Brief Introduction to Finite Difference Method

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Overview of Classical Numerical Methods

Method	Concept	Advantages	Disadvantages
Finite Difference Method (FDM)	Approximates derivatives using grid-based difference formulas. Works well on structured grids.	Simple and efficient for regular domains.	Not well-suited for complex geometries.
Finite Element Method (FEM)	Uses piecewise polynomials to approximate solutions over a mesh of elements. Good for unstructured grids.	Can handle complex geometries and boundary conditions.	More computationally expensive and harder to implement.
Finite Volume Method (FVM)	Solves PDEs using control volumes and flux conservation. Popular in fluid dynamics.	Ensures conservation of mass, energy, etc.	More complex than FDM.

Table 1: Comparison of classical numerical methods for solving PDEs.

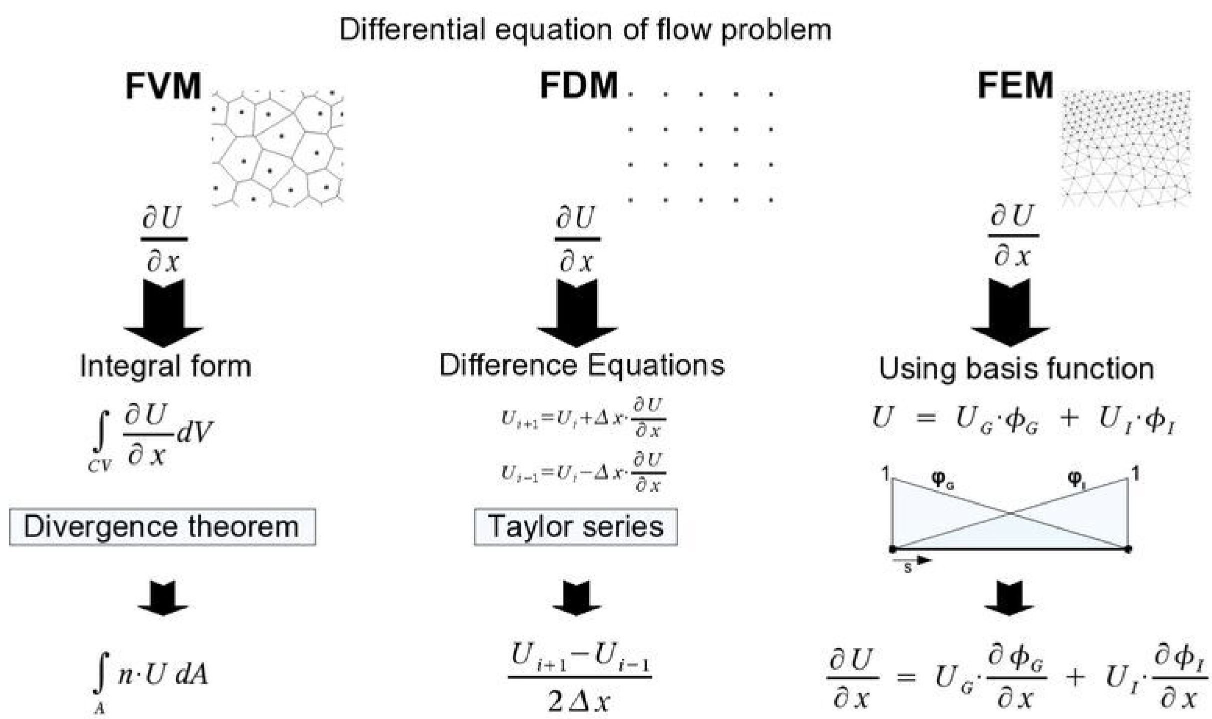

Figure 1: Structured grid for FDM, unstructured mesh for FEM, control volumes for FVM (Cardiff et. al. 2021)

0.1 Introduction to Finite Difference Method (FDM)

The **finite difference method (FDM)** replaces continuous derivatives with discrete approximations.

