Numerical Methods

For solving Partial Differential equation

Classification of PDE:

- Physical Classification:
  - Equilibrium Problems
  - Marching Problems

- Mathematical Classification:
  - Parabolic
  - Hyperbolic
  - Elliptic

Mathematical Classification:

General Second Order PDE:

$$a\frac{\partial^2 \boldsymbol{u}}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + \boldsymbol{d}\frac{\partial u}{\partial x} + \boldsymbol{e}\frac{\partial u}{\partial y} + fu = g(x,y)$$

Parabolic PDE: $b^2 - 4ac = 0$

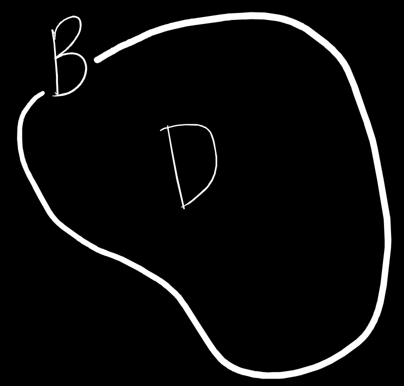
Hyperbolic: $b^2 - 4ac > 0$

Elliptic: $b^2 - 4ac < 0$

Equilibrium Problems

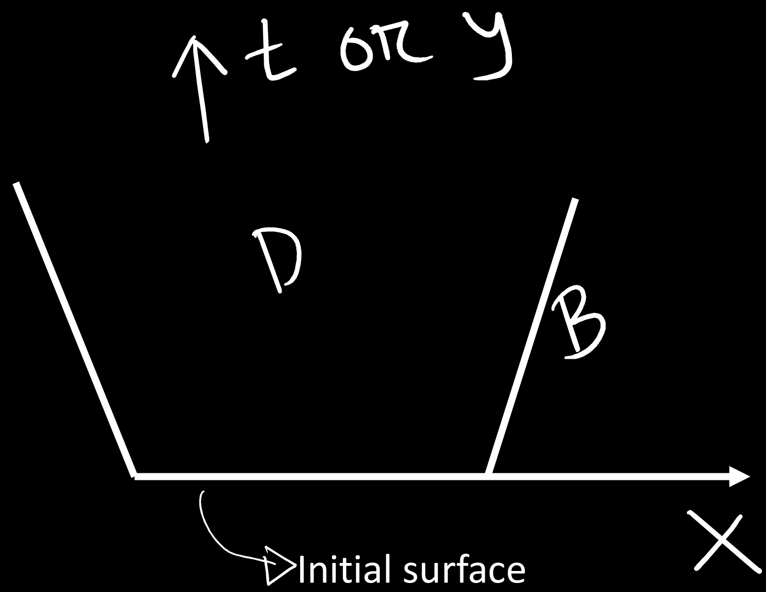
Equilibrium problems are problems in which a solution of a given PDE is desired in a closed domain subject to a prescribed set of boundary conditions. Equilibrium problems are boundary value problems.

PDEs must be satisfied in D. Boundary conditions must be satisfied on B. Mathematically, equilibrium problems are governed by elliptic PDEs.



Marching problems

- Marching problems are transient problems where the solution of a PDE is required on an open domain subject to a set of initial conditions and a set of boundary conditions.
- Generally marching problems are initial value or initial boundary value problems. Mathematically, these problems are governed by either hyperbolic or parabolic PDEs.
- The solution must be computed by marching outward from initial data surface while satisfying boundary conditions.



