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Implementation of FEM on HPC – I

Miroslav Halilovič, **Bojan Starman**, Janez Urevc, Nikolaj Mole

Faculty of Mechanical Engineering, University of Ljubljana

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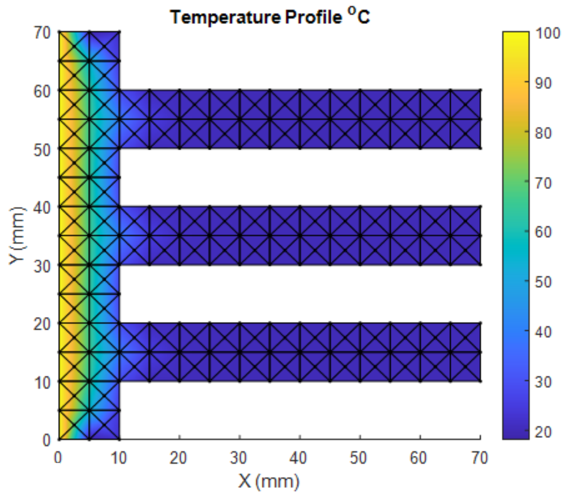
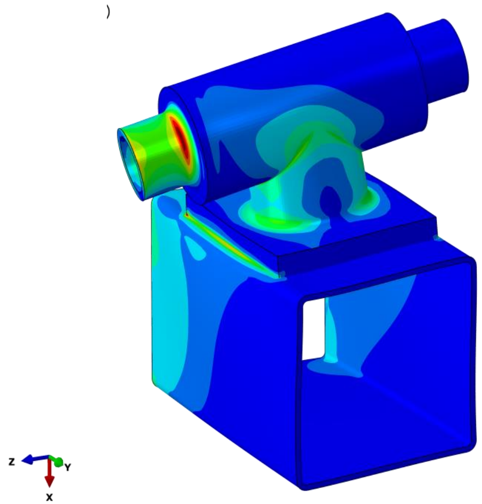
Methods for solution of Boundary Value Problem (BVP):

- Finite Difference Method (FDM)
- Finite Element Method (FEM)
- Boundary Element Method (BEM)
- Finite Volume Method (FVM)



$$k\,\Delta T(x,y) + q_v = 0$$



$$\tilde{\nabla}^T \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}$$
$$\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon} - \mathbf{D}\boldsymbol{\varepsilon}_0$$
$$\boldsymbol{\varepsilon} = \tilde{\nabla}\mathbf{u}$$

Finite Difference Method

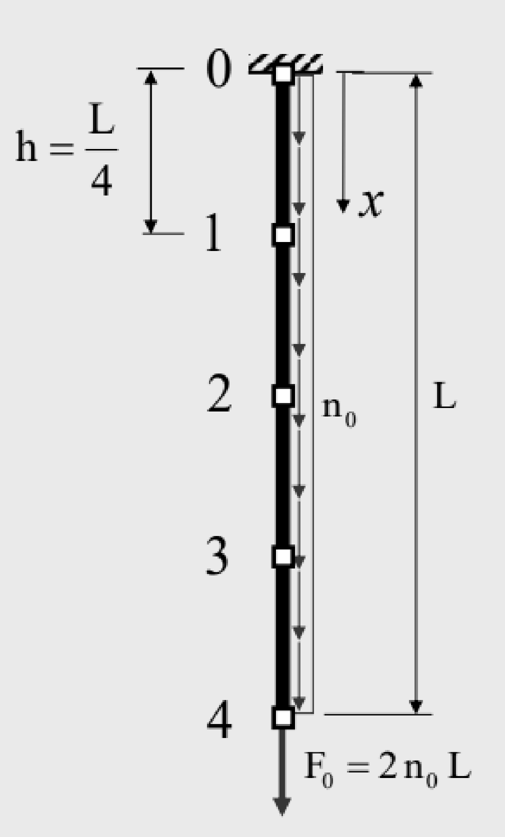
- IDEA: approximation of derivatives in governing equation and boundary conditions at points (grid)
- Approximation is derived based on the Taylor's series expansion

$$EA\, u''(x) = -n_0$$

- ADVANTAGE: simple to use
- DISADVANTAGE: irregular domains, mesh preparation

$$u(0)=0$$

$$EA\, u(L)' = F_0$$



Finite Difference Method

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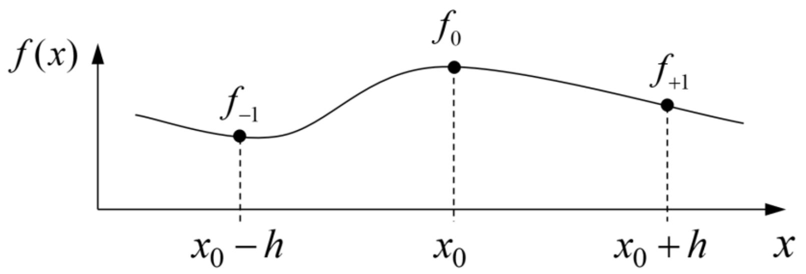
- Approximation based on the Taylor's series expansion

$$f(x_0+h) = f(x_0) + \frac{h}{1!}\frac{d^1 f(x_0)}{dx^1} + \frac{h^2}{2!}\frac{d^2 f(x_0)}{dx^2} + \frac{h^3}{3!}\frac{d^3 f(x_0)}{dx^3} + \ldots$$



$$f_{+1} \approx f_0 + h\, f_0' + \frac{h^2}{2}\, f_0''$$

$$f_{-1} \approx f_0 - h\, f_0' + \frac{h^2}{2}\, f_0''$$

$$f_0' \approx \frac{f_{+1} - f_{-1}}{2h}$$

$$f_0'' \approx \frac{f_{+1} - 2 f_0 + f_{-1}}{h^2}$$

Finite difference approximation of 1st and 2nd derivative

Finite Difference Method

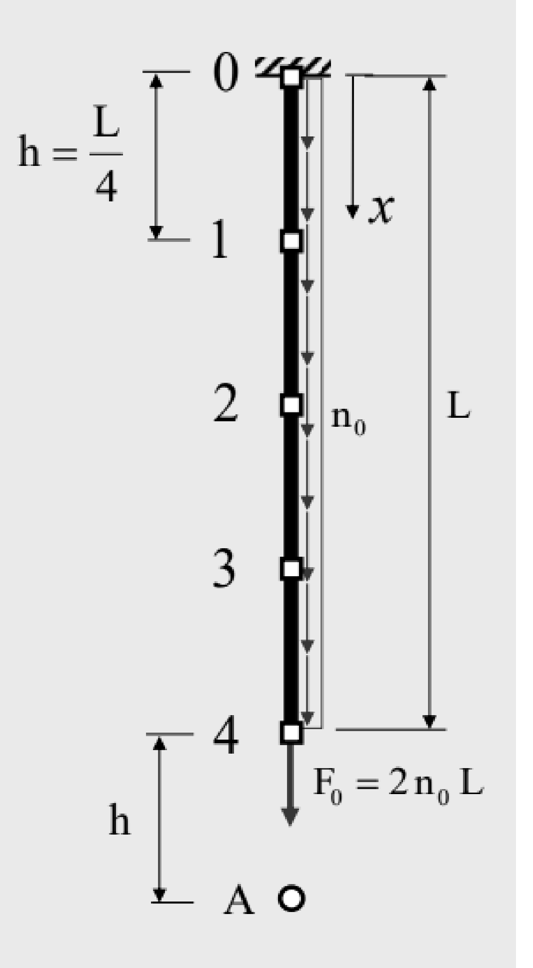
- Writing boundary conditions in discrete form:

