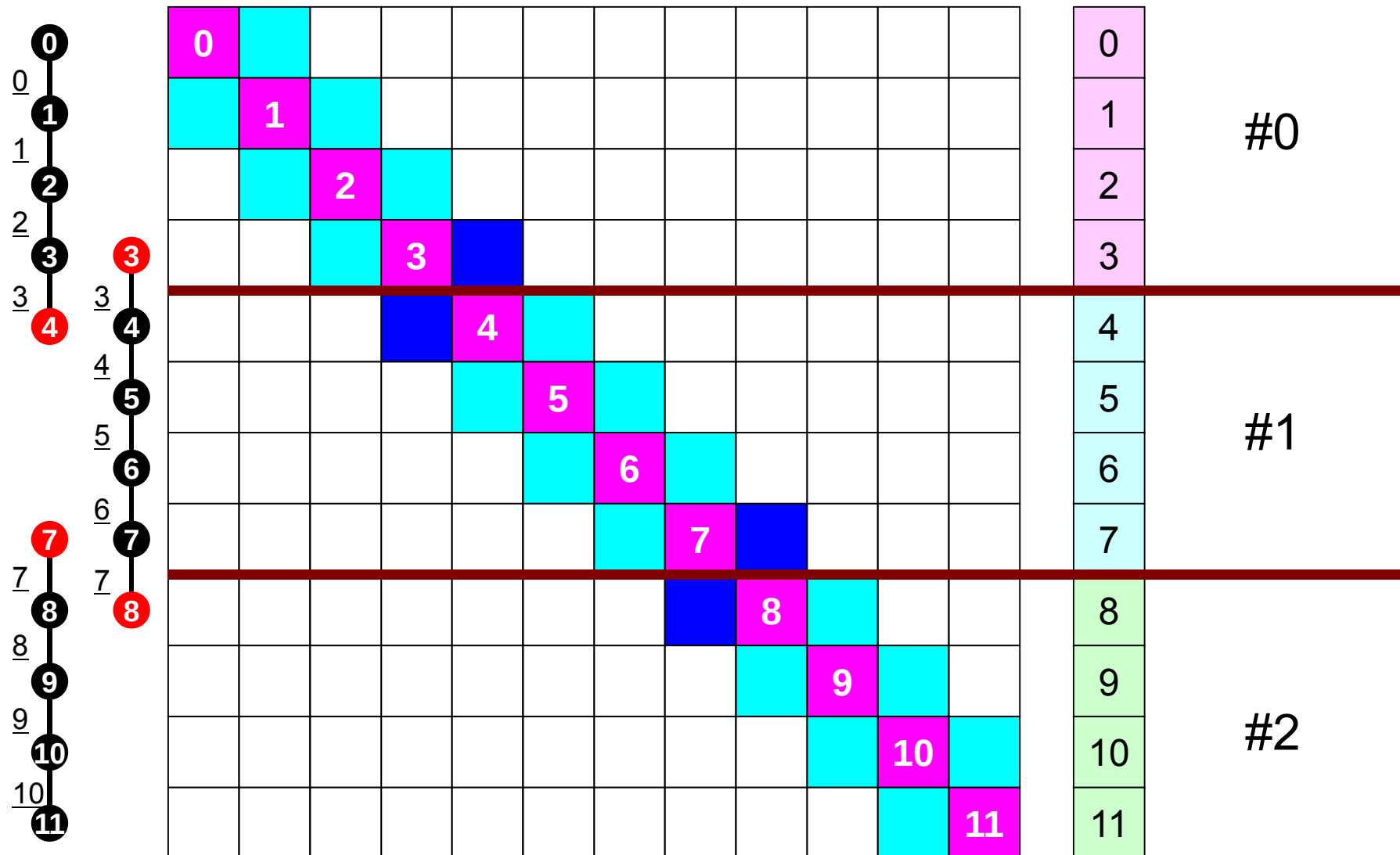
Matrices are incomplete !



