ME 747 Introduction to computational fluid dynamics

Lecture 4

Introduction to numerical methods

By Chainarong Chaktranond

Lecture schedule

Session	Topics
1	**1.Overviews of computational fluid dynamics** **-** Overviews and importance of heat transfer in real applications
2 - 3	**2. Introduction to Fortran programming** - Basic commands in Fortran programming
4	**3. Overviews of governing equations for flow and heat transfer** -Elliptic, Parabolic and Hyperbolic equations
5	**4. Introduction to numerical methods** - Finite different method, Finite volume method, Finite element method, etc.
6 – 7	**5. Introduction to solve engineering problems with finite-different method** - Taylor series expansion, Approximation of the second derivative, Initial condition and Boundary conditions

Contents

- Overviews of numerical solving methods
- Finite difference method

Introduction to numerical methods

- ❑ การกำหนดฟิสิกส์ของปัญหา (Define the physical problem)
- ❑ การกำหนดแบบจำลอง (Create a mathematical model)

  - Systems of PDEs, ODEs, algebraic equations

  - การกำหนดเงื่อนเริ่มต้น เงื่อนไขขอบเขต เพื่อให้สอดคล้องกับปัญหา (Well- posed problem)

- ❑ การสร้างแบบจำลองแบบดิสคริท (Discrete model)

  - การดิสคริไตซ์โดเมน → การสร้างกริด → การได้แบบจำลองแบบดิสคริท

  - ระบบการแก้สมการดิสคริท

- ❑ การวิเคราะห์ค่าผิดพลาดในระบบดิสคริท (Analyze errors in the discrete system)

  - ความสอดคล้อง/ตรงกับกายภาพ ความเสถียร และการวิเคราะห์การลู่เข้าของคำตอบ

Numerical solving methods

- Finite difference method
- Finite element method
- Finite volume method
- Spectral method

Main numerical methods for PDEs

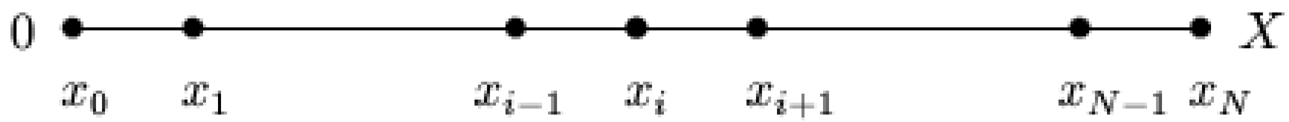
- **Finite difference method (FDM)**
  - **Advantages:**
    - Simple and easy to design the scheme
    - Flexible to deal with the nonlinear problem
    - Widely used for elliptic, parabolic and hyperbolic equations
    - Most popular method for simple geometry, ….
  - **Disadvantages:**
    - Not easy to deal with complex geometry
    - Not easy for complicated boundary conditions
    - ……..

Finite difference method

หลักการ คือ การหาค่าอนุพันธ์ในสมการอนุพันธ์ย่อยเป็นค่าประมาณโดยใช้ค่าฟังก์ชั่นเชิงเส้นที่จุดบนกริด

1 D $\quad \Omega = (0, X) \qquad u_i \approx u(x_i) \qquad i = 0, 1, 2, \ldots, N$

Grid points $\quad x_i = i\Delta x \quad$ Mesh size $\quad \Delta x = \dfrac{X}{N}$