$u(0)=0 \quad \Rightarrow u_0 = 0$

$EA\,u(L)' = F_0 \Rightarrow \quad u_A - u_3/(2\mathrm{h}) = F_0$

- Writing governing equation at discrete points 1 to 4

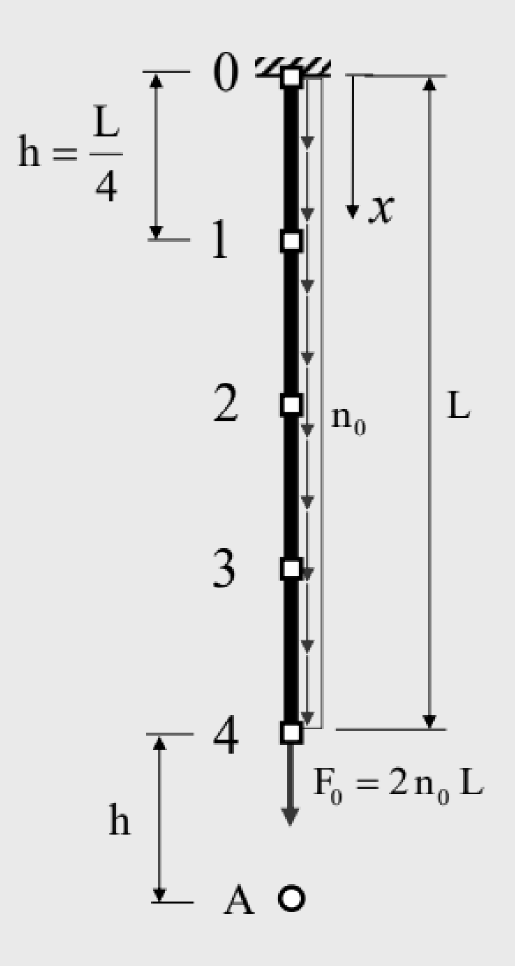
$$EA\,u''(x) = -n_0 \quad \Rightarrow \quad \begin{aligned} u_0 - 2u_1 + u_2 &= -n_0 h^2/(EA) \\ u_1 - 2u_2 + u_3 &= -n_0\, h^2/(EA) \\ u_2 - 2u_3 + u_4 &= -n_0\, h^2/(EA) \\ u_3 - 2u_4 + u_A &= -n_0\, h^2/(EA) \end{aligned}$$



- System of equations:

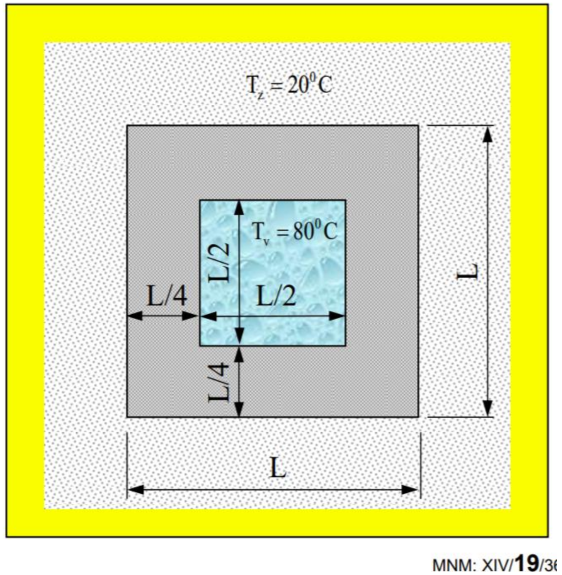
		u_0	u_1	u_2	u_3	u_4	u_A
BC pt. 0	→	1	0	0	0	0	0
BC pt. 4	→	0	0	0	−1	0	+1
GE pt. 1	→	+1	−2	+1	0	0	0
GE pt. 2	→	0	+1	−2	+1	0	0
GE pt. 3	→	0	0	+1	−2	+1	0
GE pt. 4	→	0	0	0	+1	−2	+1

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ +1 & -2 & +1 & 0 & 0 & 0 \\ 0 & +1 & -2 & +1 & 0 & 0 \\ 0 & 0 & +1 & -2 & +1 & 0 \\ 0 & 0 & 0 & +1 & -2 & +1 \end{bmatrix} \begin{Bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_A \end{Bmatrix} = \begin{Bmatrix} 0 \\ 16 \\ -1 \\ -1 \\ -1 \\ -1 \end{Bmatrix} \frac{n_0 L^2}{16EA}$$

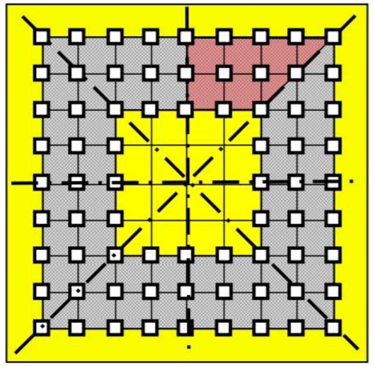


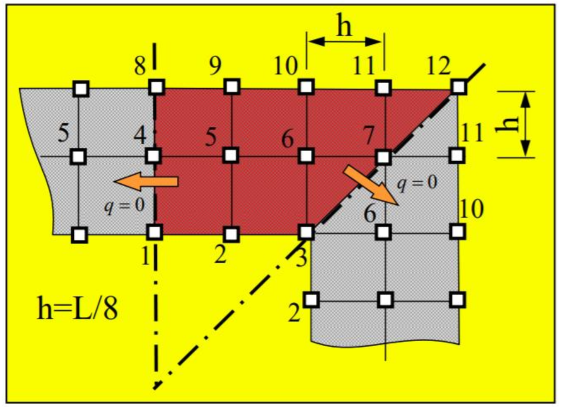
Finite Difference Method

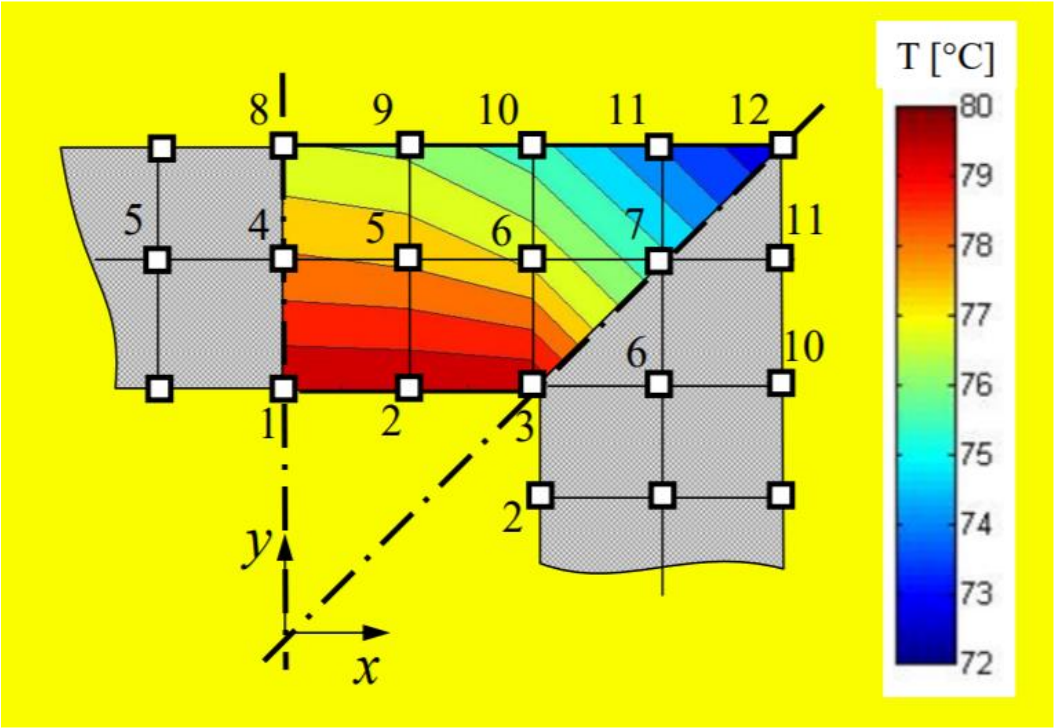
- Stationary heat transfer in 2D



$$k\ \Delta T(x,y) + q_v = 0$$







Finite Element Method

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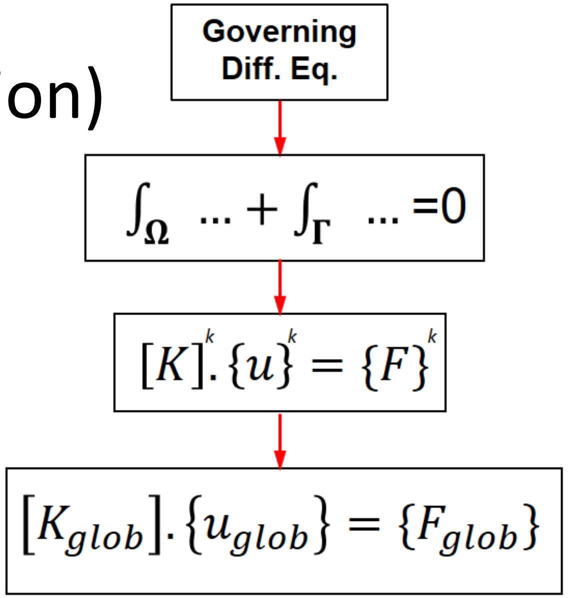
- IDEA: integral based approach
- Starting point of derivation is Weak Integral Form of governing equation
- Solution domain is discretized into sub-domains, called finite elements (FEs)
- In the FE sub-domain we approximate unknown quantities