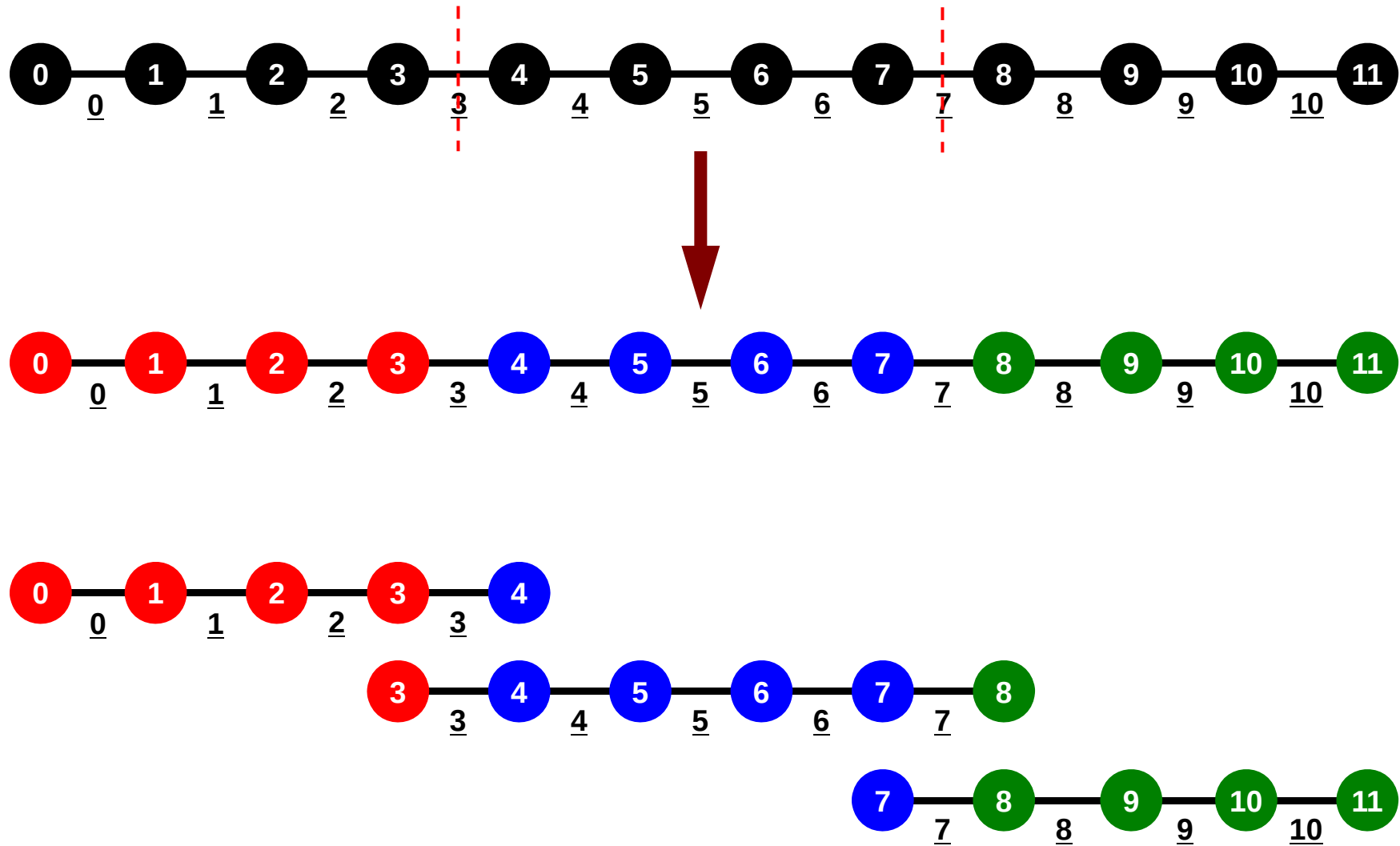
Connected Elements + External Nodes



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

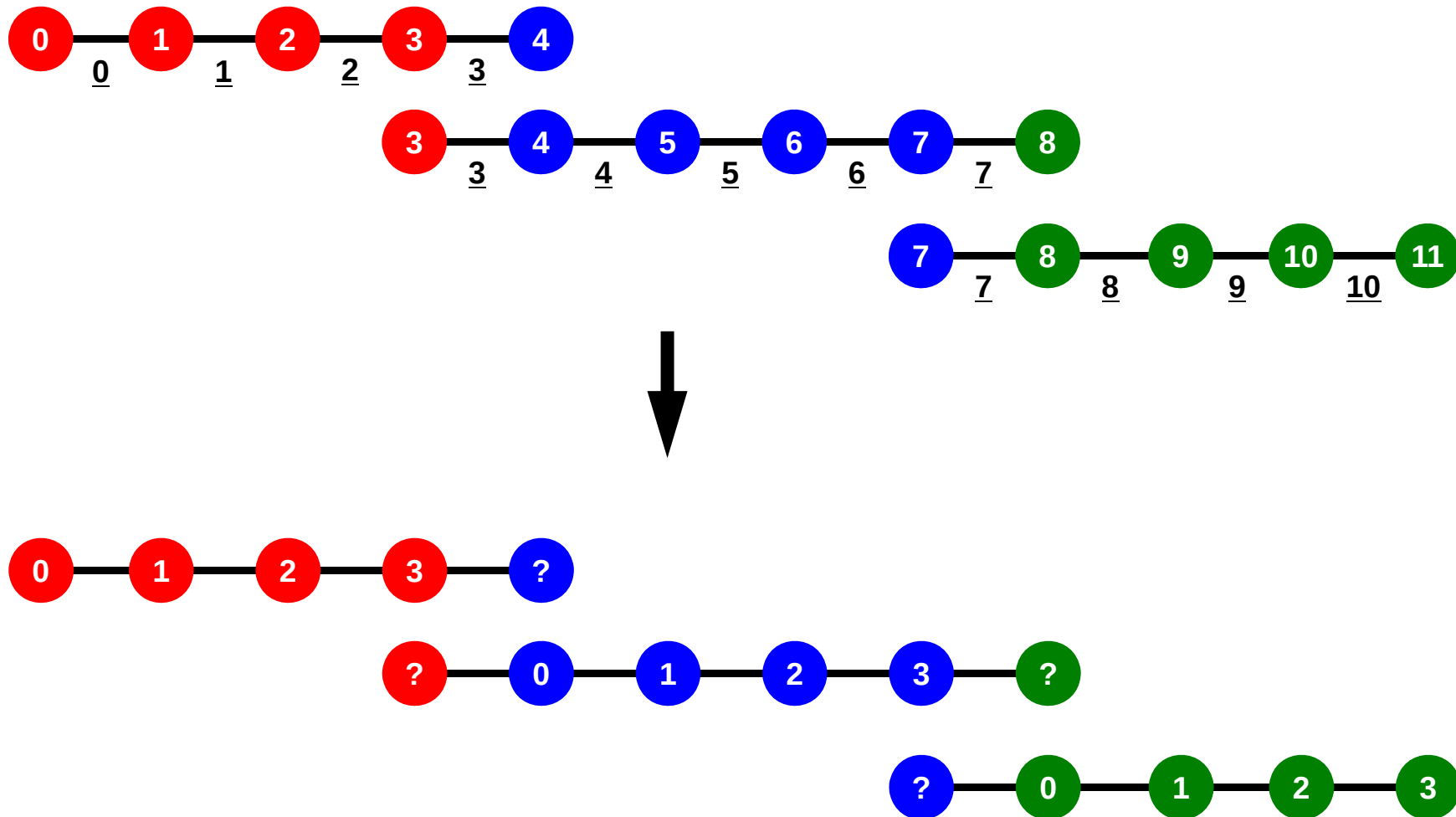


1D FEM: 12 nodes/11 elem's/3 domains



