MA4110/MA5020: Computational Methods for Fluid Flow

Lecture 8: Modified Equation Analysis: Numerical Dissipation and Dispersion

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1 Introduction

In Lecture 7, we established that numerical stability requires the amplification factor to satisfy $|G(\xi)| \leq 1$ for all resolvable Fourier wave modes $\xi = k\Delta x \in [-\pi, \pi]$. Under this criterion, the First-Order Upwind (FOU), Lax-Wendroff (LW), and Beam-Warming (BW) schemes are all stable when their Courant-Friedrichs-Lewy (CFL) conditions are met.

However, stability alone does not tell us how an algorithm distorts a physical wave as it propagates across a computational grid. In practice, two distinct numerical artifacts appear:

- **Numerical Dissipation (Diffusion):** First-order schemes damp peak amplitudes and severely smear sharp fronts over time.
- **Numerical Dispersion:** Second-order schemes preserve peak amplitudes, but generate spurious oscillations (wiggles) near steep gradients.

In this lecture, we introduce **Modified Equation Analysis**, a powerful mathematical method that reveals the exact continuous partial differential equation our discrete algebraic difference scheme is *actually* solving on the computer. We will:

1. Derive the modified equations for First-Order Upwind, Lax-Wendroff, and Beam-Warming schemes.
2. Show why even-order spatial derivatives produce dissipation, while odd-order derivatives produce dispersion.
3. Contrast **trailing oscillations** (Lax-Wendroff) with **leading oscillations** (Beam-Warming).
4. Explore the **Magic CFL number** ($\nu = 1$) where all numerical errors vanish.
5. State **Godunov's Barrier Theorem** and discuss how modern CFD overcomes it.

2 The Concept of Modified Equation Analysis

When deriving a finite difference method via Taylor series, we truncate higher-order terms to form an algebraic formula. **Modified equation analysis** reverses this perspective:

1. We substitute Taylor series expansions of all discrete nodal values ($u_j^{n+1}, u_{j\pm1}^n, \dots$) back into the difference equation.
2. This produces an equation containing the original PDE plus infinite series of higher-order time and spatial derivatives:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = C_1 \Delta t \frac{\partial^2 u}{\partial t^2} + C_2 \Delta x \frac{\partial^2 u}{\partial x^2} + \dots$$

3. Using the governing PDE itself, we systematically replace all higher-order time derivatives with equivalent spatial derivatives.
4. The resulting continuous equation is called the **Modified Equation**. It represents the true continuous physics solved by the computer up to higher order.

3 Modified Equation for First-Order Upwind (FOU)

Consider the linear advection equation with $a > 0$:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{1}$$

The backward-in-space First-Order Upwind difference formula is:

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

Expanding $u_j^{n+1} = u(x_j, t^n + \Delta t)$ and $u_{j-1}^n = u(x_j - \Delta x, t^n)$ in Taylor series about the point (x_j, t^n):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\partial u}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + \frac{\Delta t^2}{6}\frac{\partial^3 u}{\partial t^3} + \mathcal{O}(\Delta t^3) \tag{3}$$

$$\frac{u_j^n - u_{j-1}^n}{\Delta x} = \frac{\partial u}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}(\Delta x^3) \tag{4}$$

Substituting equations (3) and (4) into (2):

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = -\frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + \frac{a\Delta x}{2}\frac{\partial^2 u}{\partial x^2} - \frac{\Delta t^2}{6}\frac{\partial^3 u}{\partial t^3} - \frac{a\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + \dots \tag{5}$$

3.1 Eliminating Time Derivatives Using the Governing PDE

To convert time derivatives on the right-hand side of equation (5) into spatial derivatives, we differentiate the base PDE $\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x}$:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial t}\left(-a\frac{\partial u}{\partial x}\right) = -a\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}\right) = -a\frac{\partial}{\partial x}\left(-a\frac{\partial u}{\partial x}\right) = a^2\frac{\partial^2 u}{\partial x^2} \tag{6}$$

$$\frac{\partial^3 u}{\partial t^3} = \frac{\partial}{\partial t}\left(a^2\frac{\partial^2 u}{\partial x^2}\right) = a^2\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial t}\right) = a^2\frac{\partial^2}{\partial x^2}\left(-a\frac{\partial u}{\partial x}\right) = -a^3\frac{\partial^3 u}{\partial x^3} \tag{7}$$

Substituting these expressions into equation (5):

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \left(\frac{a\Delta x}{2} - \frac{a^2\Delta t}{2}\right)\frac{\partial^2 u}{\partial x^2} - \left(\frac{a\Delta x^2}{6} - \frac{a^3\Delta t^2}{6}\right)\frac{\partial^3 u}{\partial x^3} + \dots \tag{8}$$