- ADVANTAGE: simple to use for complex geometrical domains, useful for all types of physical problems
- DISADVANTAGE: computationally intensive method

FEM – Implementation steps

- Derivation of Weak Integral Form of Governing Equation
- Approximation of Solution Variable over Finite Element Domain
- Derivation of Finite Element Matrix Equation
- Meshing & Writing FE Matrix Equation for each FE
- The Assembly Process (Global Finite Element Matrix Equation)
- Writing Boundary Conditions
- Solution of System of Equations



FEM – Implementation steps

- **Derivation of Weak Integral Form of Governing Equation**
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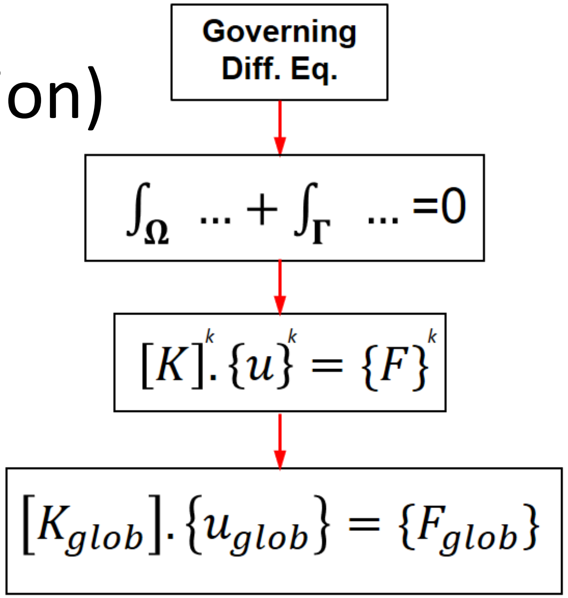


Derivation of Weak Integral Form of Governing Equation

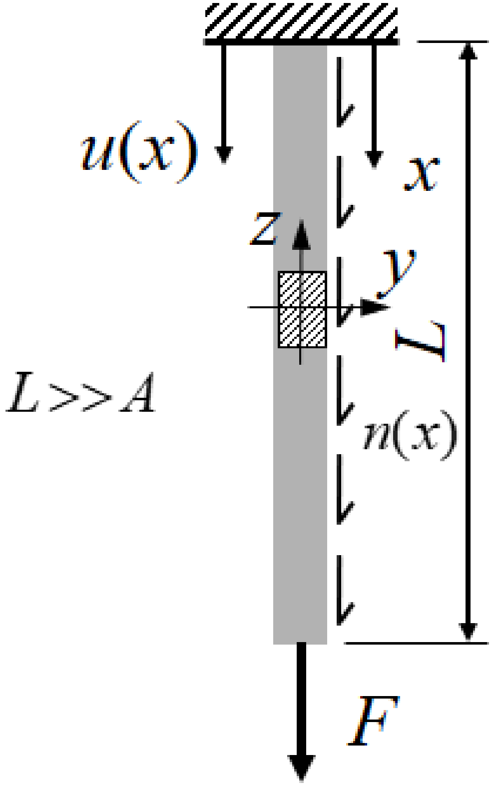
$$EA\,u''(x) = -n_0$$

Governing Equation

$$EA\,u''(x) + n_0 = 0$$

$$\int_0^{L_e} (EA\,u''(x) + n_0)v(x)\mathrm{d}x = 0$$

Strong Form



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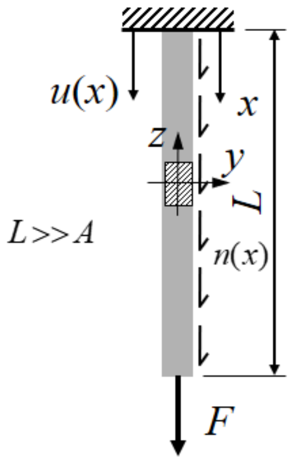
Derivation of Weak Integral Form of Governing Equation

$$\int_0^{L_e} EA\, u''(x)v(x)\mathrm{d}x = -\int_0^{L_e} n_0 v(x)\mathrm{d}x$$

Strong Form



Integration by PARTS

$$\int_0^{L_e} EA\, u'(x)v'(x)\mathrm{d}x = EAu'(L)\, v(L) - EAu'(0)v(0) + \int_0^{L_e} n_0 v(x)\mathrm{d}x$$

$N(L)$ $N(0)$

WEAK Form

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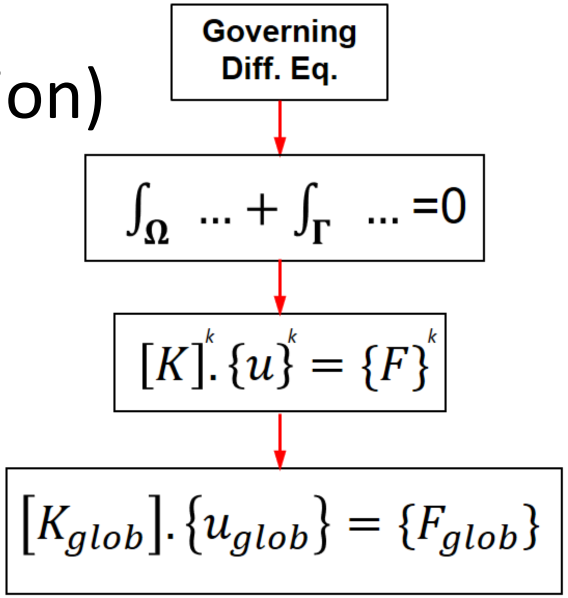
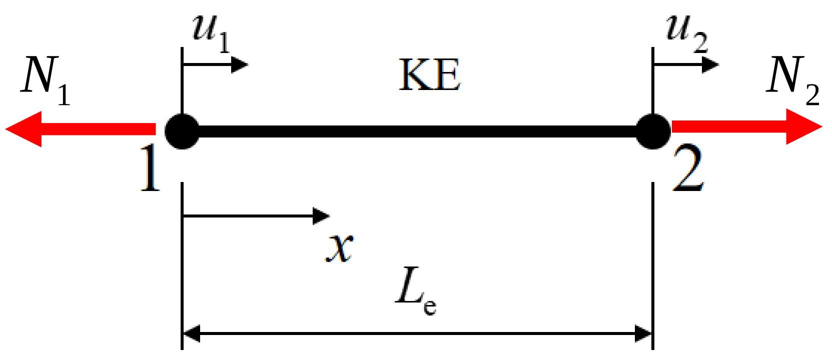


FEM – Approximation

$$\int_0^{L_e} EA\, u'(x) v'(x) \mathrm{d}x = N_2\, v(L) - N_1\, v(0) + \int_0^{L_e} n_0 v(x) \mathrm{d}x$$

Approximation of u(x)

$$u(x) \approx \hat{u}(x) = u_1 \psi_1(x) + u_2 \psi_2(x)$$



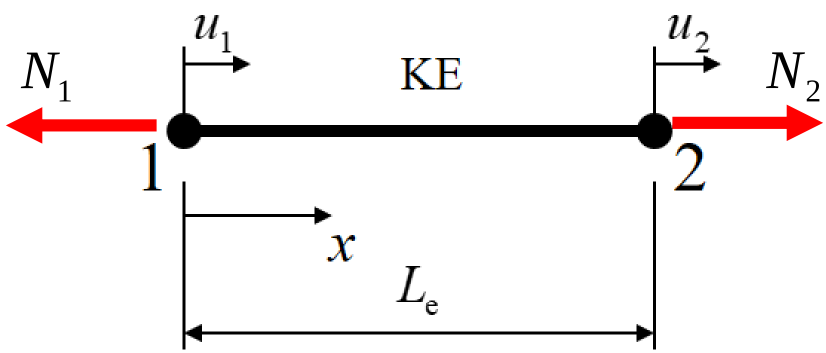
$$\hat{u}(0) = u_1 \;\Rightarrow\; \psi_1(0) = 1 \;\wedge\; \psi_1(L_e) = 0 \;\Rightarrow\; \psi_1(x) = 1 - \frac{x}{L_e}$$

$$\hat{u}(L_e) = u_2 \Rightarrow\; \psi_2(0) = 0 \;\wedge\; \psi_1(L_e) = 1 \;\Rightarrow\; \psi_2(x) = \frac{x}{L_e}$$