Local Numbering for SPMD

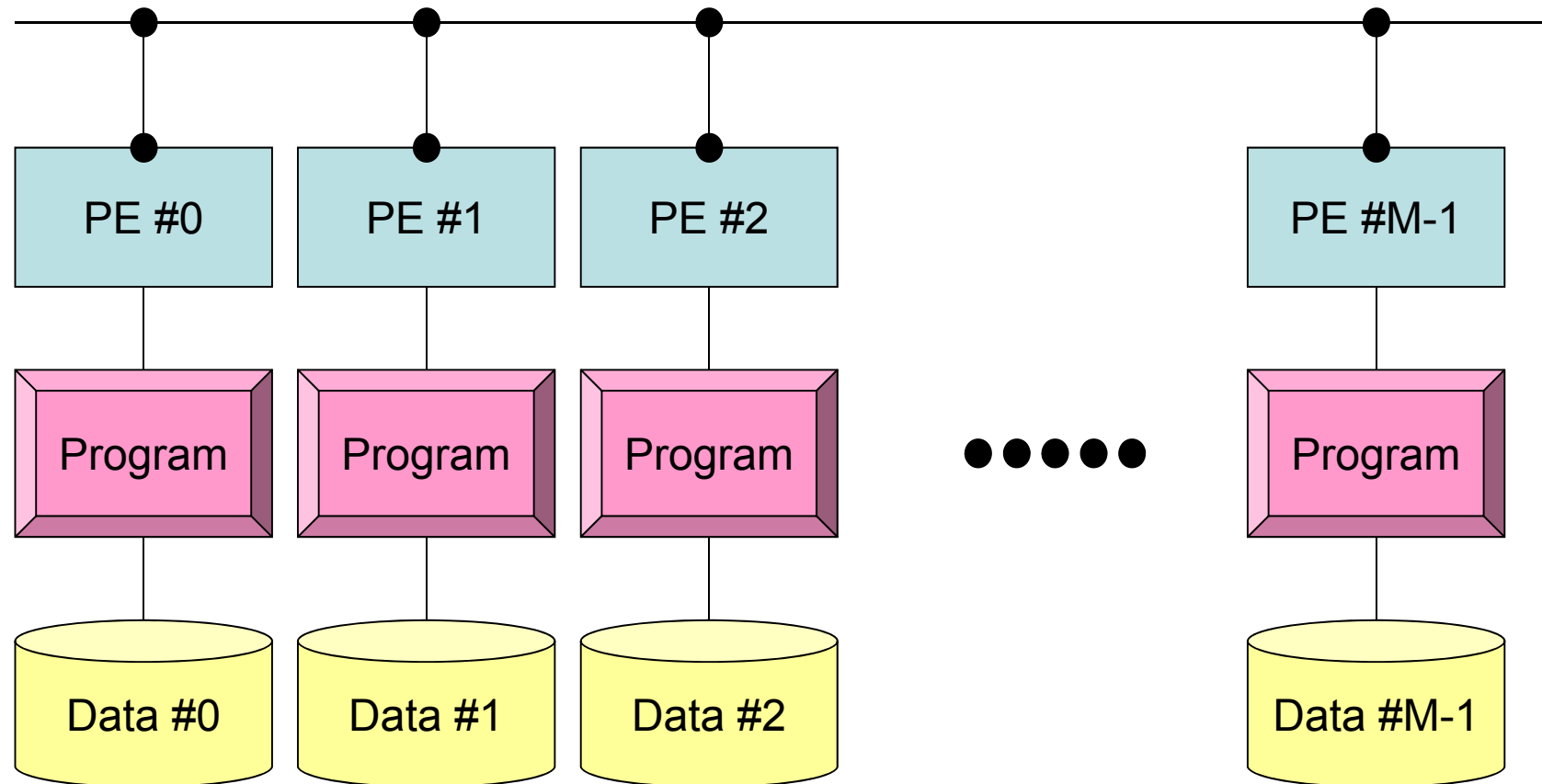
Numbering of internal nodes is 1-N (0-N-1), same operations in serial program can be applied. How about numbering of external nodes ?



