MA4110/MA5020: Computational Methods for Fluid Flow

Lecture 6: Finite Difference Methods: Foundations, Taylor Series, and Truncation Error

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1 Introduction: Moving from Continuous to Discrete

In Module 1, we analyzed fluid dynamics through the lens of continuous partial differential equations (PDEs) and exact characteristic solutions. While analytical techniques provide crucial physical insight into wave propagation, steepening, and shocks, realistic fluid flow problems with complex geometries and non-linear interactions cannot be solved in closed form.

Beginning with this lecture, we transition to **numerical discretization methods**. Our overarching strategy is:

1. Replace the continuous space-time continuum with a discrete computational grid of nodes.
2. Approximate continuous spatial and temporal derivatives by algebraic difference quotients.
3. Transform continuous PDEs into system of algebraic equations that can be solved sequentially on a computer.

In this lecture, we introduce the **Finite Difference Method (FDM)**, establish its mathematical foundation via Taylor series expansions, formally define **truncation error** and **consistency**, and construct our first numerical schemes for the linear advection equation.

2 The Computational Grid

Consider a one-dimensional space-time domain $(x, t) \in [0, L] \times [0, T]$. We discretize the continuous domain using uniform step sizes:

- **Spatial grid spacing:** $\Delta x = \frac{L}{N}$, generating spatial grid points $x_j = j\,\Delta x$ for $j = 0, 1, \ldots, N$.
- **Temporal time step:** $\Delta t = \frac{T}{M}$, generating discrete time levels $t^n = n\,\Delta t$ for $n = 0, 1, \ldots, M$.

Discrete Grid Function Notation

We denote the **exact analytical solution** evaluated at a grid node (x_j, t^n) by:

$$u(x_j, t^n) \tag{1}$$

and the **approximate numerical value** computed by our discrete algorithm by:

$$u_j^n \approx u(x_j, t^n) \tag{2}$$

Here, the subscript j represents the spatial index, and the superscript n represents the temporal index (time level).

3 Derivation of Finite Difference Operators via Taylor Series

The cornerstone of the finite difference method is the **Taylor series expansion**. Assuming $u(x, t)$ is sufficiently smooth, we expand the exact solution at neighboring spatial nodes $x_{j+1} = x_j + \Delta x$ and

$x_{j-1} = x_j - \Delta x$ about the point x_j at a fixed time level t^n:

$$u(x_{j+1}, t^n) = u(x_j, t^n) + \Delta x \frac{\partial u}{\partial x}(x_j, t^n) + \frac{\Delta x^2}{2!}\frac{\partial^2 u}{\partial x^2}(x_j, t^n) + \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}(x_j, t^n) + \dots \tag{3}$$

$$u(x_{j-1}, t^n) = u(x_j, t^n) - \Delta x \frac{\partial u}{\partial x}(x_j, t^n) + \frac{\Delta x^2}{2!}\frac{\partial^2 u}{\partial x^2}(x_j, t^n) - \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}(x_j, t^n) + \dots \tag{4}$$

3.1 First Derivative Approximations

3.1.1 Forward Difference Operator (Δ^+)

Solving equation (3) for the first spatial derivative $\frac{\partial u}{\partial x}(x_j, t^n)$:

$$\frac{\partial u}{\partial x}(x_j, t^n) = \frac{u(x_{j+1}, t^n) - u(x_j, t^n)}{\Delta x} - \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}(x_j, t^n) - \mathcal{O}(\Delta x^2) \tag{5}$$

Truncating higher-order terms gives the **Forward Difference** formula:

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_j \approx \frac{u_{j+1} - u_j}{\Delta x}} \tag{6}$$

The leading-order error is proportional to Δx. Hence, this approximation is **first-order accurate**, denoted as $\mathcal{O}(\Delta x)$.

3.1.2 Backward Difference Operator (Δ^-)

Similarly, solving equation (4) for $\frac{\partial u}{\partial x}(x_j, t^n)$:

$$\frac{\partial u}{\partial x}(x_j, t^n) = \frac{u(x_j, t^n) - u(x_{j-1}, t^n)}{\Delta x} + \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}(x_j, t^n) - \mathcal{O}(\Delta x^2) \tag{7}$$

This gives the **Backward Difference** formula:

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_j \approx \frac{u_j - u_{j-1}}{\Delta x}} \tag{8}$$

which is also **first-order accurate** with leading error $\mathcal{O}(\Delta x)$.