Shape functions

FEM – Matrix Equation

$$\int_0^{L_e} EA\, u'(x)v'(x)\mathrm{d}x = N_2\, v(L) - N_1 v(0) + \int_0^{L_e} n_0 v(x)\mathrm{d}x$$



Inserting $\hat{u}(x)$ into weak form

$$u'(x) \approx \hat{u}'(x) = u_1 \frac{-1}{L_e} + u_2 \frac{1}{L_e}$$

$$EA\int_0^{L_e} u'(x)\, v'(x)\, dx = EA\int_0^{L_e} \left[\left(u_1 \frac{-1}{L_e} + u_2 \frac{1}{L_e} \right) \right] v'(x)\, dx = N_2\, v(L) - N_1\, v(0) + \int_0^{L_e} n_0\, v(x)\, dx$$

FEM – Implementation steps

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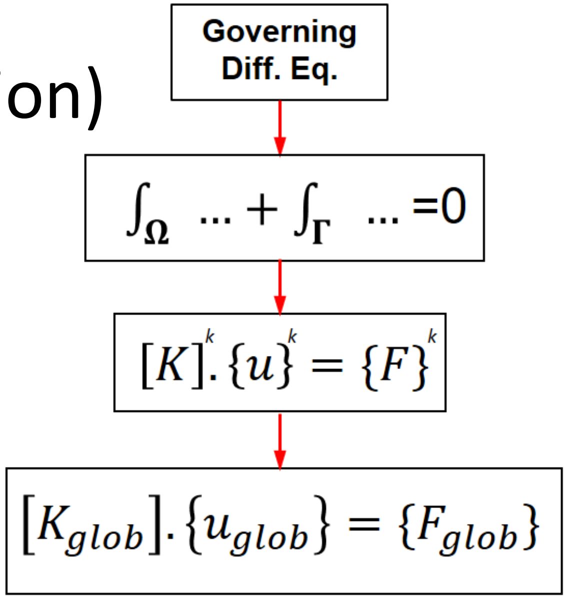

FEM – Matrix Equation

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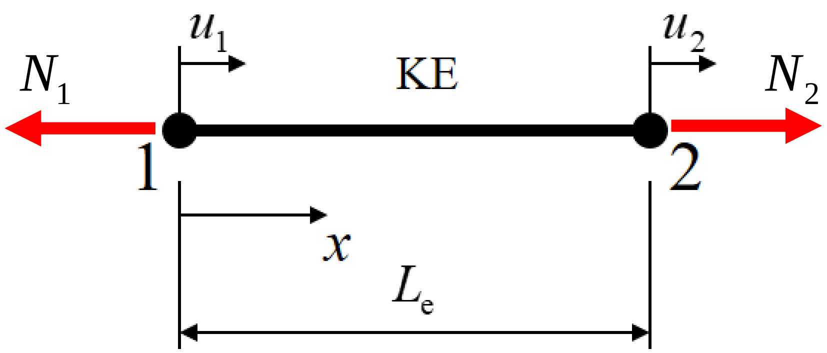
$$EA\int_0^{L_e} u'(x)\; v'(x)\; dx = EA\int_0^{L_e}\left[\left(u_1\frac{-1}{L_e}+u_2\frac{1}{L_e}\right)\right]v'(x)\; dx = N_2\, v(L) - N_1\, v(0) + \int_0^{L_e} n_0\; v(x)\, dx$$

Choice of v(x) – Galerkin approach



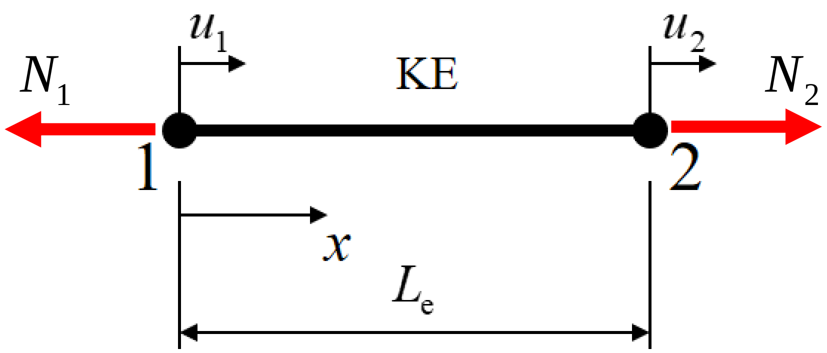
1 $$v(x) = \psi_1(x) = 1 - \frac{x}{L_e}, \qquad v'(x) = -\frac{1}{L_e}$$

$$EA\int_0^{L_e}\left[\left(u_1\frac{-1}{L_e}+u_2\frac{1}{L_e}\right)\right]\left(\frac{-1}{L_e}\right)dx = -\,N_1 + \int_0^{L_e} n_0\;\psi_1(x)\, dx \;\Rightarrow\; \frac{EA}{L_e}(u_1 - u_2) = -\,N_1 + \int_0^{L_e} n_0\;\psi_1(x)\, dx$$

FEM – Matrix Equation

$$EA\int_0^{L_e} u'(x)\, v'(x)\, dx = EA\int_0^{L_e}\left[\left(u_1\frac{-1}{L_e}+u_2\frac{1}{L_e}\right)\right]v'(x)\, dx = N_2\, v(L) - N_1\, v(0) + \int_0^{L_e} n_0\, v(x)\, dx$$

Choice of v(x) – Galerkin approach



2

$$v(x) = \psi_2(x) = \frac{x}{L_e}, \qquad v'(x) = \frac{1}{L_e}$$

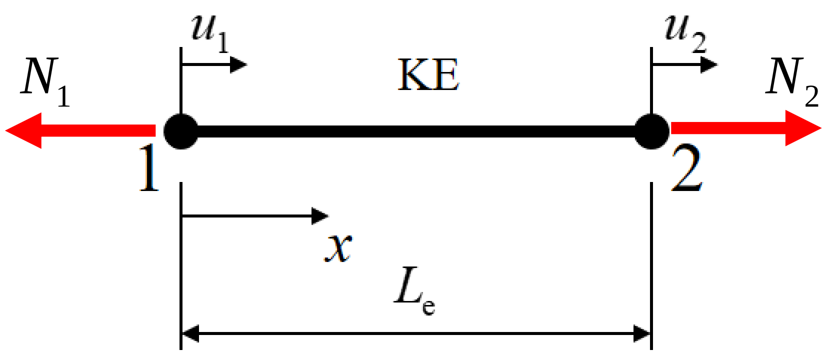
$$EA\int_0^{L_e}\left[\left(u_1\frac{-1}{L_e}+u_2\frac{1}{L_e}\right)\right]\left(\frac{1}{L_e}\right) dx = N_2 + \int_0^{L_e} n_0\, \psi_2(x)\, dx$$

$$\Rightarrow \quad \frac{EA}{L_e}\left(u_2 - u_1\right) = N_2 + \int_0^{L_e} n_0\, \psi_2(x)\, dx$$

FE Matrix Equation

1. $$\frac{EA}{L_e}(u_1 - u_2) = -N_1 + \int_0^{L_e} n_0 \, \psi_1(x)\,dx$$

2. $$\frac{EA}{L_e}(u_2 - u_1) = N_2 + \int_0^{L_e} n_0 \, \psi_2(x)\,dx$$



Finite Element Matrix Equation

$$\frac{EA}{L_e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \begin{Bmatrix} -N_1 \\ N_2 \end{Bmatrix} + \frac{n_0 L_e}{2}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