PE: Processing Element
Processor, Domain, Process

SPMD

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



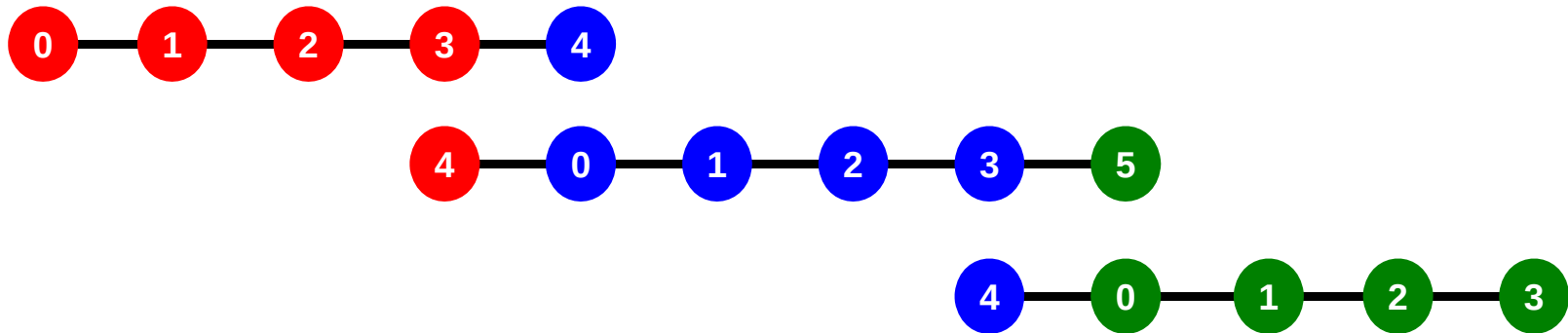
Each process does same operation for different data

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 communica

Local Numbering for SPMD

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



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, ...
    solve  $[\mathbf{M}]\mathbf{z}^{(i-1)} = \mathbf{r}^{(i-1)}$ 
     $\rho_{i-1} = \mathbf{r}^{(i-1)} \cdot \mathbf{z}^{(i-1)}$ 
    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
     $\mathbf{q}^{(i)} = [\mathbf{A}]\mathbf{p}^{(i)}$ 
     $\alpha_i = \rho_{i-1} / (\mathbf{p}^{(i)} \cdot \mathbf{q}^{(i)})$ 
     $\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + \alpha_i \mathbf{p}^{(i)}$ 
     $\mathbf{r}^{(i)} = \mathbf{r}^{(i-1)} - \alpha_i \mathbf{q}^{(i)}$ 
    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