3.1.3 Central Difference Operator (δ_x)

Subtracting equation (4) from equation (3) cancels the even-order derivative terms:

$$u(x_{j+1}, t^n) - u(x_{j-1}, t^n) = 2\Delta x \frac{\partial u}{\partial x}(x_j, t^n) + \frac{2\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3}(x_j, t^n) + \dots \tag{9}$$

Dividing by $2\Delta x$ gives:

$$\frac{\partial u}{\partial x}(x_j, t^n) = \frac{u(x_{j+1}, t^n) - u(x_{j-1}, t^n)}{2\Delta x} - \frac{\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3}(x_j, t^n) - \mathcal{O}(\Delta x^4) \tag{10}$$

This yields the standard **Central Difference** formula:

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_j \approx \frac{u_{j+1} - u_{j-1}}{2\Delta x}} \tag{11}$$

Because the $\mathcal{O}(\Delta x)$ terms canceled by symmetry, the leading truncation error is proportional to Δx^2. Thus, the central difference operator is **second-order accurate**, denoted $\mathcal{O}(\Delta x^2)$.

3.2 Second Derivative Approximation (Diffusion Operator δ_x^2)

To discretize second-order diffusion terms $\frac{\partial^2 u}{\partial x^2}$, we add equations (3) and (4):

$$u(x_{j+1}, t^n) + u(x_{j-1}, t^n) = 2u(x_j, t^n) + \Delta x^2 \frac{\partial^2 u}{\partial x^2}(x_j, t^n) + \frac{2\Delta x^4}{24} \frac{\partial^4 u}{\partial x^4}(x_j, t^n) + \dots \tag{12}$$

Solving for $\frac{\partial^2 u}{\partial x^2}(x_j, t^n)$ yields:

$$\frac{\partial^2 u}{\partial x^2}(x_j, t^n) = \frac{u(x_{j+1}, t^n) - 2u(x_j, t^n) + u(x_{j-1}, t^n)}{\Delta x^2} - \frac{\Delta x^2}{12} \frac{\partial^4 u}{\partial x^4}(x_j, t^n) - \mathcal{O}(\Delta x^4) \tag{13}$$

This defines the standard 3-point **Central Difference for Second Derivatives**:

$$\boxed{\left(\frac{\partial^2 u}{\partial x^2}\right)_j \approx \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2}} \tag{14}$$

which is **second-order accurate**, $\mathcal{O}(\Delta x^2)$.

Summary of Common Spatial Difference Operators

Operator Type	**Formula**	**Leading Error Term**	**Order**
Forward Difference (Δ^+)	$\frac{u_{j+1} - u_j}{\Delta x}$	$-\frac{\Delta x}{2} u_{xx}$	$\mathcal{O}(\Delta x)$
Backward Difference (Δ^-)	$\frac{u_j - u_{j-1}}{\Delta x}$	$+\frac{\Delta x}{2} u_{xx}$	$\mathcal{O}(\Delta x)$
Central Difference (δ_x)	$\frac{u_{j+1} - u_{j-1}}{2\Delta x}$	$-\frac{\Delta x^2}{6} u_{xxx}$	$\mathcal{O}(\Delta x^2)$
Second Central Difference (δ_x^2)	$\frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2}$	$-\frac{\Delta x^2}{12} u_{xxxx}$	$\mathcal{O}(\Delta x^2)$

4 Truncation Error and Consistency

4.1 Definition of Local Truncation Error

Consider a general linear partial differential equation written in operator form:

$$\mathcal{L}(u) = 0 \tag{15}$$

and its corresponding discrete finite difference approximation:

$$\mathcal{L}_{\Delta x, \Delta t}(u_j^n) = 0 \tag{16}$$

Definition: Local Truncation Error (LTE)

The **Local Truncation Error**, denoted τ_j^n, is the residual obtained when the **exact continuous solution** $u(x,t)$ is substituted into the discrete difference operator:

$$\tau_j^n = \mathcal{L}_{\Delta x, \Delta t}\big(u(x_j, t^n)\big) \tag{17}$$

The truncation error measures how closely the discrete algebraic operator approximates the original differential equation.