Matrix Notation

$$\mathbf{K}^k \cdot \mathbf{u}^k = \mathbf{f}^k + \mathbf{f}_{n_0}^k$$

FEM – Implementation steps

- Derivation of Weak Integral Form of Governing Equation
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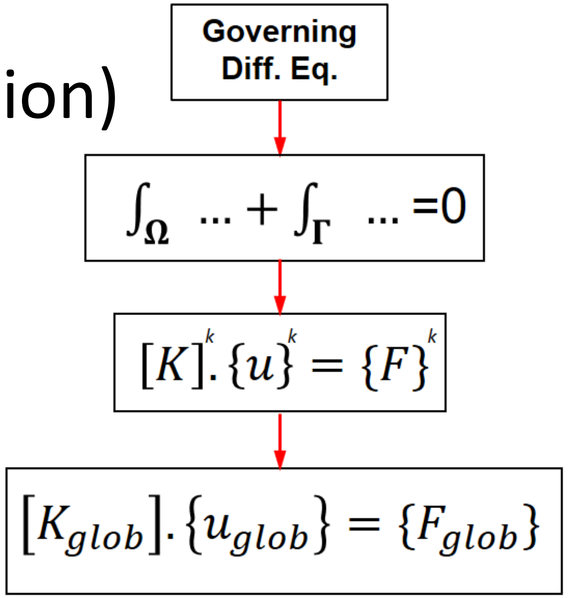
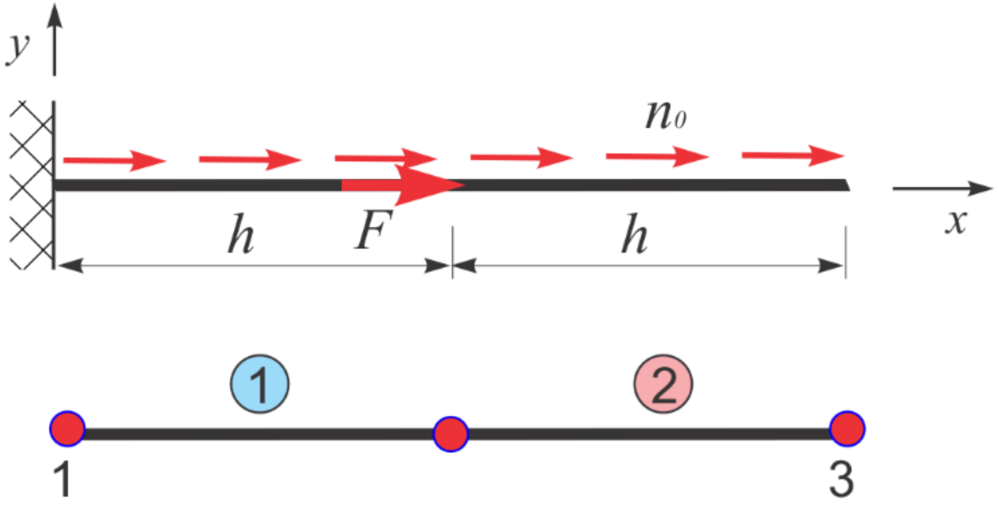


FEM – Meshing

Meshing & Writing FE Matrix Equation for each FE

$$\frac{EA}{h}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \begin{Bmatrix} -N_1^{\textcircled{1}} \\ N_2^{\textcircled{1}} \end{Bmatrix} - \frac{n_0 h}{2}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

$$\frac{EA}{h}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{Bmatrix} u_2 \\ u_3 \end{Bmatrix} = \begin{Bmatrix} -N_2^{\textcircled{2}} \\ N_3^{\textcircled{2}} \end{Bmatrix} - \frac{n_0 h}{2}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$



FEM – The Assembly Process

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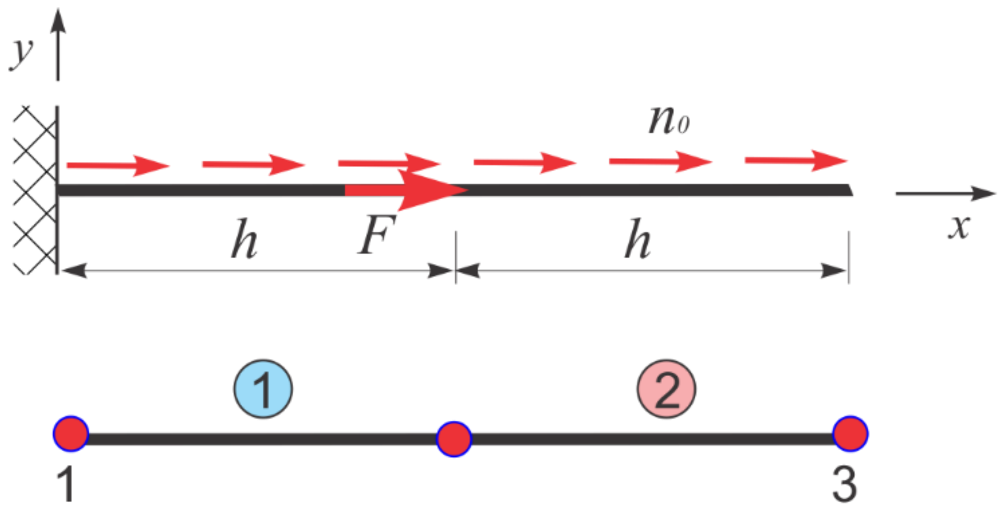
Expansion to all degrees of freedom

$$\frac{EA}{h}\begin{bmatrix}1 & -1 & 0\\ -1 & 1 & 0\\ 0 & 0 & 0\end{bmatrix}\begin{Bmatrix}u_1\\ u_2\\ u_3\end{Bmatrix}=\begin{Bmatrix}-N_1^{①}\\ N_2^{①}\\ 0\end{Bmatrix}-\frac{n_0 h}{2}\begin{Bmatrix}1\\ 1\\ 0\end{Bmatrix}$$

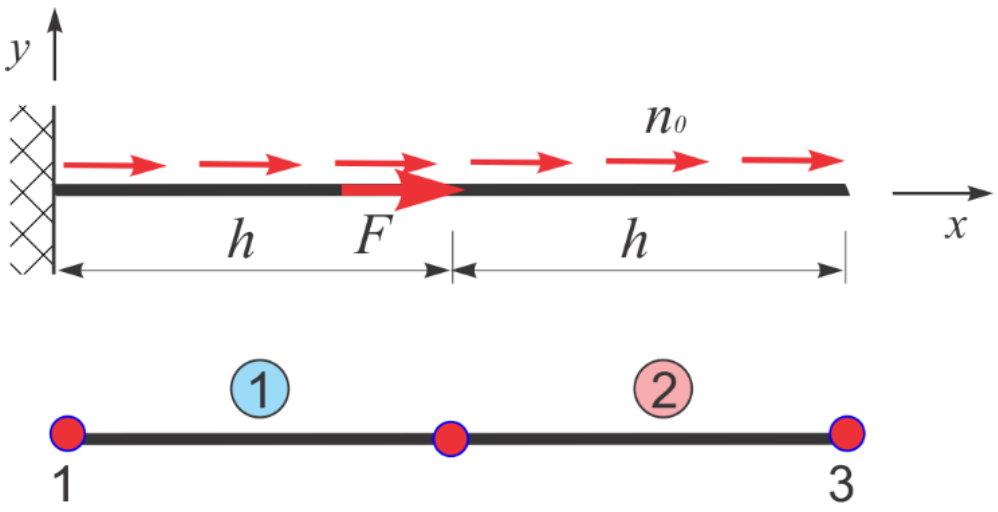
$$\frac{EA}{h}\begin{bmatrix}0 & 0 & 0\\ 0 & 1 & -1\\ 0 & -1 & 1\end{bmatrix}\begin{Bmatrix}u_1\\ u_2\\ u_3\end{Bmatrix}=\begin{Bmatrix}0\\ -N_2^{②}\\ N_3^{②}\end{Bmatrix}-\frac{n_0 h}{2}\begin{Bmatrix}0\\ 1\\ 1\end{Bmatrix}$$



FEM – The Assembly Process

Adding equations together

$$\frac{EA}{h}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 1+1 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix} = \begin{Bmatrix} -N_1^{①} \\ N_2^{①} - N_2^{②} \\ N_3^{②} \end{Bmatrix} - \frac{n_0 h}{2}\begin{Bmatrix} 1 \\ 1+1 \\ 1 \end{Bmatrix}$$



