

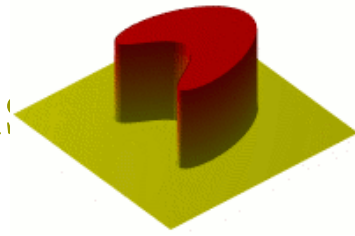
Topics on PDEs and Numerical Methods



Part 3: Finite Element Method

Guangming Yao
Department of Mathematics
Clarkson University

Three fundamental PDEs and solutions



Heat equation (parabolic): $u_t = u_{xx}$

- Solution: $u = \frac{1}{2}x^2 + t$
- Challenge: can you find another solution? $u = e^{ax+bt}$
- Fourier, 1800's
- Heat conduction

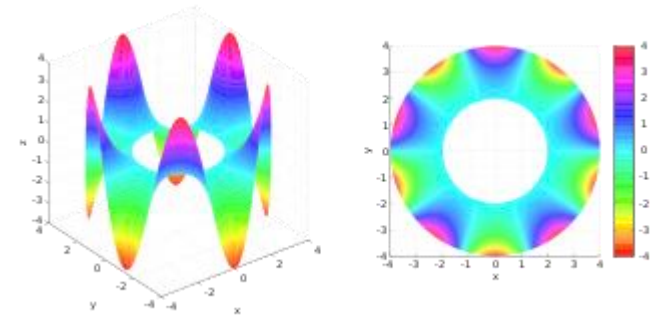
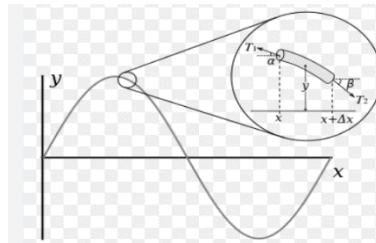
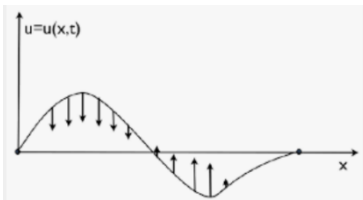
Wave equation (hyperbolic): $u_{tt} = u_{xx}$

- d'Alembert, 1740's, vibration of strings

Laplace equation (elliptic): $u_{xx} + u_{yy} = 0$

- Laplace, 1780's,
- gravitation mechanical equilibrium,
- thermal equilibrium

Vibration, [standing waves](#) in a string. The [fundamental](#) and the first 5 [overtones](#) in the [harmonic series](#).



Laplace's equation on an [annulus](#) (inner radius $r = 2$ and outer radius $R = 4$) with Dirichlet boundary conditions $u(r=2) = 0$ and $u(R=4) = 4 \sin(5 \theta)$

Common but Challenging PDEs

□ Diffusion equation

$$\nabla \cdot D \nabla C + S = 0$$

□ Solid-Mechanics

$$\nabla \cdot (\rho \vec{u} \vec{u}^T) = -\nabla P + \nabla \cdot \tau + \rho g$$

□ Navier-Stokes

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla P = \mu \nabla^2 \vec{u} + \frac{\mu}{3} \nabla(\nabla \cdot \vec{u}) + \rho g$$

□ Schrodinger

$$\nabla \cdot \left[-\frac{\hbar^2}{2m^*} \nabla \psi(\vec{r}) \right] + U(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$$

□ Dynamics Electromagnetic wave equation

$$\frac{\mu \epsilon \partial^2 \vec{E}(\vec{r}, t)}{\partial t^2} + \frac{\mu \sigma \partial \vec{E}(\vec{r}, t)}{\partial t} - \nabla^2 \vec{E}(\vec{r}, t) = -\frac{\mu \partial \vec{j}(\vec{r}, t)}{\partial t}$$

□ Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q\mathbf{E}}{\hbar} \cdot \nabla_k f = \left(\frac{\partial f}{\partial t} \right)_c$$

How to solve PDEs?

Analytically:

- Method of characteristic
- Separation of variables
- Fourier analysis---- $\sin(x)$, $\cos(x)$, Bessel's function, Legendre, ..
- Eigenfunction expansion
- Problems:
 - cannot deal with complicated geometry
 - May not converge with finite terms
 - Hard to deal with nonlinear

Numerically:

Finite difference method (FDM)

Finite element method (FEM)