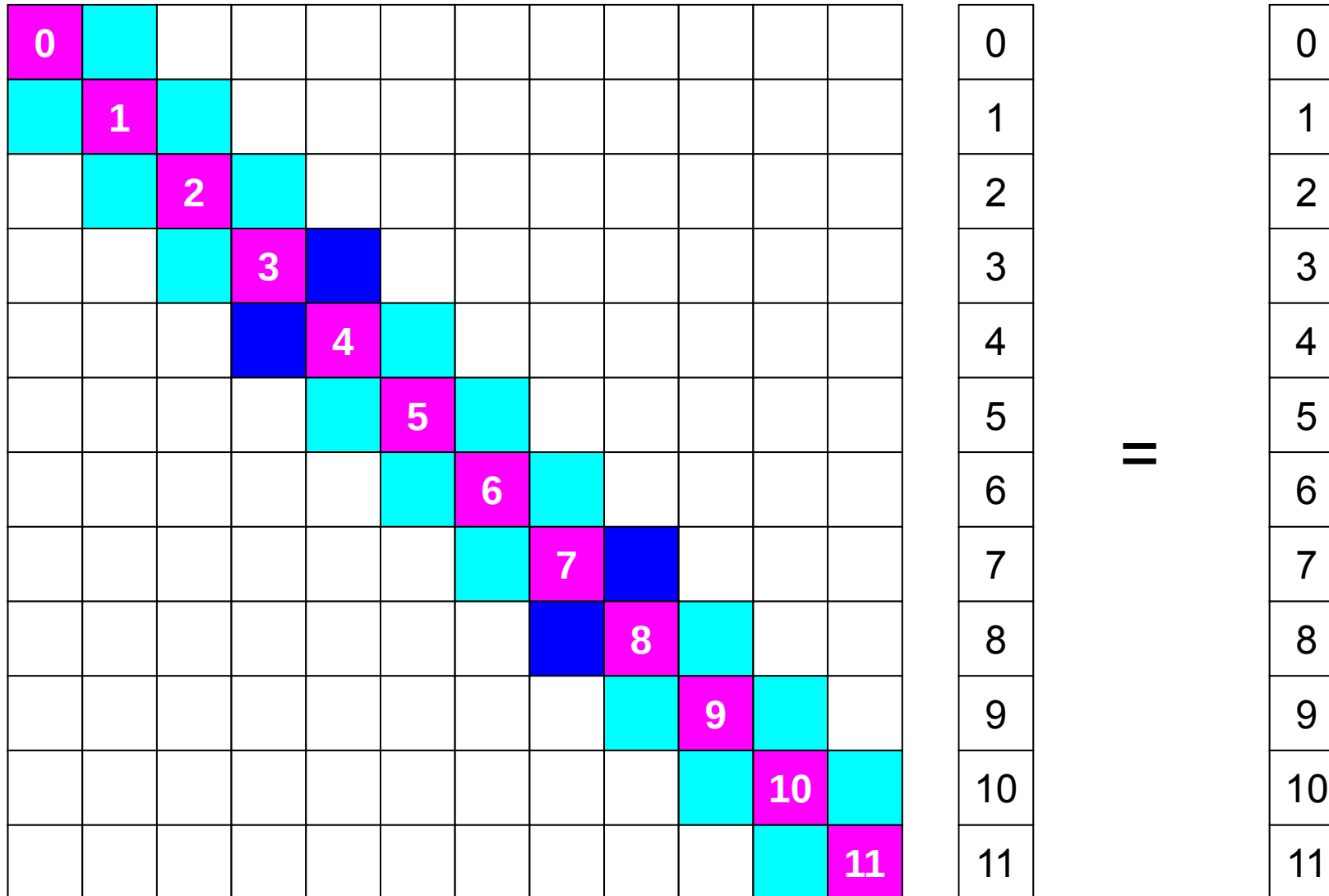
Matrix-Vector Products

Values at External Points: P-to-P Communication

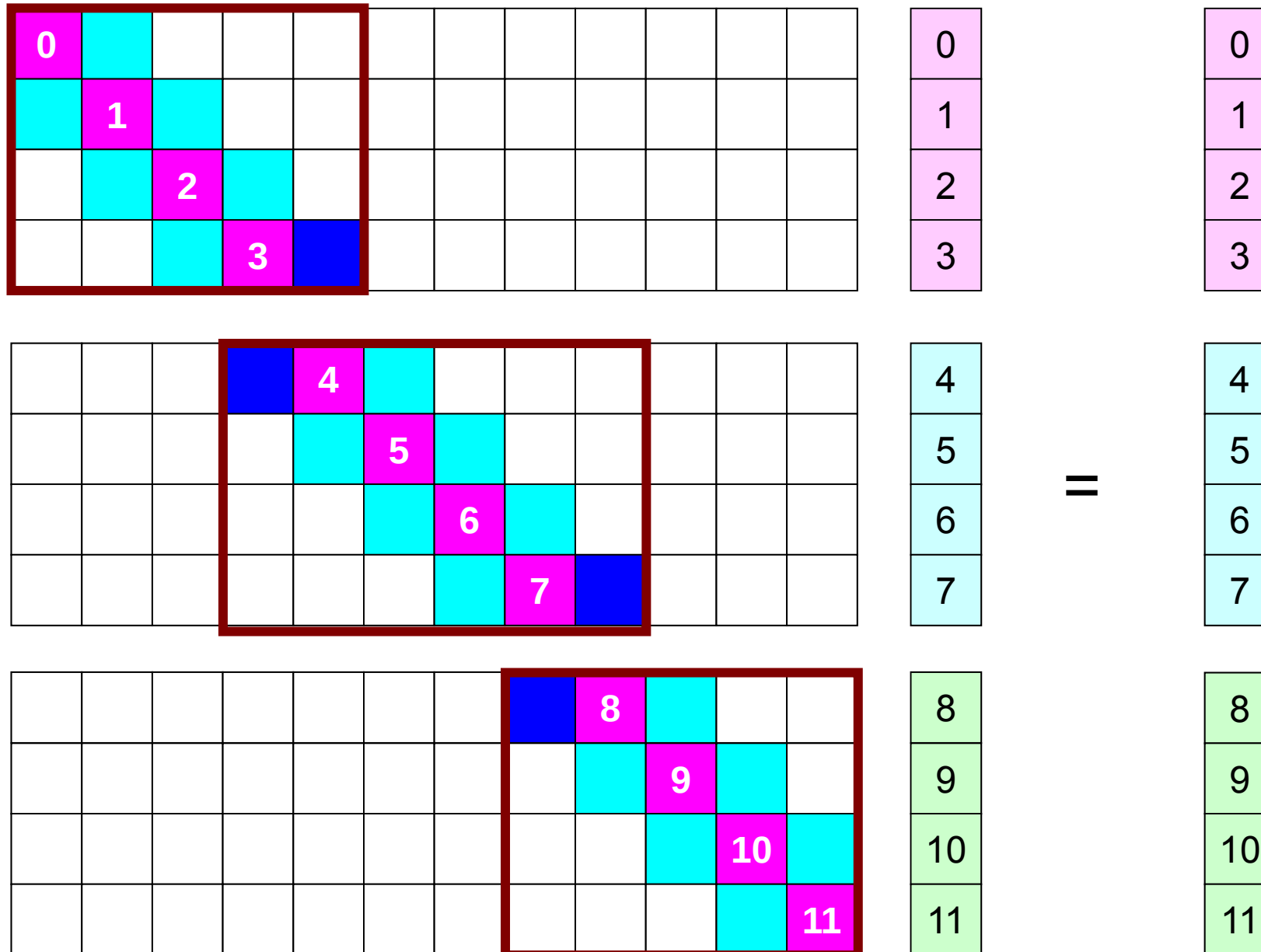
```
/*  
/-- {q} = [A] {p}  
*/  
for (i=0; i<N; i++) {  
    W[Q][i] = Diag[i] * W[P][i];  
    for (j=Index[i]; j<Index[i+1]; j++) {  
        W[Q][i] += AMat[j]*W[P][Item[j]];  
    }  
}
```