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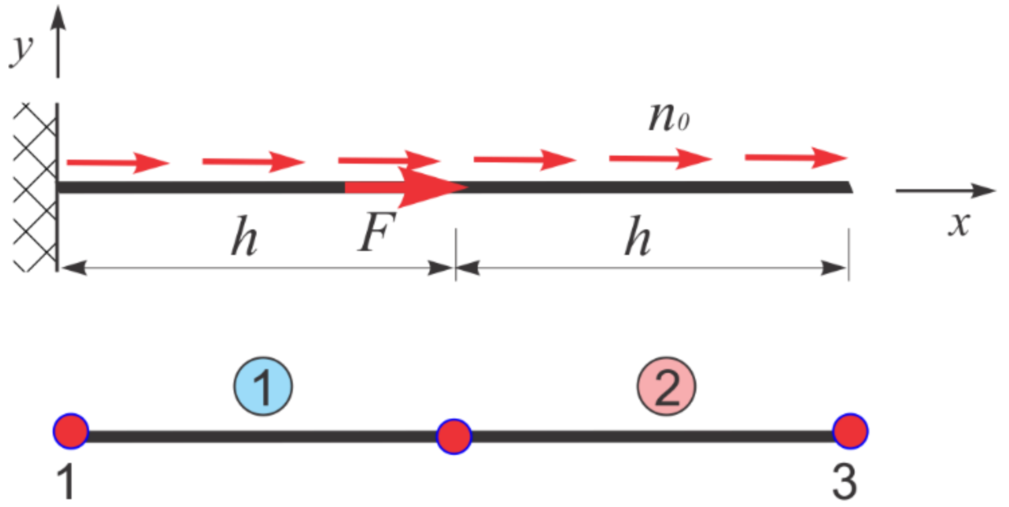
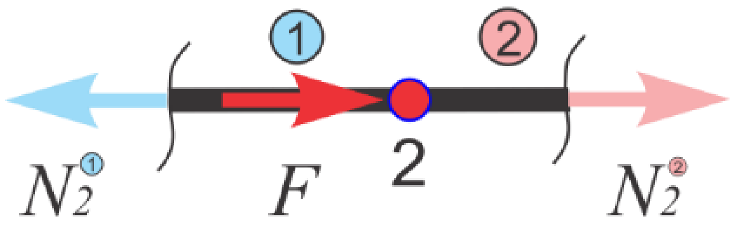
Adding equations together

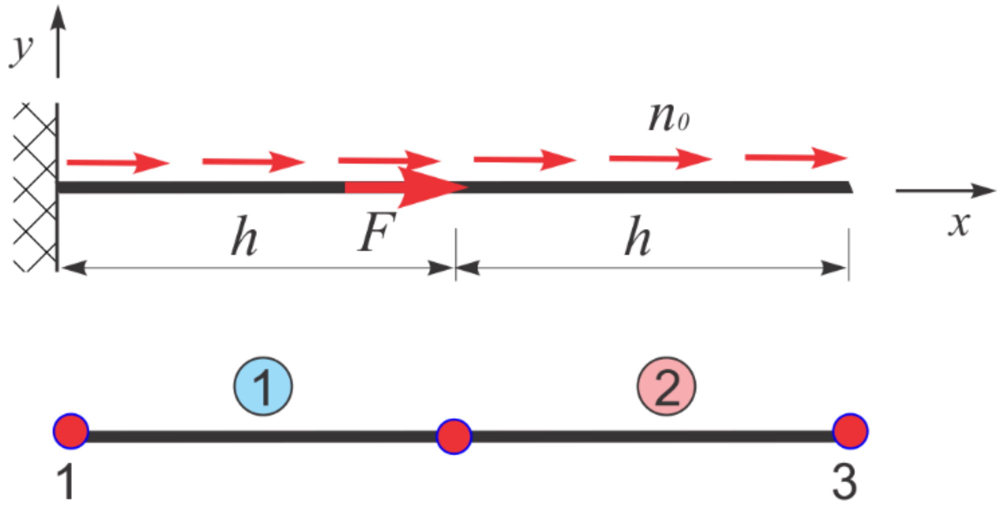
$$\frac{EA}{h}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 1+1 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix} = \begin{Bmatrix} -N_1^{①} \\ \cancel{N_2^{①} - N_2^{②}} \; F_0 \\ N_3^{②} \end{Bmatrix} - \frac{n_0 h}{2}\begin{Bmatrix} 1 \\ 1+1 \\ 1 \end{Bmatrix}$$

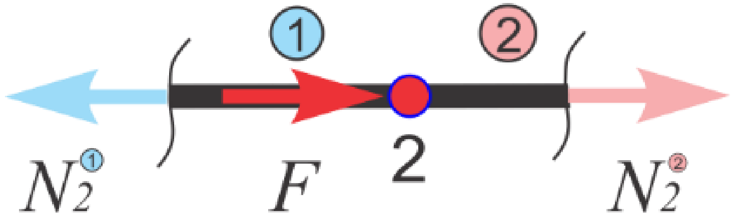


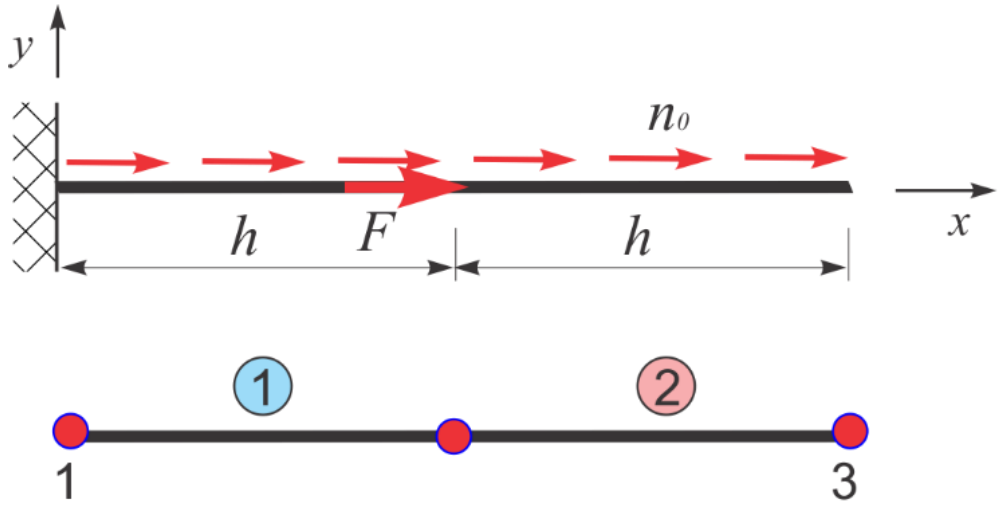


Applying boundary conditions

$$\frac{EA}{h}\begin{bmatrix}1 & -1 & 0\\ -1 & 1+1 & -1\\ 0 & -1 & 1\end{bmatrix}\begin{Bmatrix}u_1 \rightarrow 0\\ u_2\\ u_3\end{Bmatrix}=\begin{Bmatrix}-N_1^{①}\\ N_2^{①}-N_2^{②} \rightarrow F_0\\ N_3^{②} \rightarrow 0\end{Bmatrix}-\frac{n_0 h}{2}\begin{Bmatrix}1\\ 1+1\\ 1\end{Bmatrix}$$







System of equations

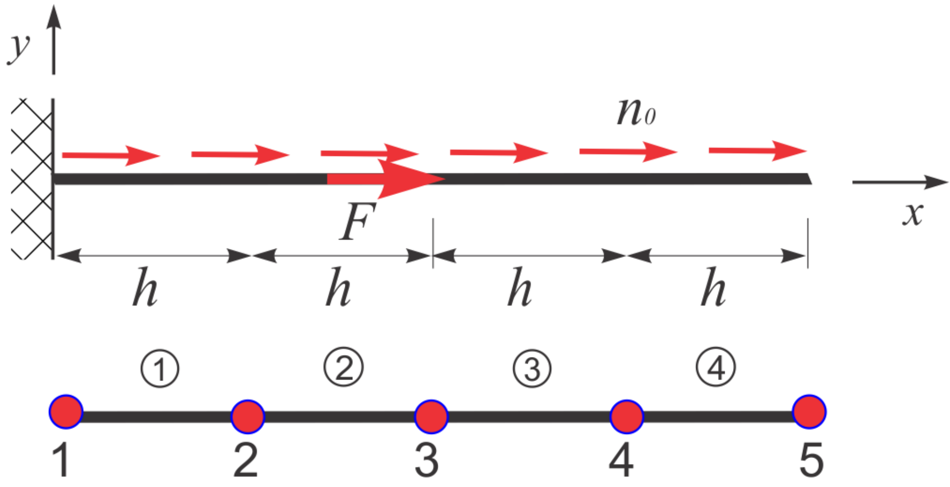
$$\frac{EA}{h}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{Bmatrix} 0 \\ u_2 \\ u_3 \end{Bmatrix} = \begin{Bmatrix} -N_1^{①} \\ F_0 \\ 0 \end{Bmatrix} - \frac{n_0 h}{2}\begin{Bmatrix} 1 \\ 2 \\ 1 \end{Bmatrix}$$