0.1.1 First-Order Derivative Approximations

Using Taylor series expansion:

$$u(x+\delta x) = u(x) + u'(x)\delta x + u''(x)\frac{\delta x^2}{2} + O(\delta x^3) \tag{1}$$

- **Forward Difference**: Take $\delta x = h$ in (1) and omit the second and higher order terms, one can obtain:
$$\frac{du}{dx} \approx \frac{u(x+h) - u(x)}{h} \tag{2}$$
  - Error: $O(h)$ (less accurate)
- **Backward Difference**: Take $\delta x = -h$ in (1) and omit second and higher order terms, we get:
$$\frac{du}{dx} \approx \frac{u(x) - u(x-h)}{h} \tag{3}$$
  - Error: $O(h)$
- **Central Difference**: Subtract the Taylor expansion of $u(x-h)$ from the Taylor expansion of $u(x+h)$, which leads to:
$$u(x+h) - u(x-h) = 2u'(x)h + O(h^3)$$
and omit higher-order terms **(Note: the second-order term disappears!)**:
$$\frac{du}{dx} \approx \frac{u(x+h) - u(x-h)}{2h} \tag{4}$$
  - Error: $O(h^2)$ **(More Accurate!)**

Illustration of Forward, Backward, and Central Differences:

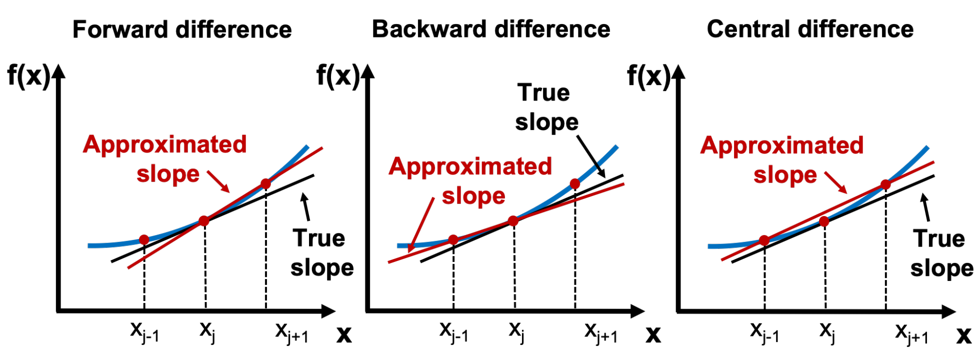

Figure 2: First-Order Derivative Approximations in FDM (Mostoufi et. al. 2022)

0.1.2 Second-Order Derivative Approximation

Let's consider the Taylor series expansion with more terms:

$$u(x+\delta x) = u(x) + u'(x)\delta x + u''(x)\frac{\delta x^2}{2} + u'''(x)\frac{\delta x^3}{6} + O(\delta x^4) \tag{5}$$

Now, let's consider adding the Taylor expansion of $u(x-h)$ to the Taylor expansion of $u(x+h)$, which leads to:

$$u(x+h) + u(x-h) = 2u(x) + u''(x)h^2 + O(h^4).$$

We notice that the first and third-order terms (as well as all odd-order terms) vanish. Similarly, we obtain the following approximation:

$$\frac{d^2u}{dx^2} \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} \tag{6}$$

This is a central difference approximation with error $O(h^2)$.

0.2 Examples of Solving PDEs Using FDM

0.2.1 1D Poisson Equation

The Poisson equation models steady-state problems in physics, such as electrostatics and heat conduction:

$$-k\frac{d^2u}{dx^2} = f(x), \quad x \in [0, L] \tag{7}$$

We assume that the boundary conditions are given by the values of u on the boundary (i.e., $x = 0, L$).

Discretization of the Domain

We first discretize the interval $[0, 1]$ into N equal-distance fragments:

$$\{0 = x_0 < x_1 < \cdots < x_N = 1\}$$

where $\Delta x = x_1 - x_0$ and $\{x_i\}_{i=0}^N$ are named as **mesh grids**.