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

	0				
		1			
			2		
				3	

0
1
2
3

=

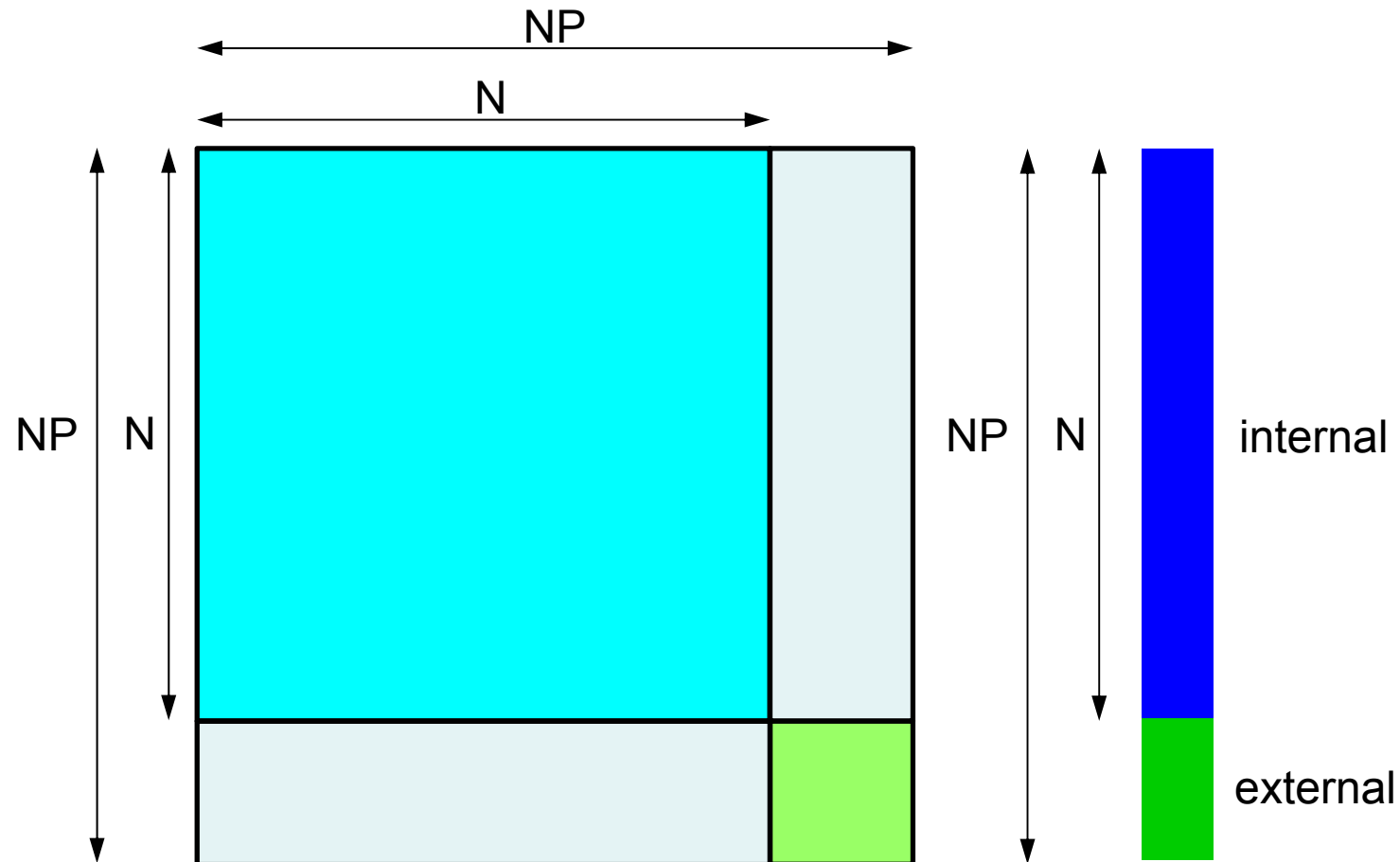
0
1
2
3

	0			
		1		
			2	
				3