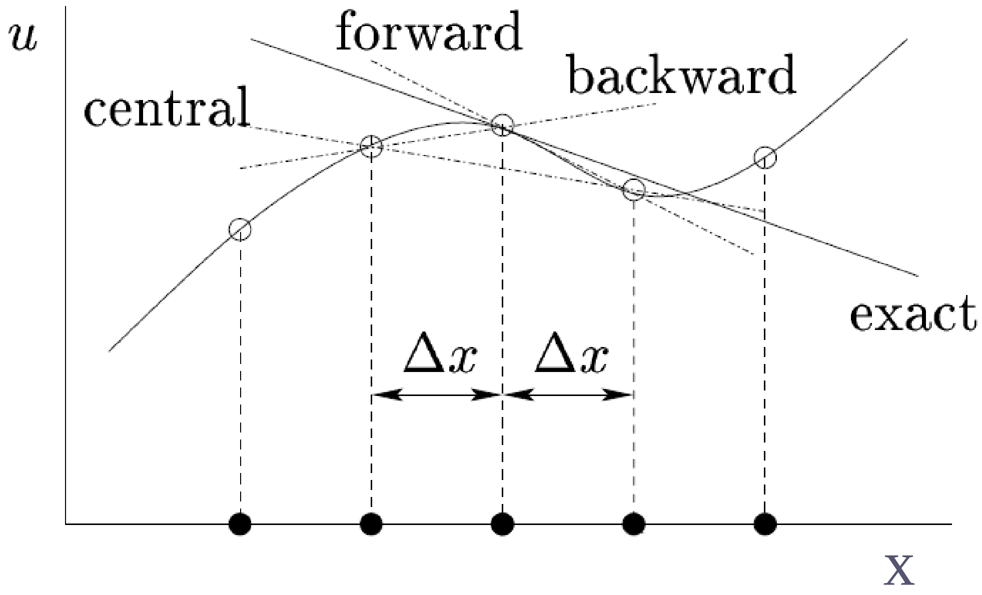


อนุพันธ์อันดับที่ 1

$$\frac{\partial u_i}{\partial x} = \lim_{\Delta x \to 0} \frac{u(x_i + \Delta x) - u(x_i)}{\Delta x} = \lim_{\Delta x \to 0} \frac{u(x_i) - u(x_i - \Delta x)}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{u(x_i + \Delta x) - u(x_i - \Delta x)}{2\Delta x}$$

การประมาณค่าอนุพันธ์อันดับที่หนึ่ง



$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1} - u_i}{\Delta x}$$

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_i - u_{i-1}}{\Delta x}$$

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

Taylor series expansion $u(x) = \sum_{n=0}^{\infty} \frac{(x-x_i)^n}{n!} \left(\frac{\partial^n u}{\partial x^n}\right)_i , \qquad u \in C^{\infty}([0, X])$

T_1 $$u_{i+1} = u_i + \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{6} + \cdots$$

T_2 $$u_{i-1} = u_i - \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{6} + \cdots$$

ค่าผิดพลาดจากการประมาณค่าอนุพันธ์อันดับที่หนึ่ง

T_1
$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

T_2
$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

Truncation error $O(\Delta x)$

$T_1 - T_2$
$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i + \dots$$

ค่าผิดจากการการคำนวณโดยการประมาณอนุพันธ์อันดับหนึ่ง

$$\epsilon_\tau = \alpha_m(\Delta x)^m + \alpha_{m+1}(\Delta x)^{m+1} + \dots \approx \alpha_m(\Delta x)^m$$

การประมาณอนุพันธ์อันดับที่สอง

Central difference scheme

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} + O(\Delta x)^2$$

Alternative derivative

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \left[\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right)\right]_i = \lim_{\Delta x \to 0} \frac{\left(\frac{\partial u}{\partial x}\right)_{i+1/2} - \left(\frac{\partial u}{\partial x}\right)_{i-1/2}}{\Delta x}$$

$$\approx \frac{\frac{u_{i+1}-u_i}{\Delta x} - \frac{u_i - u_{i-1}}{\Delta x}}{\Delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$

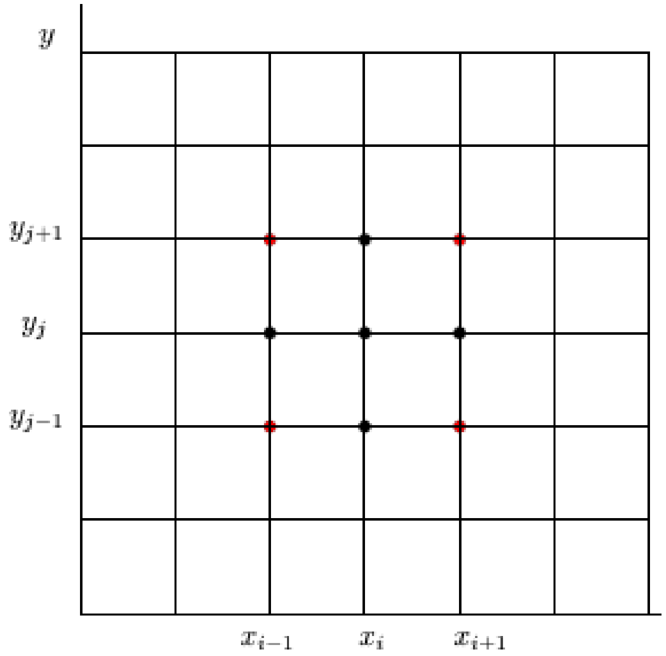
การประมาณค่าโดยอนุพันธ์ผสม

2D: $$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)$$

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

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

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



Second difference approximation

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4\Delta x \Delta y} + \mathcal{O}[(\Delta x)^2, (\Delta y)^2]$$

