ME 747 Introduction to computational fluid dynamics

Lecture 4
Introduction to numerical methods

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- 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

- Define the physical problem
- Create a mathematical model
  - Systems of PDEs, ODEs, algebraic equations
  - Specify initial and boundary conditions to match the problem (Well-posed problem)
- Discrete model
  - Discrete domain → Grid creation → Discrete model formulation
  - Error analysis in the discrete system
  - Consistency, stability, and error analysis of the solution
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

Background

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

Grid points \( x_i = i\Delta x \) Mesh size \( \Delta x = \frac{X}{N} \)

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

\( = \lim_{\Delta x \to 0} \frac{u(x_i + \Delta x) - u(x_i - \Delta x)}{2\Delta x} \)
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\[
\frac{\partial u}{\partial x}_i \approx \frac{u_{i+1} - u_i}{\Delta x}
\]

\[
\frac{\partial u}{\partial x}_i \approx \frac{u_i - u_{i-1}}{\Delta x}
\]

\[
\frac{\partial u}{\partial x}_i \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}
\]

Taylor series expansion

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

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

\[
T_2 \quad u_{i-1} = u_i - \left( \frac{\partial u}{\partial x} \right)_i \Delta x + \left( \frac{\partial^2 u}{\partial x^2} \right)_i \frac{(\Delta x)^2}{2} - \left( \frac{\partial^3 u}{\partial x^3} \right)_i \frac{(\Delta x)^3}{6} + \ldots
\]
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\[
T_1 \left( \frac{\partial u}{\partial x} \right)_i = \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2} \left( \frac{\partial^2 u}{\partial x^2} \right)_i - \frac{(\Delta x)^2}{6} \left( \frac{\partial^3 u}{\partial x^3} \right)_i + \ldots
\]

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

Truncation error \( O(\Delta x) \)

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

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\[
\epsilon_\tau = \alpha_m(\Delta x)^m + \alpha_{m+1}(\Delta x)^{m+1} + \ldots \approx \alpha_m(\Delta x)^m
\]
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

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

\[
\approx \frac{u_{i+1} - u_i}{\Delta x} - \frac{u_i - u_{i-1}}{\Delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}
\]
Second difference approximation

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

\[ u(x) = \sum_{n=0}^{\infty} \frac{(x-x_i)^n}{n!} (\frac{\partial^n u}{\partial x^n})_i, \quad u \in C^{\infty}([0, X]) \]

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

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

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

\[
\left( \frac{\partial^2 u}{\partial x^2} \right)_i = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12(\Delta x)^2} + \mathcal{O}(\Delta x)^4 \quad \text{central}
\]
Example: 1-D Poisson equation

Boundary value problem

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

One-dimensional mesh

\[x_0 \quad x_1 \quad x_{i-1} \quad x_i \quad x_{i+1} \quad x_{N-1} \quad x_N\]

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

Central difference approximation \(O(\Delta x)^2\)

\[
\begin{cases}
-u_{i-1} - 2u_i + u_{i+1} = f_i, & \forall i = 1, \ldots, N - 1 \\
u_0 = u_N = 0 & \text{Dirichlet boundary conditions}
\end{cases}
\]

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

\[
\begin{align*}
  i = 1 & \quad -\frac{u_0 - 2u_1 + u_2}{(\Delta x)^2} = f_1 \\
  i = 2 & \quad -\frac{u_1 - 2u_2 + u_3}{(\Delta x)^2} = f_2 \\
  i = 3 & \quad -\frac{u_2 - 2u_3 + u_4}{(\Delta x)^2} = f_3 \\
  \vdots & \\
  i = N - 1 & \quad -\frac{u_{N-2} - 2u_{N-1} + u_N}{(\Delta x)^2} = f_{N-1}
\end{align*}
\]

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

\[
A = \frac{1}{(\Delta x)^2} \begin{bmatrix}
  2 & -1 & & & \\
  -1 & 2 & -1 & & \\
  & -1 & 2 & -1 & \\
  & & & \ddots & \\
  & & & & 2 & -1 \\
  & & & & -1 & 2 \\
\end{bmatrix}, \quad u = \begin{bmatrix}
  u_1 \\
  u_2 \\
  u_3 \\
  \vdots \\
  u_{N-1}
\end{bmatrix}, \quad F = \begin{bmatrix}
  f_1 \\
  f_2 \\
  f_3 \\
  \vdots \\
  f_{N-1}
\end{bmatrix}
\]

The matrix \( A \) is tridiagonal and symmetric positive definite \( \Rightarrow \) invertible.
Example: 2-D Poisson equation

Boundary value problem

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

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

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

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

\[
\begin{cases}
-\frac{u_{i-1,j} + u_{i+1,j} - 4u_{i,j} + u_{i,j+1} + u_{i,j+1}}{h^2} = f_{i,j}, & \forall i, j = 1, \ldots, N - 1 \\
u_{i,0} = u_{i,N} = u_{0,j} = u_{N,j} = 0 & \forall i, j = 0, 1, \ldots, N
\end{cases}
\]
### Example: 2-D Poisson equation

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

**Row-by-row node numbering**
\[ u = [u_{1,1} \ldots u_{N-1,1} \ u_{1,2} \ldots u_{N-1,2} \ u_{1,3} \ldots u_{N-1,N-1}]^T \]
\[ F = [f_{1,1} \ldots f_{N-1,1} \ f_{1,2} \ldots f_{N-1,2} \ f_{1,3} \ldots f_{N-1,N-1}]^T \]

\[
A = \begin{bmatrix}
B & -I \\
-I & B & -I \\
& \cdots & \cdots & \cdots \\
& & -I & B & -I \\
& & & -I & B
\end{bmatrix}, \quad B = \begin{bmatrix}
4 & -1 \\
-1 & 4 & -1 \\
& \cdots & \cdots & \cdots \\
& -1 & 4 & -1 \\
& & -1 & 4
\end{bmatrix}
\]

\[
I = \begin{bmatrix}
1 & 1 \\
1 & 1 \\
\end{bmatrix}
\]

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

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

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

\[ u_t = \kappa u_{xx}, \quad 0 \leq x \leq 1, \quad t \geq 0 \]

\[ u(0, x) = f(x), \text{ Initial Condition} \]

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

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

- Discretize the spatial domain \([0, 1]\) into \(m + 2\) grid points using a uniform mesh step size \(\Delta x = 1/(m + 1)\). 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 \( \Delta t \).
- Denote the approximate solution at the grid point \((t_k, x_j)\) as \( U_{j}^{k} \).

\[
\alpha = u_0^k \ u_1^k \ u_2^k \ u_{j-1}^k \ u_j^k \ u_{j+1}^k \ u_m^k u_{m+1}^k = \beta \quad t_k = k \Delta t
\]

- 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

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

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

- 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

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

\( \phi_j \) 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

\[
\begin{align*}
\left[ \frac{\partial^2 u}{\partial x^2} \right]_p &= \left[ \frac{\partial u}{\partial x} \right]_e - \left[ \frac{\partial u}{\partial x} \right]_w \frac{x_e - x_w}{x_e - x_w} \\
\left( \frac{\partial u}{\partial x} \right)_e &= \frac{u_E - u_P}{x_E - x_P} \\
\left( \frac{\partial u}{\partial x} \right)_w &= \frac{u_P - u_W}{x_P - x_W}
\end{align*}
\]
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
- .....