Finite volume method

Reduce order method

Combination of analytical and numerical methods

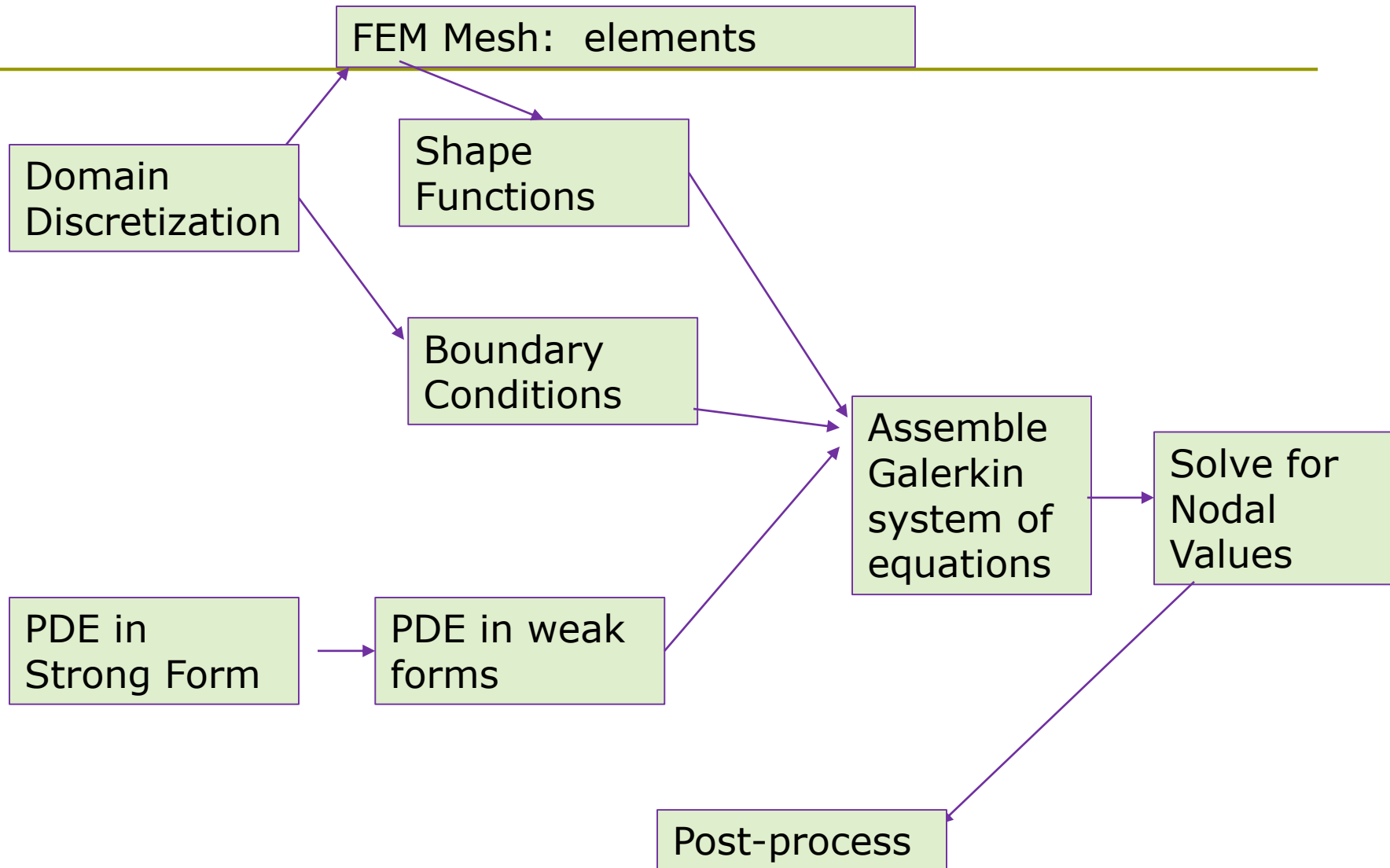
How to solve PDEs?

- **Analytic solutions** are possible for simple and special (idealized) cases only.
- To make use of the nature of the equations, **different methods are used to solve different classes of PDEs.**
- The methods discussed here are based on the **finite element** technique.
- **Methods other than FEM: FDM, Spectral Method, FVM, ...**

• **Finite Element Method (FEM)**

- **How to solve PDEs using FEM?**
 - Numerical interpolation: **shape functions**
 - Domain discretization: **mesh**
 - **Weak and strong** forms of PDE
 - Linear or nonlinear system solver

Summary of FEM Process

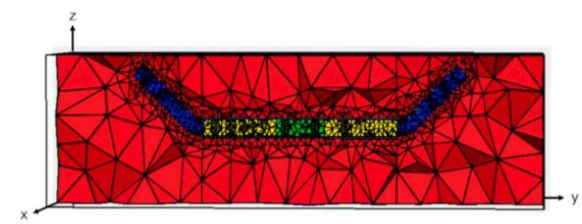


Generalization of FEM

- Divide geometry into simple elements

- Finding polynomial approximation on each element: **unknown** $a_0, a_1, a_2, \dots, a_n$
 - 1D: $\tilde{C}(x) = a_0 + a_1x + a_2x^2 + \dots$
 - 2D: $\tilde{C}(x) = a_0 + a_1x + a_2y + a_3xy + \dots$
 - 3D: $\tilde{C}(x) = a_0 + a_1x + a_2y + a_3z + \dots$
- Continuous across elements
- PDE → System of equations → Solve nodal values

Elements



- Divide geometry into simple elements

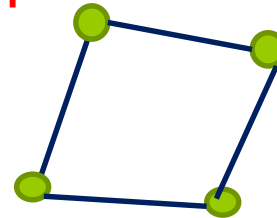
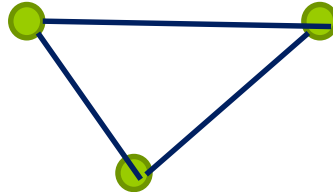
- Elements have **nodes**



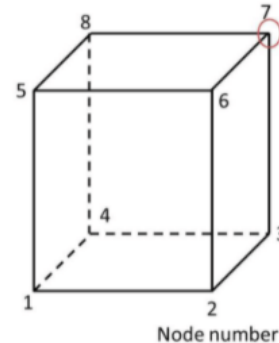
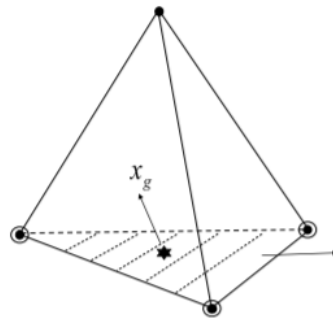
- Elements include **line segments** in 1D



- Elements include **triangular** or **quadrilateral mesh** in 2D



- Elements include tetrahedrons or hexahedrons in 3D



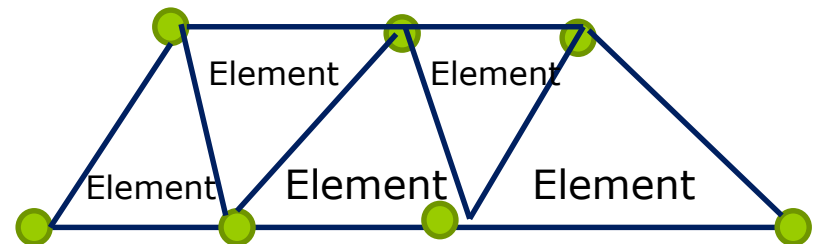
Elements

- Each element has its own coefficients:
 - One for each node: $a_0, a_1, a_2, \dots, a_n$
- Construct shape functions, meanwhile get continuous piecewise polynomial between elements:

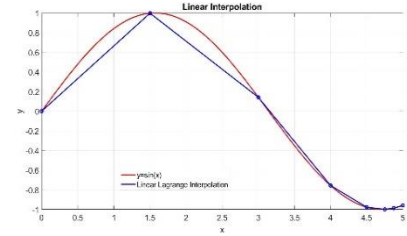
Write solution
in terms of
values at nodes