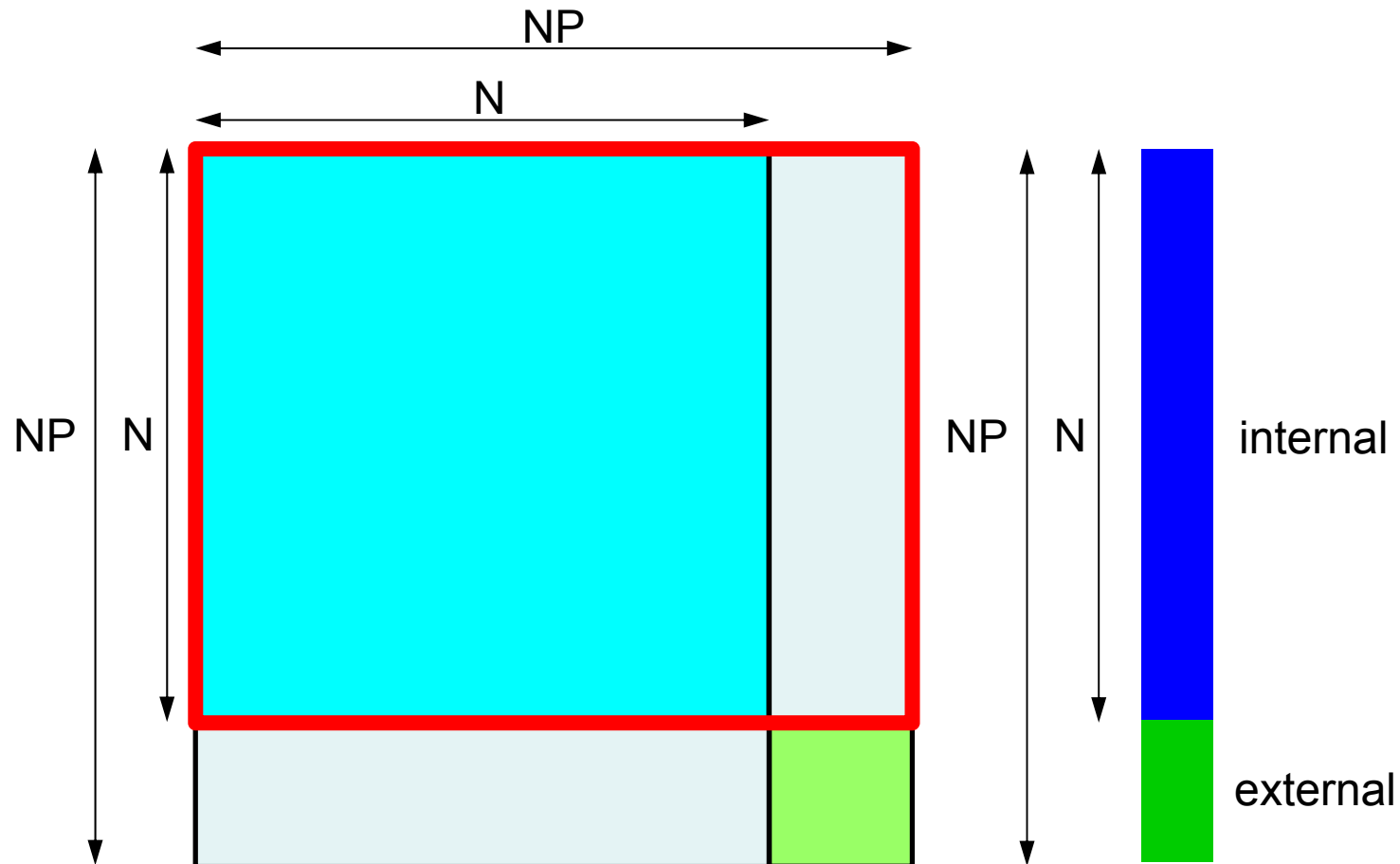
0
1
2
3

0
1
2
3

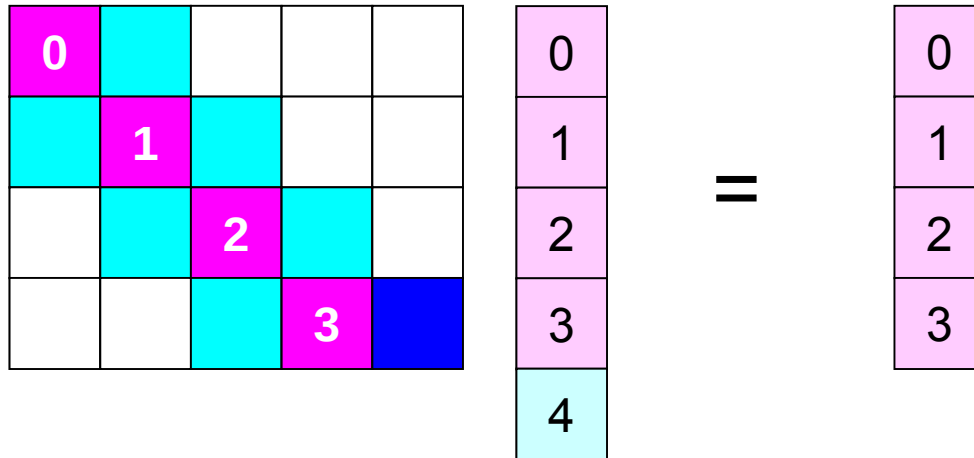
Local Matrix



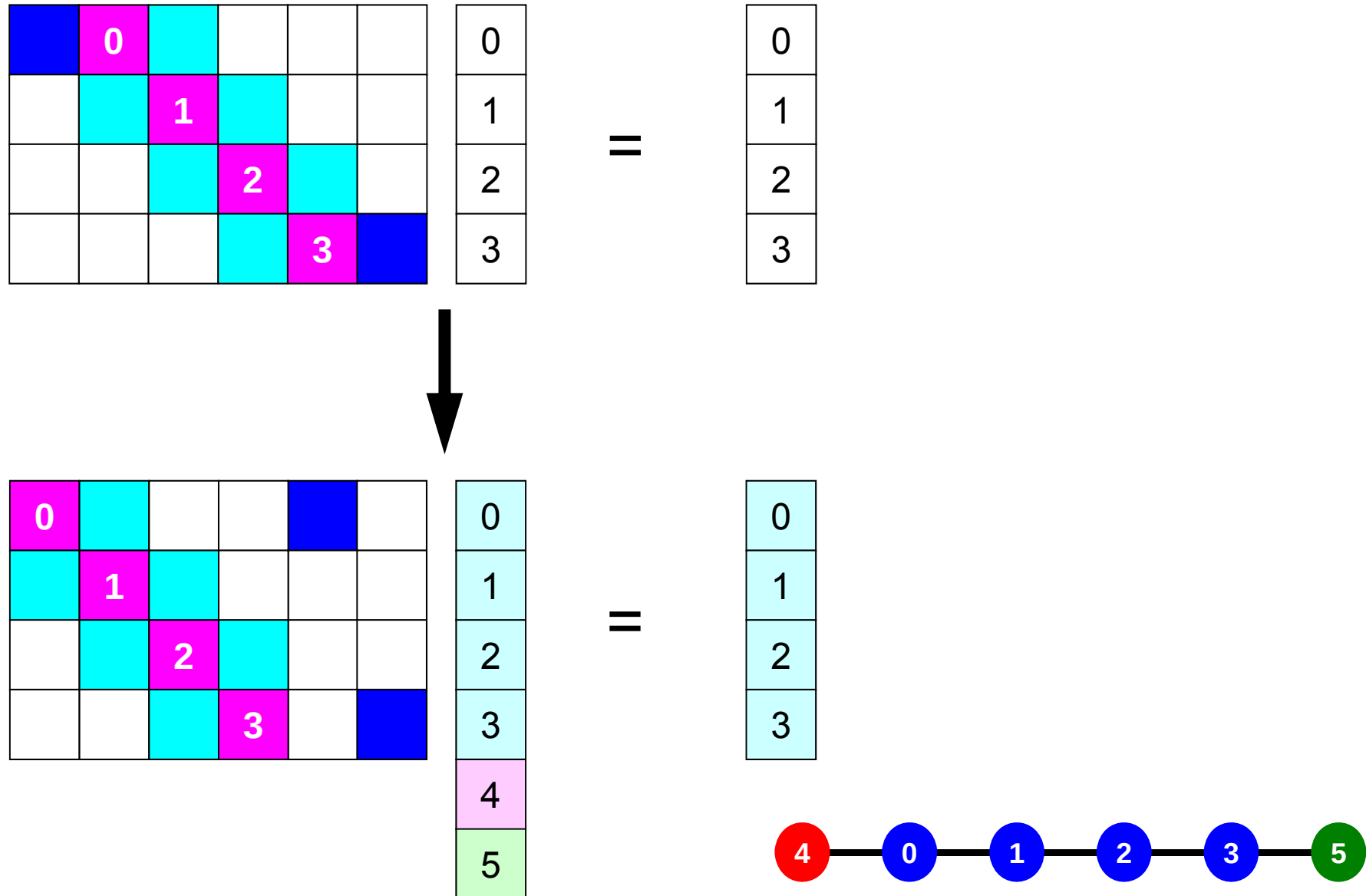
We really need these parts



Mat-Vec Products: Local Op. #0



Mat-Vec Products: Local Op. #1



Mat-Vec Products: Local Op. #2

	0				0
		1			1
			2		2
				3	3

 $=$

0
1
2
3



0					0
	1				1
		2			2
			3		3
					4

 $=$

0
1
2
3