การประมาณค่าโดยอนุพันธ์อันดับสูงๆ

Taylor series expansion $u(x) = \sum_{n=0}^{\infty} \frac{(x-x_i)^n}{n!} \left(\frac{\partial^n u}{\partial x^n}\right)_i, \qquad u \in C^\infty([0, X])$

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{2u_{i+1} + 3u_i - 6u_{i-1} + u_{i-2}}{6\Delta x} + \mathcal{O}(\Delta x)^3$$ backward

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 6u_{i+1} - 3u_i - 2u_{i-1}}{6\Delta x} + \mathcal{O}(\Delta x)^3$$ forward

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x} + \mathcal{O}(\Delta x)^4$$ central

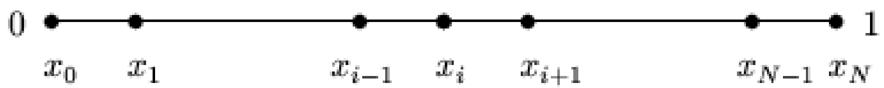
$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12(\Delta x)^2} + \mathcal{O}(\Delta x)^4$$ central

Example: 1-D Poisson equation

Boundary value problem

$$-\frac{\partial^2 u}{\partial x^2} = f \quad \text{in } \Omega = (0,1), \qquad u(0) = u(1) = 0$$

One-dimensional mesh



$$u_i \approx u(x_i), \quad f_i = f(x_i) \qquad x_i = i\Delta x, \quad \Delta x = \frac{1}{N}, \quad i = 0, 1, \ldots, N$$

Central difference approximation $\qquad \mathcal{O}(\Delta x)^2$

$$\begin{cases} -\frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} = f_i, & \forall i = 1, \ldots, N-1 \\ u_0 = u_N = 0 & \text{Dirichlet boundary conditions} \end{cases}$$

Result: the original PDE is replaced by a linear system for nodal values

Example: 1-D Poisson equation

Linear system for the central difference scheme

$$\begin{cases} i=1 & -\frac{u_0-2u_1+u_2}{(\Delta x)^2} = f_1 \\ i=2 & -\frac{u_1-2u_2+u_3}{(\Delta x)^2} = f_2 \\ i=3 & -\frac{u_2-2u_3+u_4}{(\Delta x)^2} = f_3 \\ & \cdots \\ i=N-1 & \frac{u_{N-2}-2u_{N-1}+u_N}{(\Delta x)^2} = f_{N-1} \end{cases}$$

Matrix form $\boxed{Au = F}$ $\quad A \in \mathbb{R}^{N-1\times N-1} \quad u, F \in \mathbb{R}^{N-1}$

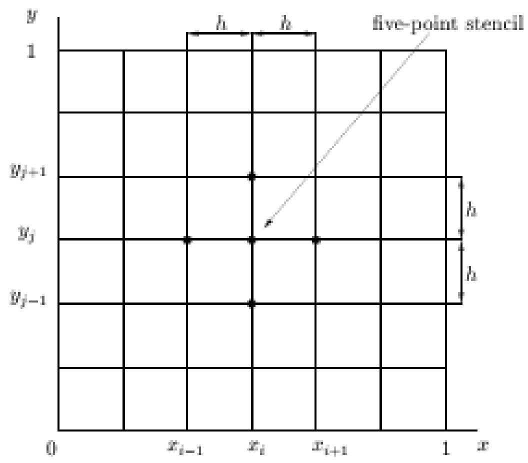
$$A = \frac{1}{(\Delta x)^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \cdots & \\ & & & -1 & 2 \end{bmatrix}, \qquad u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ u_{N-1} \end{bmatrix}, \qquad F = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \cdot \\ f_{N-1} \end{bmatrix}$$

The matrix A is tridiagonal and symmetric positive definite $\Rightarrow$ invertible.