Adjacent
elements
share nodes

Automatically
continuous
between elements



Construct shape functions in 1D



- Construct shape functions by writing solutions in terms of functions' values

Consider **single element**

2 nodes in 1D: $\tilde{C}(x) = a_0 + a_1x$

Find a_0 and a_1 by solving

$$C_1 = \tilde{C}(x_1) = a_0 + a_1x_1$$

$$C_2 = \tilde{C}(x_2) = a_0 + a_1x_2$$



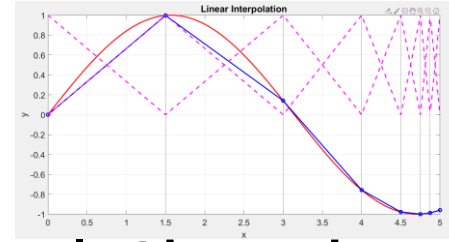
$$\text{Thus, } \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix}^{-1} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \frac{1}{x_2 - x_1} \begin{bmatrix} x_2 & -x_1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}.$$

That is:

$$\tilde{C}(x) = \frac{C_1x_2 - C_2x_1}{x_2 - x_1} + \frac{-C_1 + C_2}{x_2 - x_1}x.$$

$$\tilde{C}(x) = \frac{x_2 - x}{x_2 - x_1}C_1 + \frac{-x_1 + x}{x_2 - x_1}C_2.$$

Construct shape functions in 1D



- Construct shape functions by writing solutions in terms of functions' values

- For a **single element**



$$\tilde{C}(x) = \frac{x_2 - x}{x_2 - x_1} C_1 + \frac{-x_1 + x}{x_2 - x_1} C_2.$$

$$\tilde{C}(x) = N_1(x) C_1 + N_2(x) C_2.$$

- Shape functions**—AKA interpolation functions, basis functions for the solution:

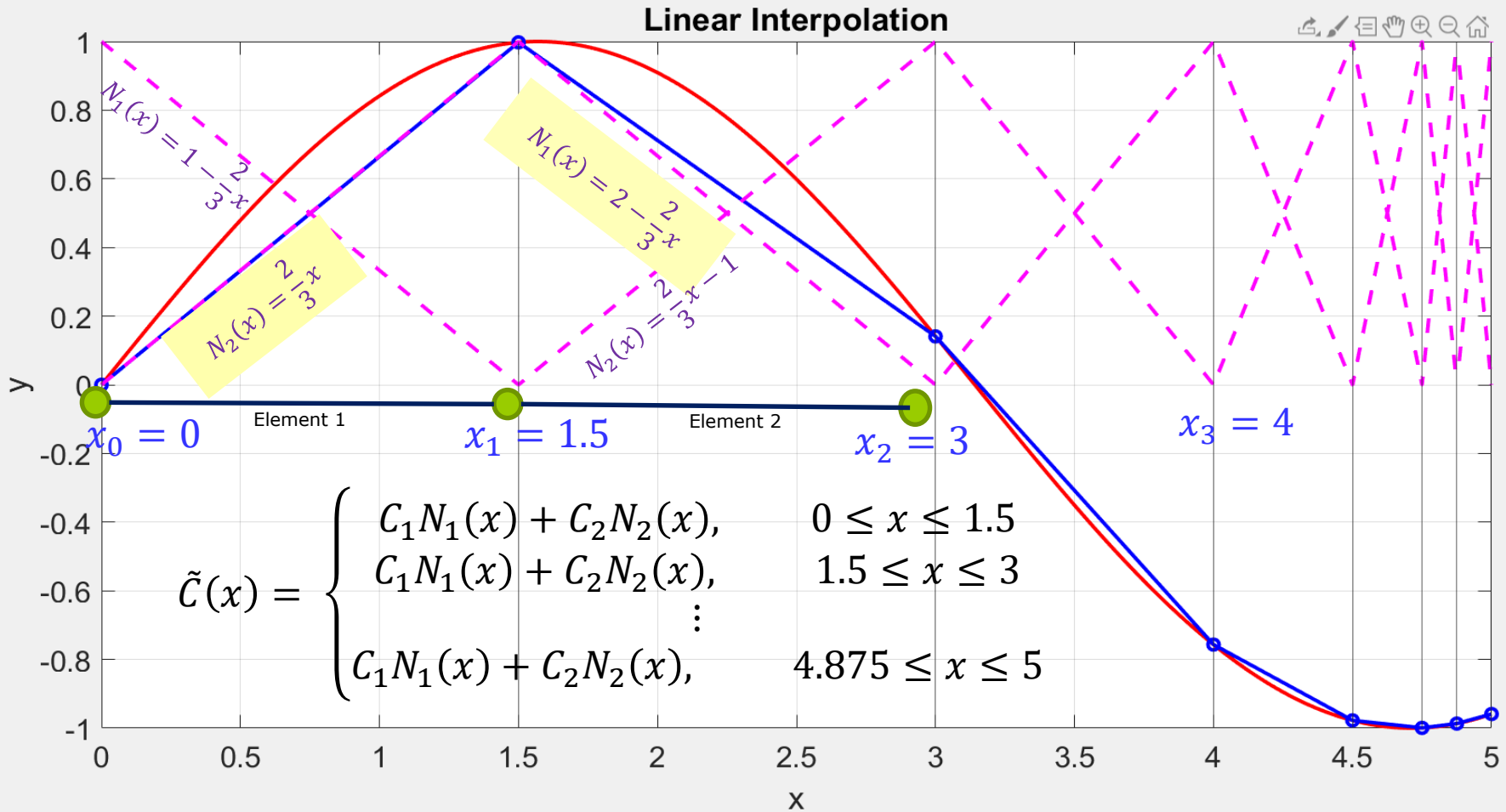
$$N_1(x) = \frac{x_2 - x}{x_2 - x_1}, N_2(x) = \frac{-x_1 + x}{x_2 - x_1}$$

- Solution is a linear combination of shape functions**

$$\tilde{C}(x) = N_1(x) C_1 + N_2(x) C_2 = \sum_{i=1}^2 N_i C_i = \vec{N} \cdot \vec{C}.$$