4.2 Definition of Consistency

Definition: Consistency

A finite difference scheme is said to be **consistent** with the partial differential equation if the local truncation error vanishes as the mesh is refined:

$$\lim_{\Delta x, \Delta t \to 0} \tau_j^n = 0 \tag{18}$$

If $\tau_j^n = \mathcal{O}(\Delta t^p) + \mathcal{O}(\Delta x^q)$, we say the scheme is of order (p, q), or **p-th order accurate in time and q-th order accurate in space**.

5 Application: Discretizing the Linear Advection Equation

To see these concepts in action, we study the 1D **linear advection equation**:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \qquad a > 0 \tag{19}$$

5.1 Forward Time, Central Space (FTCS)

Using a forward difference in time ($\mathcal{O}(\Delta t)$) and a central difference in space ($\mathcal{O}(\Delta x^2)$):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0 \tag{20}$$

5.1.1 Truncation Error Analysis for FTCS

Substituting the exact solution $u(x, t)$ into equation (20):

$$\begin{aligned}
\tau_j^n &= \frac{u(x_j, t^n + \Delta t) - u(x_j, t^n)}{\Delta t} + a\frac{u(x_j + \Delta x, t^n) - u(x_j - \Delta x, t^n)}{2\Delta x} \\
&= \left[\frac{\partial u}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + \mathcal{O}(\Delta t^2)\right] + a\left[\frac{\partial u}{\partial x} + \frac{\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}(\Delta x^4)\right] \\
&= \underbrace{\left(\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}\right)}_{=0 \text{ (exact PDE)}} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + a\frac{\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + \dots \\
&= \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + a\frac{\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}(\Delta t^2, \Delta x^4)
\end{aligned} \tag{21}$$

Because $\lim_{\Delta x, \Delta t \to 0} \tau_j^n = 0$, the FTCS scheme is **consistent** with order of accuracy $\mathcal{O}(\Delta t, \Delta x^2)$.

Important Warning regarding FTCS

Although FTCS is formally consistent and second-order accurate in space, we will prove in Lecture 7 that for pure advection ($u_t + au_x = 0$), **FTCS is unconditionally unstable for any time step $\Delta t > 0$!** Consistency alone does not guarantee a functioning numerical scheme.

5.2 The First-Order Upwind Scheme (FOU)

From our study of characteristics in Lecture 4, we know that for $a > 0$, physical information propagates from left to right ($x(t) = x_0 + at$). Therefore, to update the solution at x_j, we should look in the **upwind** direction (x_{j-1}).

Using a forward difference in time and a **backward difference in space** (for $a > 0$):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0 \qquad (a > 0) \tag{22}$$

5.2.1 Explicit Update Formula and the CFL Number

Let us define the non-dimensional **Courant-Friedrichs-Lewy (CFL) number** (or Courant number):

$$\boxed{\nu = \frac{a\,\Delta t}{\Delta x}} \tag{23}$$

Rearranging equation (22) gives the explicit update formula:

$$\boxed{u_j^{n+1} = u_j^n - \nu\left(u_j^n - u_{j-1}^n\right) = (1-\nu)u_j^n + \nu u_{j-1}^n} \tag{24}$$

Physical and Geometric Interpretation of Upwinding

When $0 \leq \nu \leq 1$, the update formula (24) is a **convex combination** of the current state u_j^n and the upstream state u_{j-1}^n (since $(1-\nu) \geq 0$ and $\nu \geq 0$ with sum $= 1$).

- When $\nu = 1$ ($\Delta t = \Delta x/a$): $u_j^{n+1} = u_{j-1}^n$, which is the **exact shift** along the characteristic line!
- When $\nu \leq 1$: the numerical domain of dependence $[x_{j-1}, x_j]$ contains the physical characteristic foot $x_0 = x_j - a\Delta t$, satisfying the fundamental **CFL condition**.