Matrix Notation

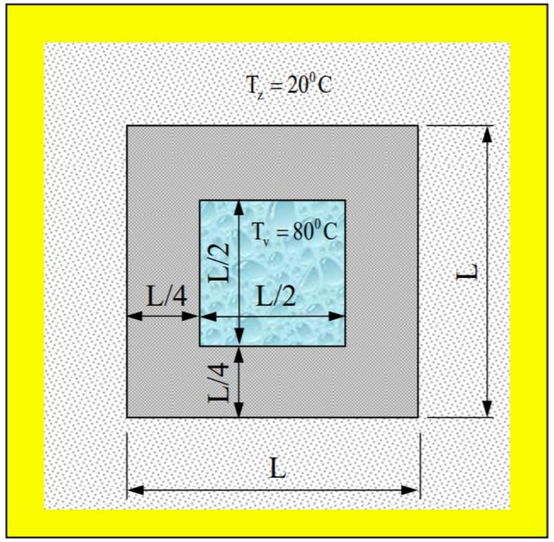
$$\mathbf{K}^{glob} \cdot \mathbf{u}^{glob} = \mathbf{f}^{glob} + \mathbf{f}_{n_0}^{glob}$$

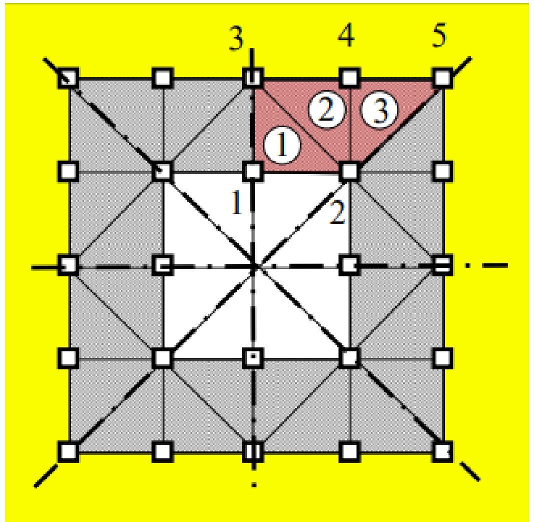
System of equations

$$\frac{EA}{h}\begin{bmatrix}1 & -1 & 0 & 0 & 0\\ -1 & 2 & -1 & 0 & 0\\ 0 & -1 & 2 & -1 & 0\\ 0 & 0 & -1 & 2 & -1\\ 0 & 0 & 0 & -1 & 1\end{bmatrix}\begin{Bmatrix}0\\ u_2\\ u_3\\ u_4\\ u_5\end{Bmatrix}=\begin{Bmatrix}-N_1^{①}\\ 0\\ F\\ 0\\ 0\end{Bmatrix}-\frac{n_0 h}{2}\begin{Bmatrix}1\\ 2\\ 2\\ 2\\ 1\end{Bmatrix}$$



- Stationary heat transfer in 2D





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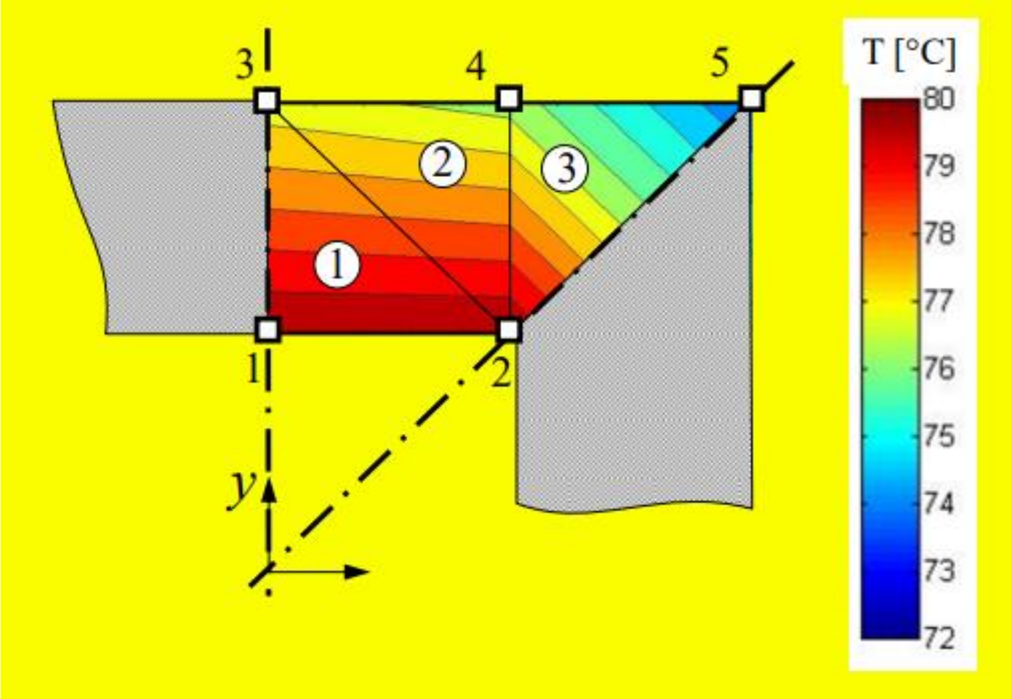

$$k\,\Delta T(x,y) + q_v = 0$$

Boundary Element Method

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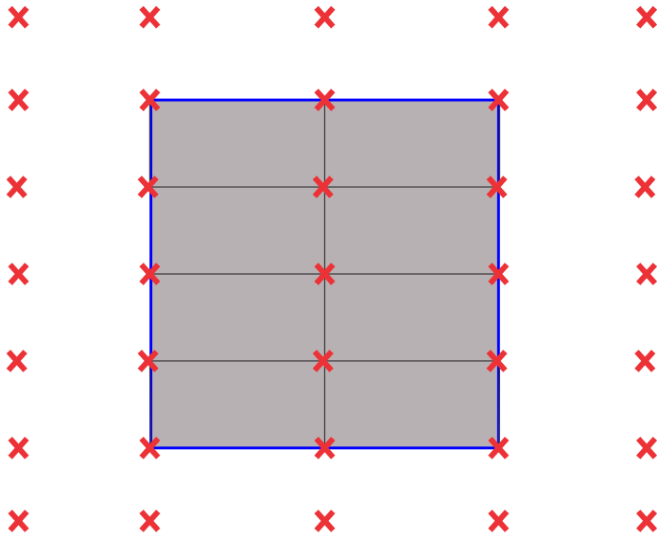
- IDEA: integral based approach
- Starting point of derivation is Inverse Integral Form of governing equation
- Solution boundary is discretized into sub-domains, called boundary elements (BEs)
- In the BE sub-domain (only boundary!) we approximate unknown quantities

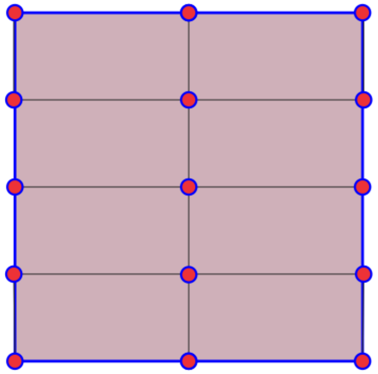
- ADVANTAGE: solution of governing field equations is converted into searching unknown quantities on boundary
- Suitable for solution of potential problems & infinite problems
- DISADVANTAGE: full and non-symmetrical matrices

Boundary Element Method

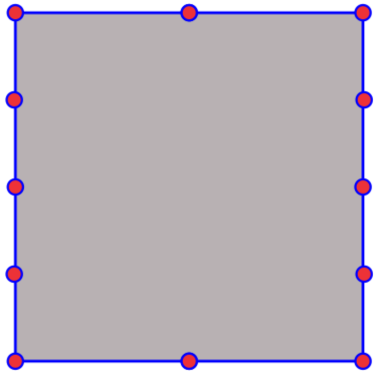
- Basic differences between BVP solution methods