Exa 1: Interpolation

$$C(x) = \sin(x), 0 \leq x \leq 5$$




Approximation includes all spatial dependence: $\tilde{C}(x) = \sum_i N_i C_i = \vec{N} \cdot \vec{C}$

- Depend on coordinates of nodes
- $N_i = 1$ at node i , $N_i = 0$ at all other nodes
- Zero outside their element

Exa 1: Interpolation--higher order shape functions

Order 1

Linear lagrange



C_1
 x_1

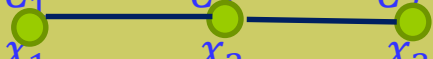
C_2
 x_2

2 nodes, 2 DOF

$$\tilde{C}(x) = a_0 + a_1x$$

Order 2

Quadratic line segment



C_1
 x_1

C_2
 x_2


C_3
 x_3

3 nodes, 3 DOF

$$\tilde{C}(x) = a_0 + a_1x + a_2x^2$$

Order 3

Cubic line segment



C_1
 x_1

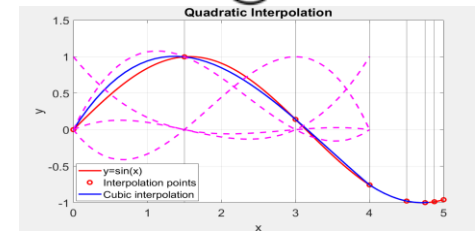
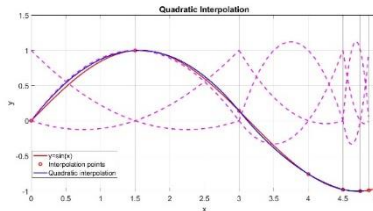
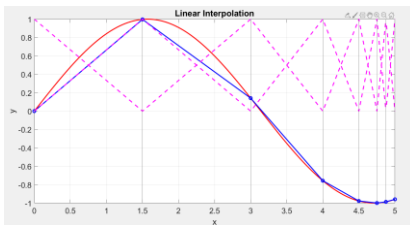
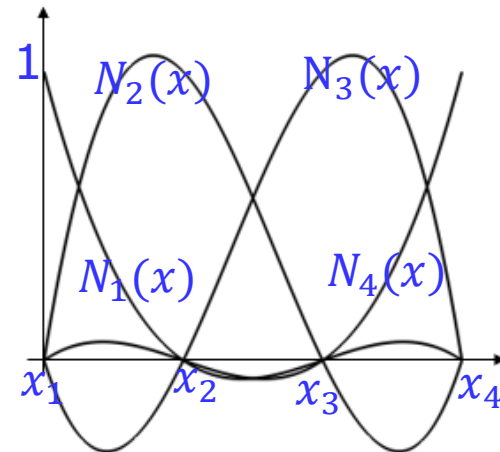
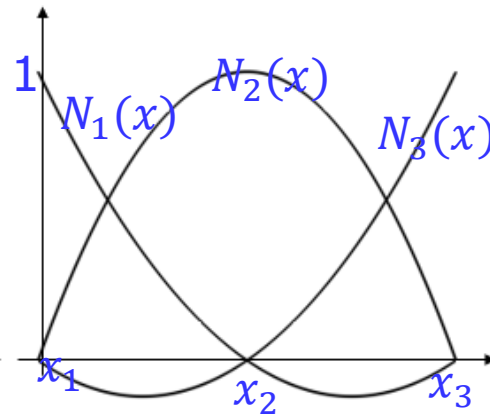
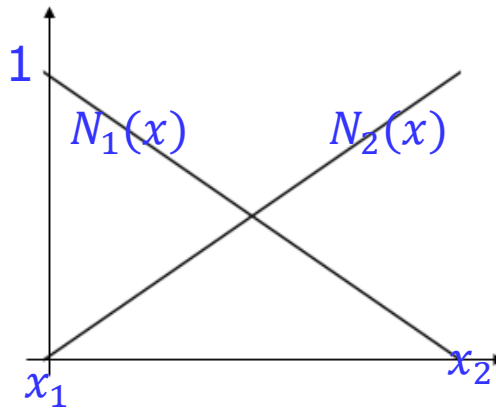
C_2
 x_2

C_3
 x_3

C_4
 x_4

4 nodes, 4 DOF

$$\tilde{C}(x) = a_0 + a_1x + a_2x^2 + a_3x^3$$

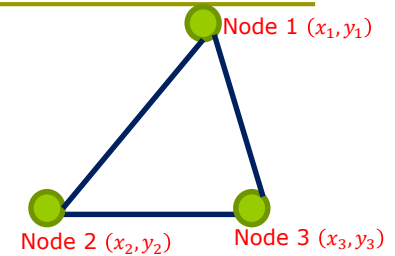


Construct shape functions in 2D

- Construct shape functions by writing solutions in terms of functions' values

Consider **single element**

3 nodes in 2D: $\tilde{C}(x, y) = a_0 + a_1x + a_2y$



Find a_0, a_1 and a_2 (3 degree of freedom DOF):