Solution of PDE

- Analytic Solution
- Approximate Solution/ Numerical Solution

Numerical solution

- Advantages:
    - Can be applied on complex geometry
    - Some of the PDE nearly impossible to solve analytically. Numerical methods must be used on those problem
    - Easy to apply
- Disadvantages:
    - It gives approximate result
    - Sometime needs lots of time
    - Solving process can be computationally costly

Types of numerical methods

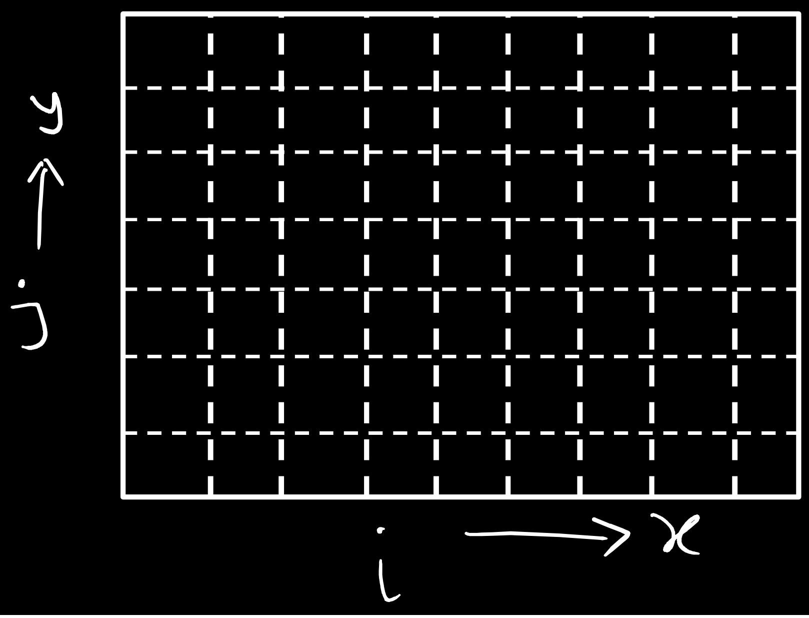
- Finite Difference Method (FDM)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)

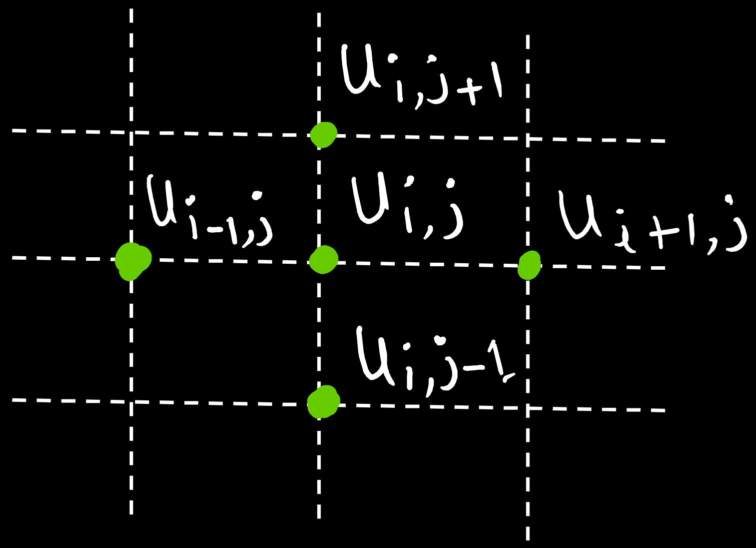
Some definition

- Discretization: In applied mathematics, discretization is the process of transferring continuous functions, models, variables, and equations into discrete counterparts.
- Truncation Error: A truncation error is the difference between an actual and a truncated or cut-off value.
- Round off Error: A round-off error, is a mathematical miscalculation or quantization error caused by altering a number to an integer or one with fewer decimals.
- Discretization Error: An error caused by replacing the continuous problem by a discrete problem. It is defined as the difference between exact solution of PDE and exact solution of FDE when both are round off error free.

FDM: Definition

- In FDM, the continuous problem is discretized so that the dependent variables are considered to exist only at a discrete points.