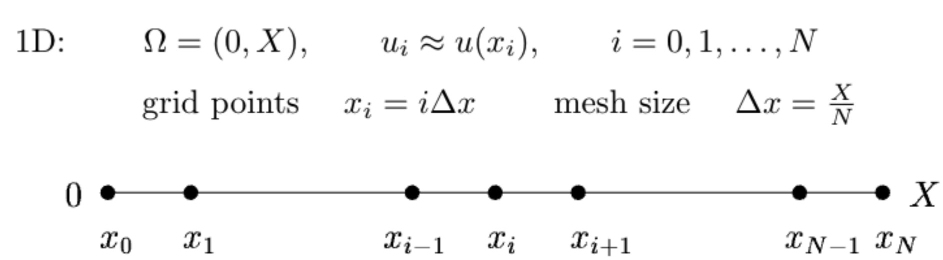

Figure 3: The discretization of the domain

Discretize the Equations and Form a Linear System

With the second-order derivative approximation (6), we can discretize the PDE (7) as follows:

$$-k\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta x^2} = f(x_i), \quad i = 1, \cdots, N-1 \tag{8}$$

We denote

$$\vec{u} = [u_1, u_2, \cdots, u_{N-1}]^T,$$

then (8) can be formulated as the following linear system:

$$-\begin{bmatrix} -\frac{2k}{\Delta x^2} & \frac{k}{\Delta x^2} & & \\ \frac{k}{\Delta x^2} & -\frac{2k}{\Delta x^2} & \ddots & \\ & \ddots & \ddots & \frac{k}{\Delta x^2} \\ & & \frac{k}{\Delta x^2} & -\frac{2k}{\Delta x^2} \end{bmatrix} \vec{u} = \begin{bmatrix} \frac{k}{\Delta x^2}u_0 \\ 0 \\ \vdots \\ 0 \\ \frac{k}{\Delta x^2}u_N \end{bmatrix} + \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{N-2}) \\ f(x_{N-1}) \end{bmatrix} \tag{1}$$

We denote it as:

$$A\tilde{u} = b,$$

which can be solved using various methods depending on the properties of A, such as direct methods (e.g., LU Decomposition, Cholesky Decomposition) or iterative methods (e.g., Jacobi Method, Gauss-Seidel Method).

0.2.2 1D Heat Equation

The 1D heat equation (also known as the diffusion equation) is given by:

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$$

where:

- $u(x,t)$ represents the temperature at position x and time t,
- k is the thermal diffusivity of the material.

The equation describes how heat diffuses over time in a 1D rod.

Initial and Boundary Conditions: We solve this equation in the domain $x \in [0,1]$ with:

- Initial Condition: $u(x,0) = \sin(\pi x)$ (Initial temperature distribution),
- Boundary Conditions:
  - $u(0,t) = 0$ (Fixed temperature at $x = 0$),
  - $u(1,t) = 0$ (Fixed temperature at $x = 1$).

Discretization of the Domain (Only the Spatial Domain)

We first discretize the interval $[0, 1]$ into N equal-distance fragments:

$$\{0 = x_0 < x_1 < \cdots < x_N = 1\}$$

where $\Delta x = x_1 - x_0$.

Discretize the Equations and Form the Linear System

We denote $u_i = u(x_i, t)$ and approximate the PDE as

$$\frac{du_i}{dt} = k\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}, \quad i = 1, \cdots, N-1 \tag{9}$$

We denote

$$\vec{u}(t) = [u_1, u_2, \cdots, u_{N-1}]^T,$$

Then, the equations (9) can be reformulated as the following linear system:

$$\frac{d\vec{u}(t)}{dt} = \begin{bmatrix} -\frac{2k}{\Delta x^2} & \frac{k}{\Delta x^2} & & \\ \frac{k}{\Delta x^2} & -\frac{2k}{\Delta x^2} & \ddots & \\ & \ddots & \ddots & \frac{k}{\Delta x^2} \\ & & \frac{k}{\Delta x^2} & -\frac{2k}{\Delta x^2} \end{bmatrix} \vec{u} + \begin{bmatrix} \frac{k}{\Delta x^2}u_0 \\ 0 \\ \vdots \\ 0 \\ \frac{k}{\Delta x^2}u_N \end{bmatrix} \tag{2}$$

We denote it as:

$$\frac{d\tilde{u}}{dt} = A\tilde{u} + b.$$

This is a **first-order linear ordinary differential equation (ODE) system**, which can be solved with numerical methods like **Euler's method** or **Runge-Kutta**.