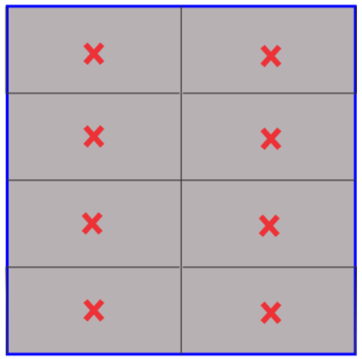
finite differences



finite elements



boundary elements



finite volumes

Finite Volume Method

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- IDEA: integral based approach
- Starting point of derivation is Integral Form of governing equation, where the integral over solution domain is converted in surface integral around the domain
- Solution domain is discretized into sub-domains, called finite volumes (cells or control volumes)
- The unknown solution variable is constant over the cell (calculated at the centre)

- ADVANTAGE: solution of governing field equations is converted into searching unknown quantity in the cell centre.
- Continuity requirements are simply fulfilled.
- Similar to FDM, Suitable for solution of heat transfer & fluid flow problems
- DISADVANTAGE: fulfilment of boundary conditions related to solution variable

Finite Volume Method

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- Presentation on the stationary heat transfer problem

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+q_V=0$$

$$div\left[k\, grad(T)\right]=-q_V$$

$$\int_{\Omega} div\left[k\, grad(T)\right]\, d\Omega=-\int_{\Omega} q_V\; d\Omega$$

Integration over the domain

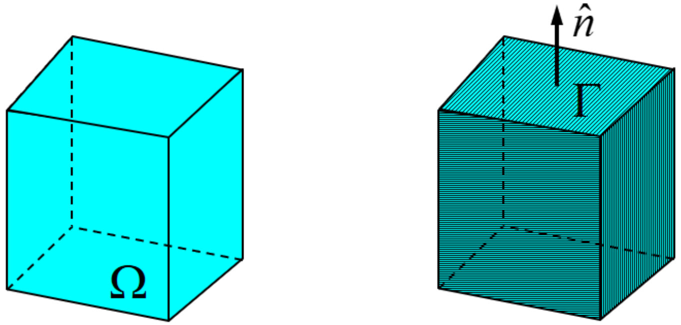
Finite Volume Method

- Green-Gauss theorem

$$\int_{\Omega} div\left[k\, grad(T)\right]\, d\Omega = \int_{\Gamma} k\, grad(T)\, \hat{n}\, d\Gamma$$

$$\int_{\Omega} div\left[k\, grad(T)\right]\, d\Omega = -\int_{\Omega} q_V\, d\Omega$$

$$\int_{\Gamma} k\, grad(T)\, \hat{n}\, d\Gamma = -\int_{\Omega} q_V\, d\Omega$$



$$\int_{\Omega} div\left[k\, grad(T)\right]\, d\Omega = \int_{\Gamma} k\, grad(T)\, \hat{n}\, d\Gamma$$

Heat balance over control volume

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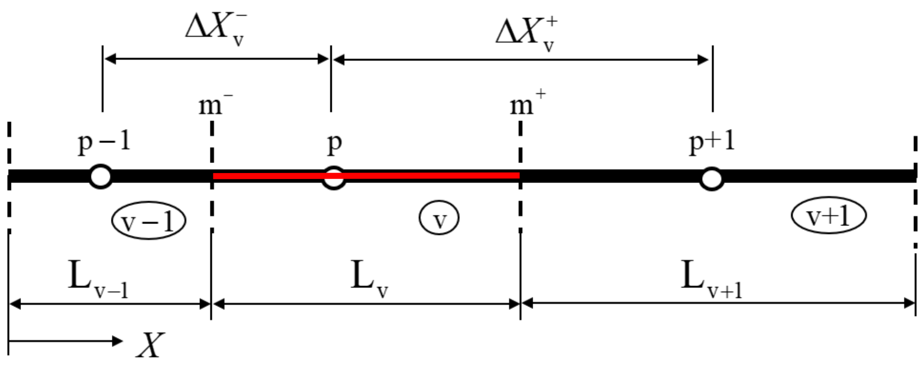
- Reduction to 1D $T = T(x)$

$$\int_{\Gamma} k\, grad(T)\, \hat{n}\, d\Gamma = -\int_{\Omega} q_V\, d\Omega \;\Rightarrow\; \int_{\Gamma} k \frac{dT}{dx} n_x\, d\Gamma = -\int_0^L q_V\, A dx$$

Since the temperature is unknown, we use approximation

$$\int_{\Gamma_v} k \frac{dT}{dx} n_x\, d\Gamma \approx \left[\left(\frac{k\,A}{\Delta X_v} \right)_{m^+} (T_{p+1} - T_p) \right] - \left[\left(\frac{k\,A}{\Delta X_v} \right)_{m^-} (T_p - T_{p-1}) \right]$$



Finite Volume Method

- Reduction to 1D $T = T(x)$

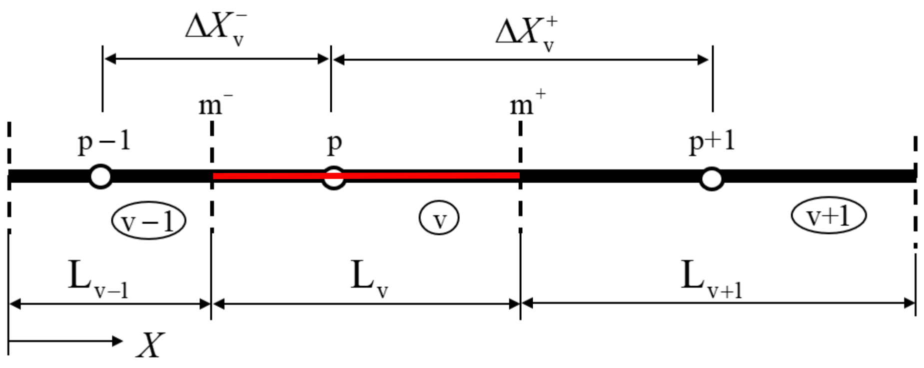
$$\int_{\Gamma} k\, grad(T)\, \hat{n}\, d\Gamma = -\int_{\Omega} q_V \, d\Omega \quad \Rightarrow \quad \int_{\Gamma} k \frac{dT}{dx} n_x \, d\Gamma = -\int_0^L q_V \, A dx$$

Right-hand side of the equation, we approximate as

$$-\int_0^{L_v} q_V \, A dx \approx -(q_V)_p \, A_p \, L_v$$

Finite volume equation

$$\left[\left(\frac{k A}{\Delta X_v}\right)_{m^+} (T_{p+1} - T_p)\right] - \left[\left(\frac{k A}{\Delta X_v}\right)_{m^-} (T_p - T_{p-1})\right] = -(q_V)_p \, A_p \, L_v$$

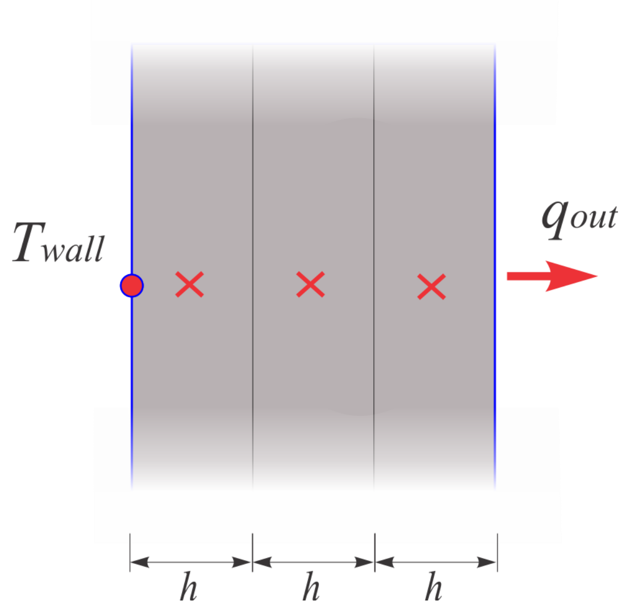


Finite Volume Method

- System of equations

$$\frac{k}{h}\begin{bmatrix}-3 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1\end{bmatrix}\begin{Bmatrix}T_1 \\ T_2 \\ T_3\end{Bmatrix}=\begin{Bmatrix}-2k/hT_{wall} \\ 0 \\ -q_{out}\end{Bmatrix}$$

Heat transfer problem



Thank you for your attention!

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