$$C_1 = \tilde{C}(x_1, y_1) = a_0 + a_1x_1 + a_2y_1$$

$$C_2 = \tilde{C}(x_2, y_2) = a_0 + a_1x_2 + a_2y_2$$

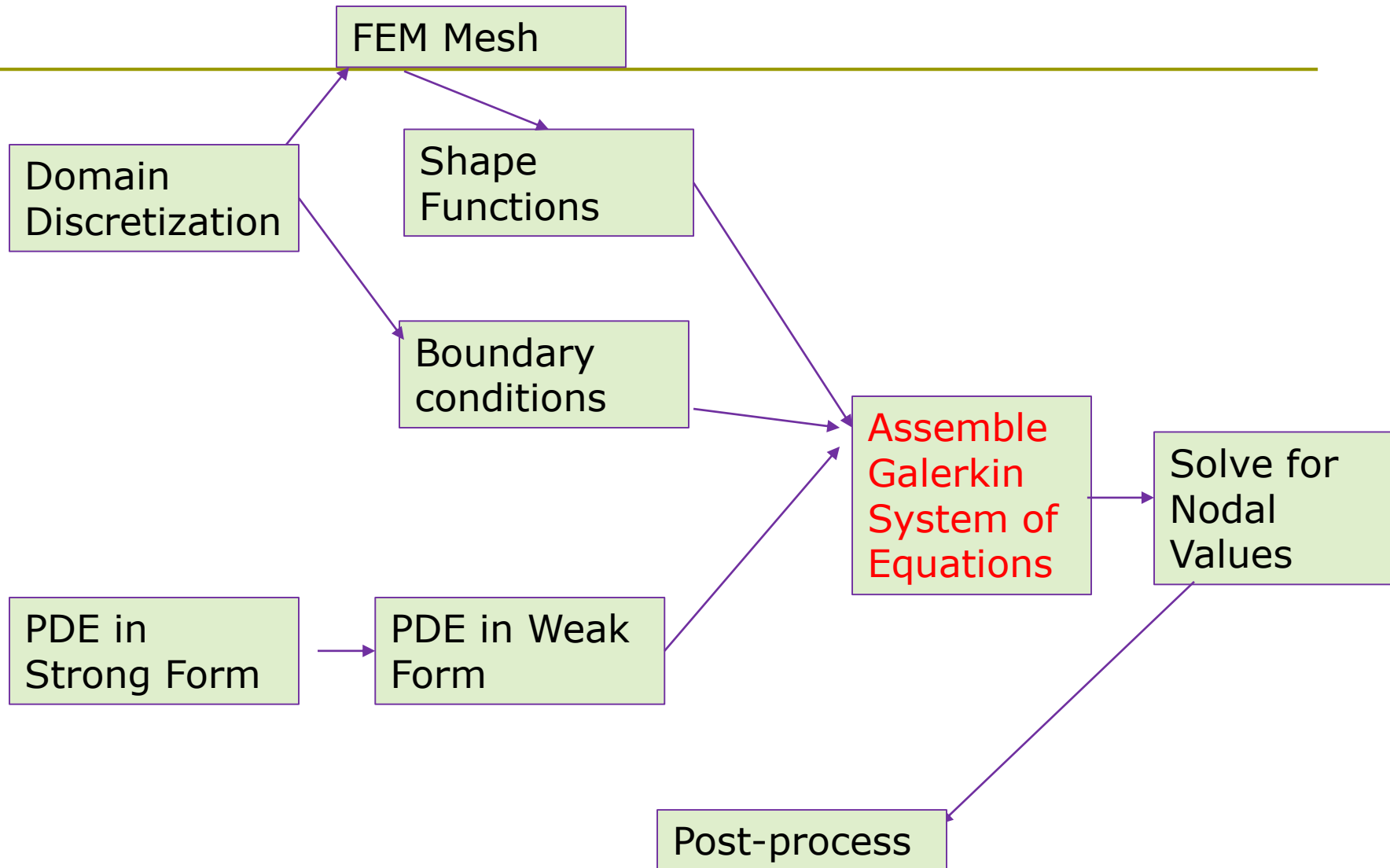
$$C_3 = \tilde{C}(x_3, y_3) = a_0 + a_1x_3 + a_2y_3$$

$$\rightarrow \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}^{-1} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} = \frac{1}{x_2y_3 + x_1y_2 + x_3y_1 - x_2y_1 - x_3y_2 - x_1y_3} \begin{bmatrix} x_2y_3 - x_3y_2 & x_3y_1 - x_1y_3 & x_1y_2 - x_2y_1 \\ y_2 - y_3 & y_3 - y_1 & y_1 - y_2 \\ x_3 - x_2 & x_1 - x_3 & x_2 - x_1 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \end{bmatrix}.$$

Collect $C_1, C_2,$ & C_3 to get shape functions:

$$\tilde{C}(x) = N_1(x, y)C_1 + N_2(x, y)C_2 + N_3(x, y)C_3 = \sum_j N_j C_j = \vec{N} \cdot \vec{C}.$$

Summary of FEM Process



Exa 2: Steady state heat eqn

$$\nabla \cdot \mathbf{F} = \frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z}$$

$$\nabla f = \left\langle \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right\rangle$$

Strong form of PDE:

$$\nabla \cdot k \nabla C - S = 0 \text{ on } \Omega$$

Diffusion eqn

$$k \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - S = 0 \text{ if } k \text{ is constant}$$

- Step 1. Use $\tilde{C} \approx C$, now PDE with residual R

$$\nabla \cdot k \nabla \tilde{C} - S = R \text{ on } \Omega$$

- Step 2. Want weighted error

$$\int w \nabla \cdot k \nabla \tilde{C} - w S d\Omega = 0. \quad \leftarrow \text{Derivative twice}$$

- Step 3. Use Cal III identity:

$$\nabla (a \vec{b}) = \nabla a \cdot \vec{b} + a \nabla \vec{b} \text{ for } a = w, \vec{b} = k \nabla \tilde{C}$$

$$\int \nabla \cdot w k \nabla \tilde{C} - \nabla w \cdot k \nabla \tilde{C} - w S d\Omega = 0.$$

Weaker constraints on solution

- Step 4. Apply Divergence Theorem

$$\int \nabla \cdot w k \nabla \tilde{C} = \oint_{\Omega} \hat{n}_{\Omega} \cdot w k \nabla \tilde{C} d\Omega$$

- Step 5. **Weak form** of diffusion equation Derivative once

$$\oint_{\Omega} \hat{n}_{\Omega} \cdot w k \nabla \tilde{C} d\Omega - \int \nabla w \cdot k \nabla \tilde{C} - w S d\Omega = 0.$$

Exa 2: Boundary Condition

$$D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - S = 0 \text{ if } D \text{ is constant}$$

$$\nabla \cdot D \nabla C - S = 0 \text{ on } \Omega$$

- Assume a tank with no leaks, i.e. zero flux BC

$$\hat{n}_\Omega \cdot k \nabla C = 0.$$

- Weak form without BC

$$\oint_\Omega \hat{n}_\Omega \cdot w k \nabla \tilde{C} d\Omega - \int \nabla w \cdot k \nabla \tilde{C} - w S d\Omega = 0.$$