FDM: an intuition

Definition of Derivative:

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

For small Δx we can write,

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

FDM: An intuition

- Forward Difference:

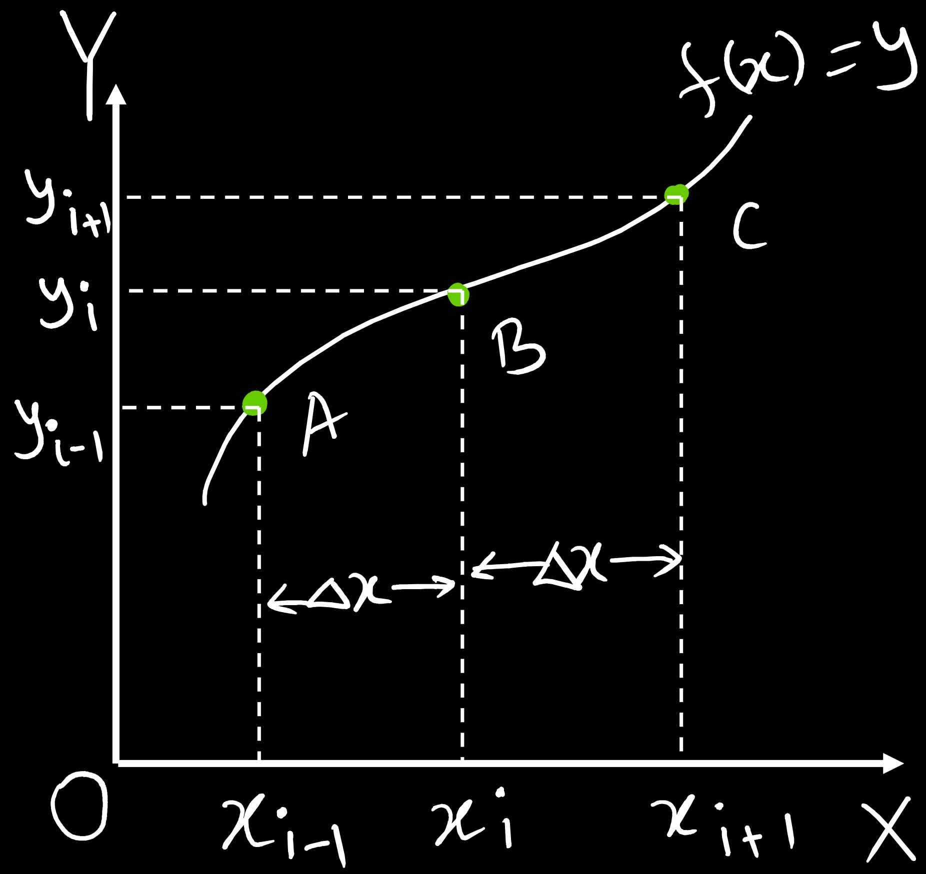
$$\frac{dy}{dx} = \frac{y_{i+1} - y_i}{\Delta x}$$

- Backward Difference:

$$\frac{dy}{dx} = \frac{y_i - y_{i-1}}{\Delta x}$$

- Central Difference:

$$\frac{dy}{dx} = \frac{y_{i+1} - y_{i-1}}{2(\Delta x)}$$



FDM FOR PDE

Definition of derivative of a function u(x , y) at x = x_0 and y = y_0

$$\left(\frac{\partial u}{\partial x}\right)_0 = \lim_{\Delta x \to 0} \frac{u(x_0 + \Delta x, y_0) - u(x_0, y_0)}{\Delta x}$$

TAYLOR Series

$$f(x+a) = f(x) + \frac{a}{1!}\frac{\partial f}{\partial x} + \frac{a^2}{2!}\frac{\partial^2 f}{\partial x^2} + \frac{a^3}{3!}\frac{\partial^3 f}{\partial x^3} + \cdots$$

Developing a Taylor series expansion for $U(x_0 + \Delta x, y_0)$ about the point $U(x_0, y_0)$

$$u(x_0 + \Delta x, y_0) = u(x_0, y_0) + \frac{\Delta x}{1!}\left(\frac{\partial u}{\partial x}\right)_0 + \frac{(\Delta x)^2}{2!}\left(\frac{\partial^2 u}{\partial x^2}\right)_0 + \cdots$$