5.2.2 Truncation Error and Modified Equation for Upwind

Let us compute the local truncation error of the upwind scheme:

$$\begin{aligned}
\tau_j^n &= \frac{u(x_j, t^n + \Delta t) - u(x_j, t^n)}{\Delta t} + a\frac{u(x_j, t^n) - u(x_j - \Delta x, t^n)}{\Delta x} \\
&= \left[\frac{\partial u}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + \dots\right] + a\left[\frac{\partial u}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + \dots\right] \\
&= \underbrace{\left(\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}\right)}_{=0} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} - a\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + \mathcal{O}(\Delta t^2, \Delta x^2)
\end{aligned} \tag{25}$$

Using the continuous PDE relation $\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} \implies \frac{\partial^2 u}{\partial t^2} = a^2\frac{\partial^2 u}{\partial x^2}$, we can express the leading time derivative in terms of space:

$$\tau_j^n = \frac{a^2\Delta t}{2}\frac{\partial^2 u}{\partial x^2} - \frac{a\Delta x}{2}\frac{\partial^2 u}{\partial x^2} = -\frac{a\Delta x}{2}(1-\nu)\frac{\partial^2 u}{\partial x^2} + \mathcal{O}(\Delta t^2, \Delta x^2) \tag{26}$$

This reveals that the upwind scheme actually solves the **modified equation**:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \underbrace{\frac{a\Delta x}{2}(1-\nu)}_{\text{Numerical Diffusion Coefficient } \alpha_{\text{num}}} \frac{\partial^2 u}{\partial x^2} \tag{27}$$

The discretization introduces an artificial **numerical diffusion** (or artificial viscosity) that smooths out sharp gradients!

6 The Fundamental Triad: Consistency, Stability, Convergence

When designing and analyzing any numerical method for differential equations, three core properties must be satisfied:

1. **Consistency:** The discrete algebraic operator approximates the original differential equation as grid spacing vanishes ($\tau_j^n \to 0$ as $\Delta x, \Delta t \to 0$).

2. **Stability:** Spurious numerical round-off and truncation errors are not amplified as the computation proceeds forward in time ($n \to \infty$).

3. **Convergence:** The numerical solution approaches the exact continuous solution at every point (x, t) as the grid is refined:

$$\lim_{\Delta x, \Delta t \to 0} |u_j^n - u(x_j, t^n)| = 0 \tag{28}$$

The Lax Equivalence Theorem

For a well-posed linear initial value problem and a consistent linear finite difference scheme,

$$\boxed{\textbf{Consistency} + \textbf{Stability} \iff \textbf{Convergence}}$$

Significance: It is typically straightforward to verify consistency via Taylor series and stability via algebraic techniques (such as Von Neumann analysis, covered in Lecture 7). The Lax Equivalence Theorem guarantees that together, they automatically ensure that the numerical solution converges to the true physical solution.

7 Exercises

Exercises for Lecture 6

E1. Higher-Order One-Sided Differences: Use Taylor series expansions of $u(x_j + \Delta x)$ and $u(x_j + 2\Delta x)$ to derive a **second-order accurate one-sided forward difference** approximation for $\frac{\partial u}{\partial x}(x_j)$ of the form:

$$\left(\frac{\partial u}{\partial x}\right)_j \approx \frac{c_0 u_j + c_1 u_{j+1} + c_2 u_{j+2}}{\Delta x}$$

Determine the constants c_0, c_1, c_2 and find the leading-order truncation error term.

E2. Upwinding for Negative Wave Speeds: Consider the linear advection equation $u_t + a u_x = 0$ with negative speed $a < 0$.

(a) Explain physically why a backward difference in space is inappropriate when $a < 0$.

(b) Formulate the correct first-order upwind scheme using a forward difference in space.

(c) Write down the explicit update equation in terms of the CFL number $\nu = \frac{a\Delta t}{\Delta x}$.

E3. Truncation Error for the Heat Equation: Consider the 1D diffusion/heat equation:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \qquad \alpha > 0$$

Discretize this equation using Forward-Time Central-Space (FTCS):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \alpha \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

(a) Use Taylor series expansions to derive the leading-order local truncation error τ_j^n.

(b) State the order of accuracy of the scheme in time and space.

(c) Define the diffusion number $r = \frac{\alpha \Delta t}{\Delta x^2}$ and write the explicit update formula for u_j^{n+1} in terms of r.

References

[1] John D. Anderson. *Computational Fluid Dynamics: The Basics with Applications*. McGraw-Hill, New York, NY, 1995.

[2] Randall J. LeVeque. *Finite Volume Methods for Hyperbolic Problems*. Cambridge University Press, Cambridge, UK, 2002.