- Weak form with no flux

$$\int \nabla w \cdot k \nabla \tilde{C} + w S d\Omega = 0.$$

$$k \int \frac{\partial w}{\partial x} \frac{\partial \tilde{C}}{\partial x} + \frac{\partial w}{\partial y} \frac{\partial \tilde{C}}{\partial y} + w S d\Omega = 0$$

- Other possible BCs:

Dirichlet, Neumann, Robin, Mixed, Cauchy

Fixed values

Flux/Natural

Exa 2: Galerkin Finite-Element Method

- Galerkin: $w(\vec{x}) = N_i$ for all i (all basis functions)

$$\int \nabla w \cdot k \nabla \tilde{C} + w S d\Omega = 0.$$

- Recall interpolation when given nodal values \vec{c} :

$$\int \nabla N_i \cdot k \sum_j C_j \nabla N_j + N_i S d\Omega = 0$$

$$\tilde{C}(x) = \sum_j N_j C_j = \vec{N} \cdot \vec{C}$$

$$\int k \sum_j \nabla N_i \cdot \nabla N_j d\Omega C_j = - \int N_i S d\Omega$$

$$\nabla \tilde{C} = \vec{C} \cdot \nabla \vec{N} = \sum_j C_j \nabla N_j$$

In Matrix Form

$[K]$

\vec{C}

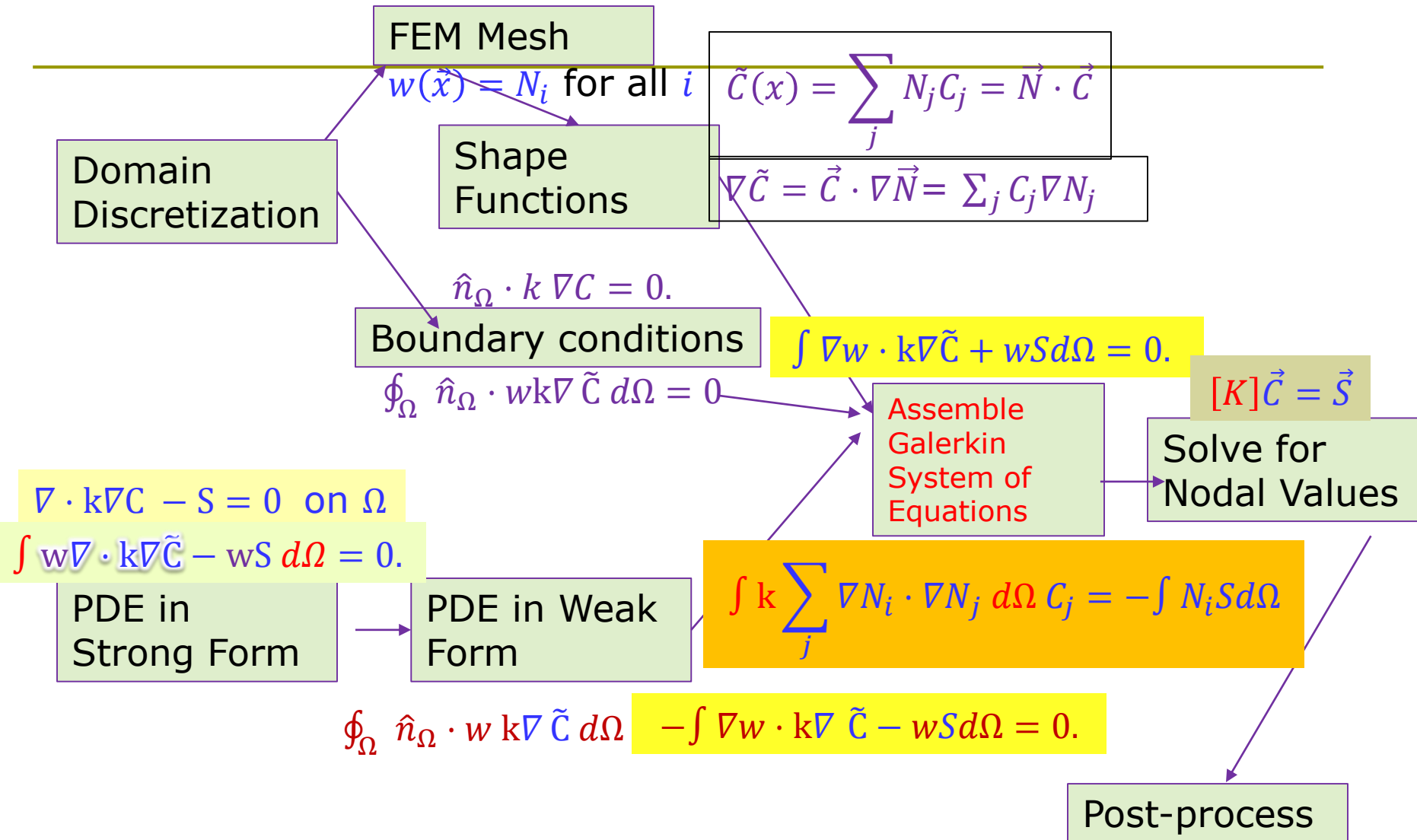
\vec{S}

$$[K] \vec{C} = \vec{S}$$