Or, $\left(\frac{\partial u}{\partial x}\right)_0 = \frac{u(x_0+\Delta x, y_0) - u(x_0, y_0)}{\Delta x} - \frac{\Delta x}{2!}\left(\frac{\partial^2 u}{\partial x^2}\right)_0 - \cdots$

Switching to i , j notation

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + T \cdot E \cdot$$

T.E. is order of Δx and can be denoted by O(x).

FD formula for u(x , y) of first order

Forward Difference Formula:

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x}$$

Backward Difference Formula:

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x}$$

Central Difference Formula:

$$\left(\frac{\partial u}{x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$

For second order approximation

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + O[(\Delta x)^2]$$

Neglecting T. E. part:

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$

Convergence, Consistency, Stability

- Convergence: means the solution to the finite difference method approaches to exact solution of PDE when the mesh is refined.
- Consistency: A FDM is consistence if by reduction of the mesh and time step size, the truncation error terms could be made to approach zero
- Stability: A FDM is stable if the error decay as computation proceeds from one marching step to the next . Stability of a FDM can be assessed using Von Neumann stability analysis.

Explicit and Implicit method

- Explicit method: A formula which express one unknown value at a given node in terms of the known preceding values.
  - FTCS method
  - Durfort-Frankel Method

- Implicit Method: A method in which the computation of many present unknown values necessitates the solution of a set of simultaneous equations is called implicit method.
  - Crank-Nicolson Method

Steps of FDM

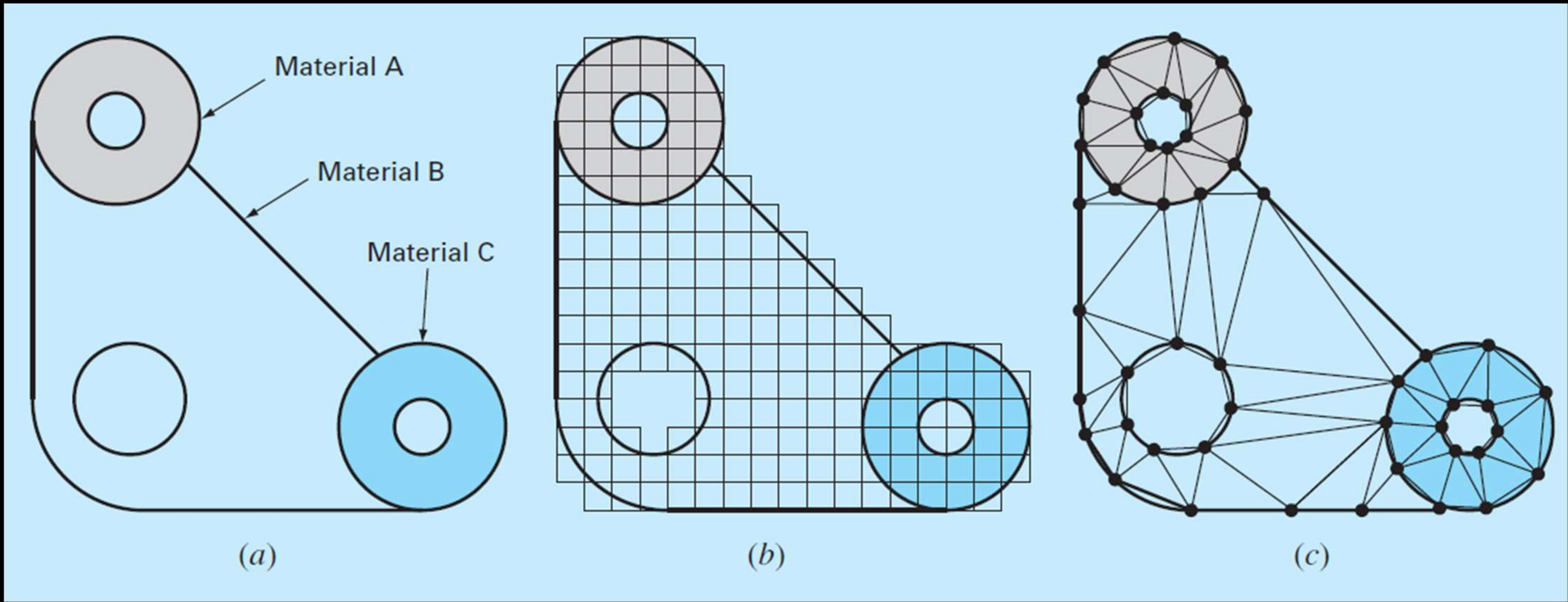
- Discretizing the Domain
- Converting the PDE into Difference equations
- Choosing an appropriate method(explicit or implicit)
- Solving
- Post processing