Example: 2-D Poisson equation

Boundary value problem

$$\begin{cases} -\dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial^2 u}{\partial y^2} = f & \text{in } \Omega = (0,1)\times(0,1) \\ u = 0 & \text{on } \Gamma = \partial\Omega \end{cases}$$



Uniform mesh: $\Delta x = \Delta y = h, \quad N = \frac{1}{h}$

$$u_{i,j} \approx u(x_i, y_j), \quad f_{i,j} = f(x_i, y_j), \qquad (x_i, y_j) = (ih, jh), \quad i, j = 0, 1, \ldots, N$$

Central difference approximation $\qquad \mathcal{O}(h^2)$

$$\begin{cases} -\frac{u_{i-1,j}+u_{i,j-1}-4u_{i,j}+u_{i+1,j}+u_{i,j+1}}{h^2} = f_{i,j}, & \forall i, j = 1, \ldots, N-1 \\ u_{i,0} = u_{i,N} = u_{0,j} = u_{N,j} = 0 & \forall i, j = 0, 1, \ldots, N \end{cases}$$

Example: 2-D Poisson equation

Linear system $\boxed{Au = F}$ $\quad A \in \mathbb{R}^{(N-1)^2 \times (N-1)^2} \quad u, F \in \mathbb{R}^{(N-1)^2}$

row-by-row node numbering

$$u = [u_{1,1} \dots u_{N-1,1} \; u_{1,2} \dots u_{N-1,2} \; u_{1,3} \dots u_{N-1,N-1}]^T$$

$$F = [f_{1,1} \dots f_{N-1,1} \; f_{1,2} \dots f_{N-1,2} \; f_{1,3} \dots f_{N-1,N-1}]^T$$

$$A = \begin{bmatrix} B & -I & & & \\ -I & B & -I & & \\ & \dots & \dots & & \\ & & -I & B & -I \\ & & & -I & B \end{bmatrix}, \qquad B = \begin{bmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \dots & \dots & & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{bmatrix}$$

$$I = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & \cdot & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}$$

The matrix A is sparse, block-tridiagonal (for the above numbering) and SPD.

$$\text{cond}_2(A) = \frac{|\lambda_{\max}|}{|\lambda_{\min}|} = \mathcal{O}(h^{-2})$$

Caution: convergence of iterative solvers deteriorates as the mesh is refined

FDM for Parabolic PDEs: The Heat Equation

- Consider the initial-boundary value problem for the heat equation

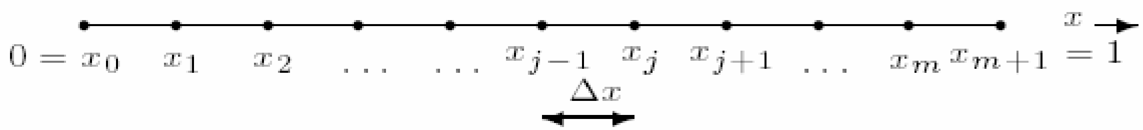
$$u_t = \kappa u_{xx}, \; 0 \le x \le 1, \; t \ge 0$$

$$u(0,x) = f(x), \; \text{Initial Condition}$$

$$u(t,0) = \alpha, \; \text{Boundary Condition at } x = 0$$

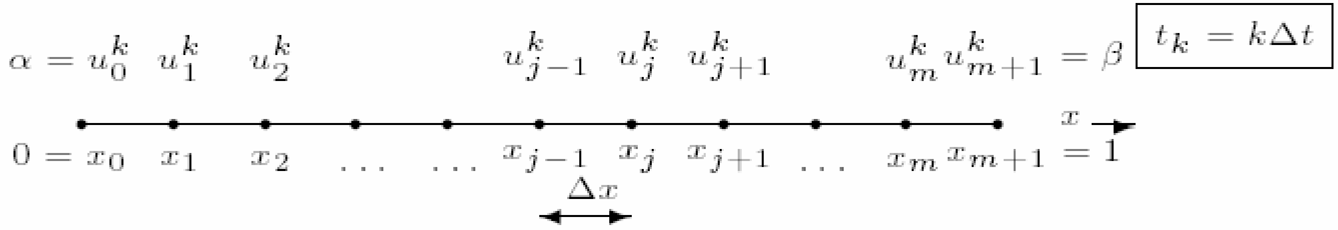
$$u(t,1) = \beta, \; \text{Boundary Condition at } x = 1$$

- Discretize the spatial domain $[0,1]$ into $m+2$ grid points using a uniform mesh step size $\boxed{\Delta x = 1/(m+1)}$. Denote the spatial grid points by $x_j, j = 0, 1, \ldots m+1$.