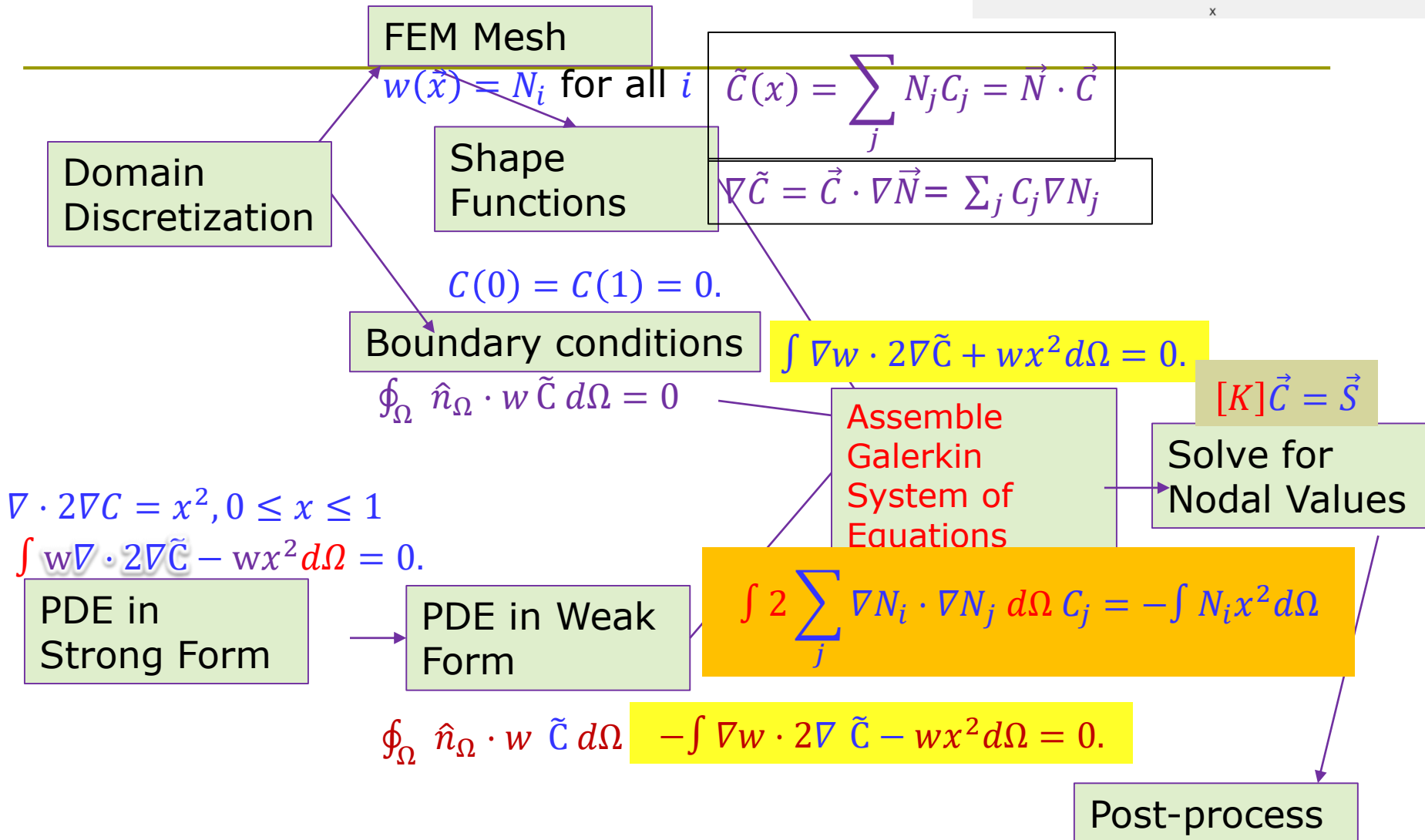
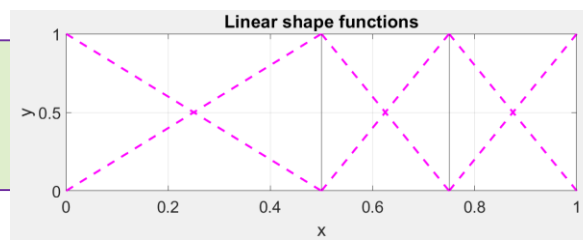
- Calculate integral as sum of integral of each element:

$$\int d\Omega = \sum \int d\Omega_{element}$$

Exa 2: Steady state heat eqn -- summary

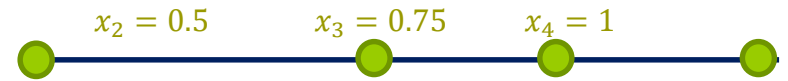


Exa 3: 1D Diffusion



Exa 3: 1D diffusion

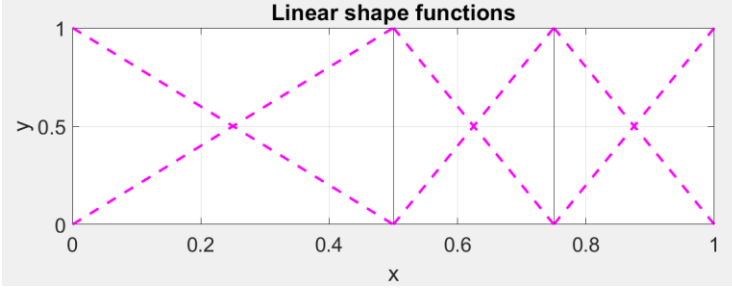
$x_1 = 0$



- Solve ODE: $\nabla \cdot 2\nabla C = x^2, 0 \leq x \leq 1$
 $C(0) = C(1) = 0.$

- Galerkin linear shape function gives

$$\int 2 \sum_j \nabla N_i \cdot \nabla N_j d\Omega C_j = -\int N_i x^2 d\Omega$$



- $$\begin{cases} \sum_j (\int 2 \nabla N_1 \cdot \nabla N_j d\Omega_1) C_j = -\int N_1 x^2 d\Omega_1 \\ \sum_j (\int 2 \nabla N_2 \cdot \nabla N_j d\Omega_1) C_j = -\int N_2 x^2 d\Omega_1 - \int N_2 x^2 d\Omega_2 \\ \sum_j (\int 2 \nabla N_3 \cdot \nabla N_j d\Omega_1) C_j = -\int N_3 x^2 d\Omega_2 - \int N_3 x^2 d\Omega_3 \\ \sum_j (\int 2 \nabla N_4 \cdot \nabla N_j d\Omega_1) C_j = -\int N_4 x^2 d\Omega_3 \end{cases}$$