Finite Element Method

Motivation: In finite difference method we divide the solution domain into finite numbers of discrete grid point. Then PDE is written for each grid point and derivatives is replaced by Difference formula. This method is easy to understand but has some short comings. It is difficult to apply FDM to the problems involving irregular geometry, unusual boundary conditions, or heterogenous composition.

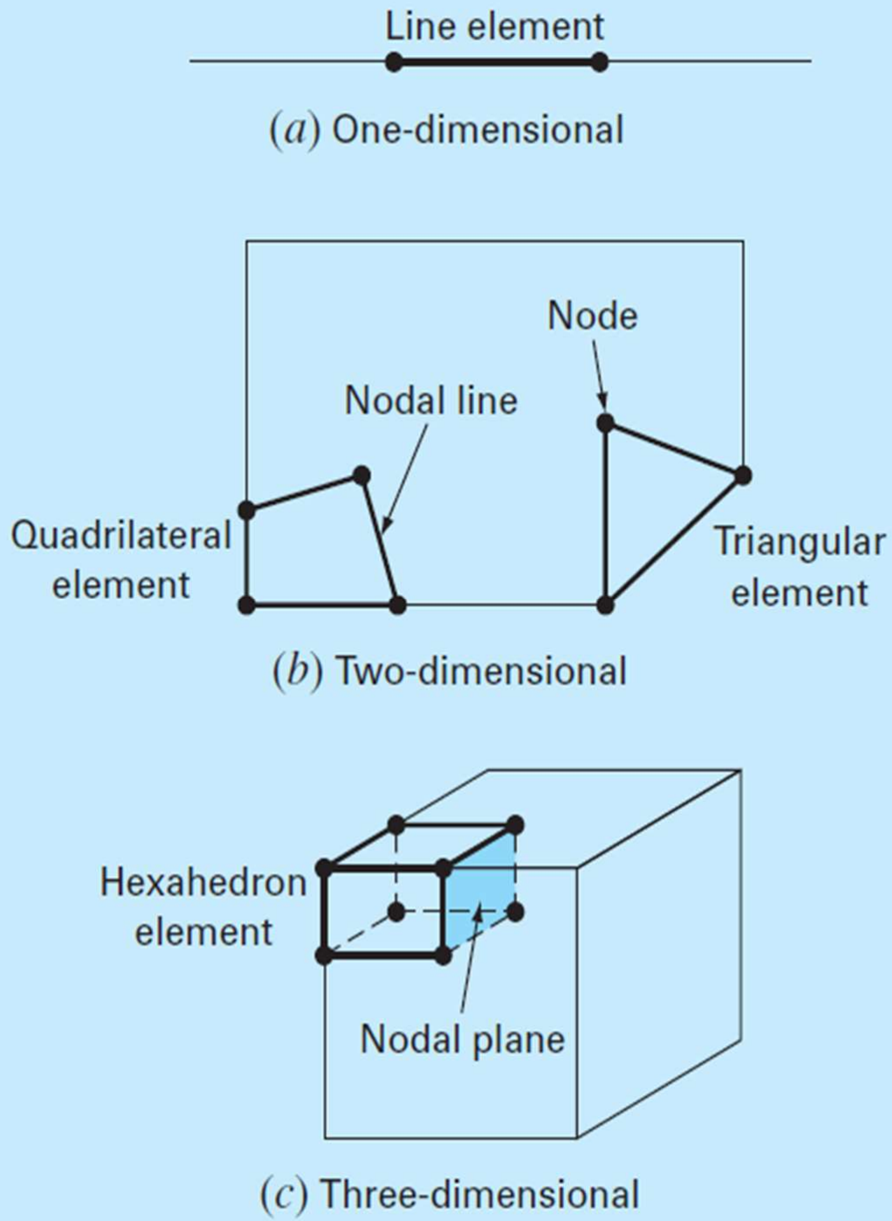
The FEM provides an alternative that is better suited for such systems. In contrast to FDM, the FEM divides the solution domain into simply shaped regions, or "elements"