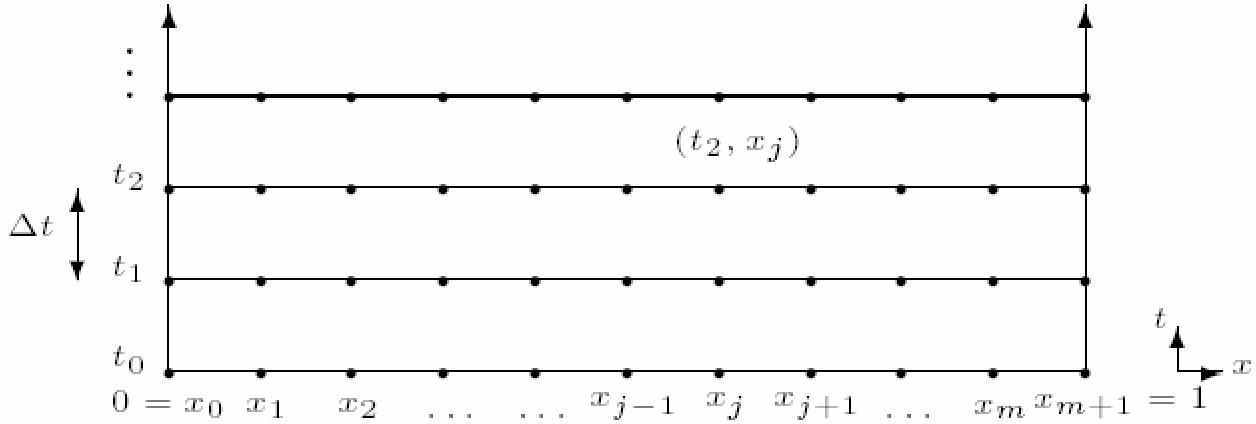


FDM for Parabolic PDEs: The Heat Equation

- Similarly discretize the temporal domain into temporal grid points $t_k = k\Delta t$ for suitably chosen time step Δt.
- Denote the approximate solution at the grid point (t_k, x_j) as U_j^k.



- The space-time grid can be represented as



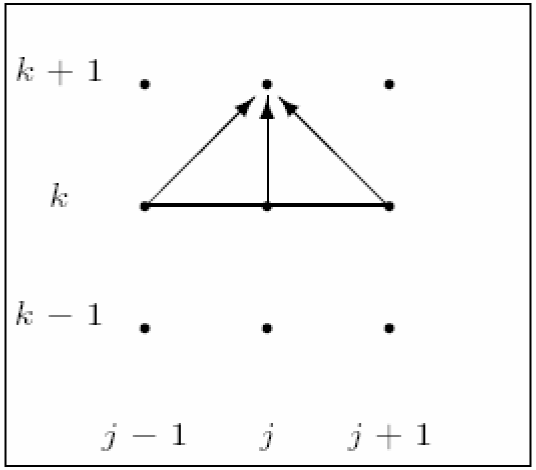
FDM for Parabolic PDEs: The Heat Equation

- Replace u_t by a forward difference in time and u_{xx} by a central difference in space to obtain the explicit FDM
-

$$\frac{U_j^{k+1} - U_j^k}{\Delta t} = \kappa \frac{U_{j+1}^k - 2U_j^k + U_{j-1}^k}{(\Delta x)^2}$$

$$\Longrightarrow U_j^{k+1} = U_j^k + \frac{\kappa \Delta t}{(\Delta x)^2} \left(U_{j+1}^k - 2U_j^k + U_{j-1}^k \right), \; j = 1, 2, \ldots m$$

- Associated to this scheme is a Computational Stencil



Main numerical methods

- **Finite element method (FEM)**
  - **Advantages:**
    - Flexible to deal with problems with complex geometry and complicated boundary conditions
    - Keep physical laws in the discretized level
    - Rigorous mathematical theory for error analysis
    - Widely used in mechanical structure analysis, computational fluid dynamics (CFD), heat transfer, electromagnetics, …
  - **Disadvantages:**
    - Need more mathematical knowledge to formulate a good and equivalent variational form