- $$\begin{cases} (\int 2 \nabla N_1 \cdot \nabla N_1 d\Omega_1) C_1 + (\int 2 \nabla N_1 \cdot \nabla N_2 d\Omega_2) C_2 = -\int N_1 x^2 d\Omega_1 \\ (\int 2 \nabla N_2 \cdot \nabla N_1 d\Omega_1) C_1 + (\int 2 \nabla N_2 \cdot \nabla N_2 d\Omega_2) C_2 + (\int 2 \nabla N_2 \cdot \nabla N_3 d\Omega_3) C_3 = -\int N_2 x^2 d\Omega_1 - \int N_2 x^2 d\Omega_2 \\ (\int 2 \nabla N_3 \cdot \nabla N_2 d\Omega_2) C_2 + (\int 2 \nabla N_3 \cdot \nabla N_3 d\Omega_3) C_3 + (\int 2 \nabla N_3 \cdot \nabla N_4 d\Omega_4) C_4 = -\int N_3 x^2 d\Omega_2 - \int N_3 x^2 d\Omega_3 \\ (\int 2 \nabla N_4 \cdot \nabla N_3 d\Omega_3) C_3 + (\int 2 \nabla N_4 \cdot \nabla N_4 d\Omega_4) C_4 = -\int N_4 x^2 d\Omega_3 \end{cases}$$

$$\begin{bmatrix} 4 & -4 & 0 & 0 \\ -4 & 12 & -8 & 0 \\ 0 & -8 & 16 & -8 \\ 0 & 0 & -8 & 8 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = \begin{bmatrix} 0.0104 \\ 0.0742 \\ 0.1432 \\ 0.1055 \end{bmatrix} \Rightarrow \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0.01823 \\ 0.01806 \\ 0 \end{bmatrix}$$

Exa 4: Heat conduction equation

$$\left(\frac{\partial \rho C T(\vec{r}, t)}{\partial t} - \nabla \cdot k \nabla T(\vec{r}, t) = f(\vec{r}, t) \right)$$

Weak form: $\int_{\Omega} w \left(\frac{\partial \rho C \tilde{T}(\vec{r}, t)}{\partial t} - \nabla \cdot k \nabla \tilde{T}(\vec{r}, t) = f(\vec{r}, t) \right) d\Omega$

Galerkin FEM: $\int_{\Omega} N_i(\vec{r}) \left(\frac{\partial \rho C \tilde{T}(\vec{r}, t)}{\partial t} - \nabla \cdot k \nabla \tilde{T}(\vec{r}, t) = f(\vec{r}, t) \right) d\Omega$

$$\int_{\Omega} N_i(\vec{r}) \left(\frac{\partial \rho C \tilde{T}(\vec{r}, t)}{\partial t} - \nabla \cdot k \nabla \tilde{T}(\vec{r}, t) = f(\vec{r}, t) \right) d\Omega$$

$$\int_{\Omega} N_i(\vec{r}) \frac{\partial \rho C \tilde{T}}{\partial t} d\Omega - \oint_{\Omega} \hat{n}_{\Omega} \cdot N_i(\vec{r}) k \nabla \tilde{T} d\Omega + \int_{\Omega} \nabla N_i(\vec{r}) \cdot k \nabla \tilde{T} d\Omega = \int_{\Omega} N_i(\vec{r}) f(\vec{r}, t) d\Omega$$

$$\int_{\Omega} N_i(\vec{r}) \frac{\partial \rho C \tilde{T}}{\partial t} d\Omega + \int_{\Omega} \nabla N_i(\vec{r}) \cdot k \nabla \tilde{T} d\Omega = \int_{\Omega} N_i(\vec{r}) f(\vec{r}, t) d\Omega + \oint_{\Omega} \hat{n}_{\Omega} \cdot N_i(\vec{r}) k \nabla \tilde{T} d\Omega.$$

Assume $\tilde{T}(\vec{r}, t) = \sum_j N_j T_j(t)$, we have the following system of ODEs:

$$\sum_j \frac{\partial T_j(t)}{\partial t} \rho C \int_{\Omega} N_i N_j d\Omega + \sum_j T_j(t) \int_{\Omega} \nabla N_i \cdot k \nabla N_j d\Omega = \int_{\Omega} N_i f(\vec{r}, t) d\Omega + \oint_{\Omega} \hat{n}_{\Omega} \cdot N_i k \sum_j \nabla N_j T_j(t) d\Omega.$$

c_{ij}

g_{ij}

b_i

Exa 4: Heat conduction equation

$$\left(\frac{\partial \rho C T(\vec{r}, t)}{\partial t} - \nabla \cdot k \nabla T(\vec{r}, t) = f(\vec{r}, t) \right)$$

- Weak form: $\int_{\Omega} w \left(\frac{\partial \rho C \tilde{T}(\vec{r}, t)}{\partial t} - \nabla \cdot k \nabla \tilde{T}(\vec{r}, t) = f(\vec{r}, t) \right) d\Omega$
- Assume $\tilde{T}(\vec{r}, t) = \sum_j N_j T_j(t)$, we have the following system of ODEs:

$$\underbrace{\sum_j \frac{dT_j(t)}{dt} \rho C \int_{\Omega} N_i N_j d\Omega}_{c_{ij}} + \underbrace{\sum_j T_j(t) \int_{\Omega} \nabla N_i \cdot k \nabla N_j d\Omega}_{g_{ij}} = \underbrace{\int_{\Omega} N_i f(\vec{r}, t) d\Omega + \oint_{\Omega} \hat{n}_{\Omega} \cdot N_i k \sum_j \nabla N_j T_j(t) d\Omega}_{b_i}$$

- In matrix form: for all i ,

$$\sum_j c_{ij} \frac{dT_j}{dt} + \sum_j g_{ij} T_j = b_i$$

- System of ODEs can be solved by any ODE solver, such as explicit finite difference, implicit finite difference, Backwards differentiation formula (BDF) method, Generalized alpha method, Different Runge-Kutta methods.

What to know about FEM

- Solution is a linear combination of shape functions

- Mesh needs to match application
- More elements improves accuracy
- Higher order improves accuracy
- Solving system of equations takes most time
 - More DOF = more work
- Solution shouldn't depend on mesh
 - Mesh isn't real → try multiple meshes
 - User judgement → doe results make sense?
- FEM is generally used for spatial discretization

□ Reference:

- Andrew Prudil, Lecture Notes, Cybertraining Workshop at Clarkson University.

□ Good read:

- [Comprehensive Introduction to Physics, PDEs, and Numerical Modeling \(comsol.com\)](#)