Gasket with irregular geometry and heterogeneous composition



INTRODUCTION TO ELEMENT

In finite element method the region is divided into small pieces. These pieces are called elements. Elements can be one, two or three dimensional. The points of intersection of the lines that make up the sides of the elements are referred to as nodes and the sides themselves are called nodal lines or planes.



(a) One-dimensional

(b) Two-dimensional

(c) Three-dimensional

Steps in FEM

- **Discretization:** This steps involves discretizing the solution domain into finite elements.
- **Element Equations**
    - Choice of Approximation Functions: Mathematically easy to calculate approximate function is polynomial. Simplest polynomial is one order polynomial that is straight line. This function must pass through the end points of an element.

$$u(x) = a_0 + a_1 x \qquad ....(1)$$

Let x_1 and x_2 are end points of an element.

$$u_1 = a_0 + a_1 x_1 \qquad ....(2)$$

$$u_2 = a_0 + a_1 x_2 \qquad ....(3)$$

Steps in FEM (Element Equations Continued)

Solving equation (2) and (3) we get

$$a_0 = \frac{u_1 x_2 - u_2 x_1}{x_2 - x_1} \text{ and } a_1 = \frac{u_2 - u_1}{x_2 - x_1}$$

So equation (1) reduces to $u = N_1 u_1 + N_2 u_2$ ... (4)

Where, $N_1 = \frac{x_2 - x}{x_2 - 1}$ and $N_2 = \frac{x - x_1}{x_2 - x_1}$

Equation (4) is called shape function and N_1 and N_2 are called interpolation function.

Steps in FEM (Element Equations continued)

Obtaining an Optimal Fit of the Function to the Solution:

After choosing interpolation function, the equation governing the behavior of the element must be developed. Most used method to develop this equation is weighted residual method which gives a set of linear equations. The set of linear equations can be expressed by matrix form,

$$[k]\{u\} = \{F\}$$

[k] = an element property or stiffness matrix,

{u} = a column vector of unknowns at the nodes,

{F} = a column vector reflecting the effect of any external influences applied at the nodes.

Steps in FEM

- **Assembly:** After derivation of element equations of all element, they must be linked together to characterize whole system.

  Assembled equations of the whole system: [K] {u'} = {F'} ....(5)

- **Boundary Conditions:** Then boundary conditions incorporated to equation (5) and expressed as $[\bar{k}]\{u'\} = \{\overline{F'}\}$ …(6)

- **Solutions:** Then system of linear equations (6) is solved by LU decomposition or any iterative method.

- **Postprocessing:** Then result can be shown in tabular form or graphically.

Reference

- Numerical methods for Scientists and Engineers, third edition by K. Sankara Rao
- Numerical methods for Scientists and Engineers, seventh edition by Steven C. Chapra, Raymond P. Canale
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Thank You