Finite element methods

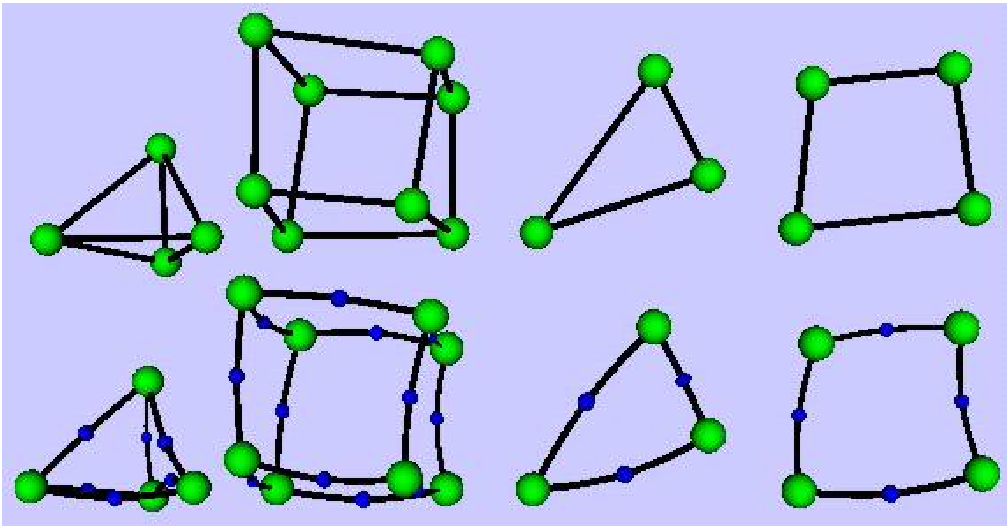
Basic idea

$$u(x) \approx \hat{u}(x) = \sum_{j=1}^{M} u_j \phi_j(x)$$

ϕ_j basic functions

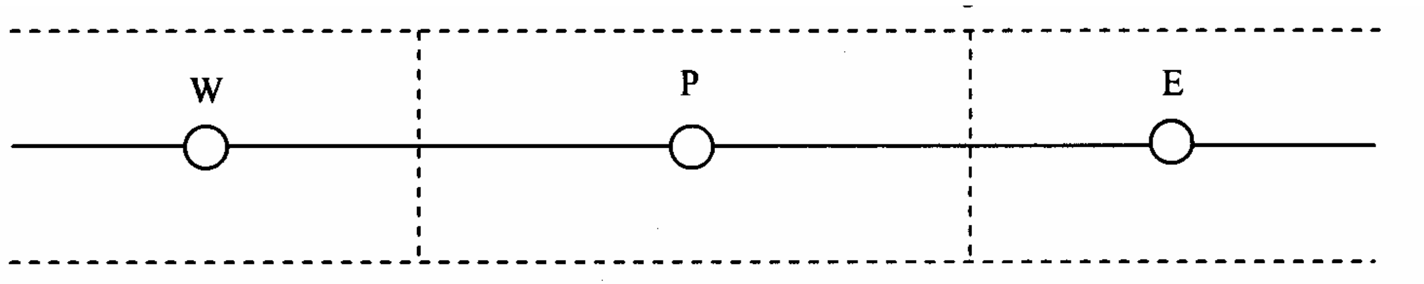
u_j M unknowns: ต้อง M สมการ

Discretizing derivative results in linear system



Main numerical methods

- **Finite volume method (FVM)**
  - Flexible to deal with problems with complex geometry and complicated boundary conditions
  - Keep physical laws in the discretized level
  - Widely used in CFD



$$\left[\frac{\partial^2 u}{\partial x^2}\right]_P = \frac{\left[\left(\frac{\partial u}{\partial x}\right)_e - \left(\frac{\partial u}{\partial x}\right)_w\right]}{x_e - x_w} \qquad \left(\frac{\partial u}{\partial x}\right)_e = \frac{u_E - u_P}{x_E - x_P} \qquad \left(\frac{\partial u}{\partial x}\right)_w = \frac{u_P - u_W}{x_P - x_W}$$

Main numerical methods

- **Spectral method**

Advantage

- High (spectral) order of accuracy
- Usually restricted for problems with regular geometry
- Widely used for linear elliptic and parabolic equations on regular geometry
- Widely used in quantum physics, quantum chemistry, material sciences,

Disadvantage

- Not easy to deal with nonlinear problem
- Not easy to deal with hyperbolic problem
- …..