Recalling the CFL number $\nu = \frac{a\Delta t}{\Delta x}$, we factor out common terms:

$$\boxed{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \underbrace{\frac{a\Delta x}{2}(1-\nu)}_{\text{Artificial Diffusion } \alpha_{\text{num}}}\frac{\partial^2 u}{\partial x^2} - \underbrace{\frac{a\Delta x^2}{6}(1-\nu^2)}_{\text{Numerical Dispersion } \beta_{\text{num}}}\frac{\partial^3 u}{\partial x^3} + \dots} \tag{9}$$

Physical Meaning of the Upwind Error Terms

- **Leading Error ($\frac{\partial^2 u}{\partial x^2}$):** The coefficient $\alpha_{\text{num}} = \frac{a\Delta x}{2}(1-\nu)$ has the dimensions of kinematic viscosity (m^2/s). For any stable CFL number $0 < \nu < 1$, $\alpha_{\text{num}} > 0$. The scheme acts exactly like a physical diffusion process, smearing out sharp gradients and reducing wave peaks over time.

- **Disappearance of Diffusion at $\nu = 1$:** If $\nu = 1$, $\alpha_{\text{num}} = 0$ and $\beta_{\text{num}} = 0$. The discrete scheme becomes mathematically exact!

4 Second-Order Schemes: Lax-Wendroff vs. Beam-Warming

4.1 Lax-Wendroff (Second-Order Central)

Recall the Lax-Wendroff scheme from Lecture 7:

$$u_j^{n+1} = u_j^n - \frac{\nu}{2}(u_{j+1}^n - u_{j-1}^n) + \frac{\nu^2}{2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \tag{10}$$

Lax-Wendroff was constructed specifically to eliminate the $\mathcal{O}(\Delta x)$ artificial diffusion term. Expanding up to fourth order:

$$\boxed{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = -\underbrace{\frac{a\Delta x^2}{6}(1-\nu^2)}_{\text{Negative Dispersion Error}}\frac{\partial^3 u}{\partial x^3} - \frac{a^2\Delta t\Delta x^2}{8}(1-\nu^2)\frac{\partial^4 u}{\partial x^4} + \dots} \tag{11}$$

Sign of the third derivative: Notice the leading error has a **negative sign** ($-\frac{a\Delta x^2}{6}(1-\nu^2)$). For a harmonic wave $u \sim e^{\mathrm{i}(kx-\omega t)}$, this causes short waves to travel **slower** than the physical speed a. Consequently, dispersive oscillations fall behind the wave, appearing as **trailing oscillations**!

4.2 Beam-Warming (Second-Order Upwind)

In 1976, Richard Beam and Robert Warming proposed a second-order accurate scheme that uses fully **upwind (one-sided backward)** spatial differences:

$$\boxed{u_j^{n+1} = u_j^n - \frac{\nu}{2}\left(3u_j^n - 4u_{j-1}^n + u_{j-2}^n\right) + \frac{\nu^2}{2}\left(u_j^n - 2u_{j-1}^n + u_{j-2}^n\right)} \tag{12}$$

Beam-Warming is stable for $0 \le \nu \le 2$. Applying Taylor series expansions to equation (12) yields its modified equation:

$$\boxed{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = +\underbrace{\frac{a\Delta x^2}{6}(2-3\nu+\nu^2)}_{\text{Positive Dispersion Error}}\frac{\partial^3 u}{\partial x^3} - \dots} \tag{13}$$

Striking Contrast with Lax-Wendroff: For $0 < \nu < 1$, the coefficient $(2-3\nu+\nu^2) = (1-\nu)(2-\nu) > 0$ is **positive**! A positive third derivative error causes short waves to travel **faster** than the physical speed a. Consequently, dispersive oscillations outrun the wave, appearing as **leading oscillations** ahead of the shock front!

Summary: Trailing vs. Leading Oscillations

- **Lax-Wendroff (Central 2nd-order):** Leading error is $-\frac{\partial^3 u}{\partial x^3} \implies$ High frequencies lag $\implies$ **Trailing (post-shock) wiggles**.
- **Beam-Warming (Upwind 2nd-order):** Leading error is $+\frac{\partial^3 u}{\partial x^3} \implies$ High frequencies lead $\implies$ **Leading (pre-shock) wiggles**.

5 The "Magic" CFL Number ($\nu = 1$)

What happens when the time step is chosen such that the CFL number is exactly unity:

$$\nu = \frac{a\,\Delta t}{\Delta x} = 1 \iff \Delta t = \frac{\Delta x}{a} \tag{14}$$

Let us evaluate each scheme at $\nu = 1$:

1. **Upwind:** $u_j^{n+1} = u_j^n - 1(u_j^n - u_{j-1}^n) = \mathbf{u_{j-1}^n}$. Error coefficients: $\alpha_{\text{num}} \propto (1-\nu) = 0$.

2. **Lax-Wendroff:** $u_j^{n+1} = u_j^n - \frac{1}{2}(u_{j+1}^n - u_{j-1}^n) + \frac{1}{2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n) = \mathbf{u_{j-1}^n}$. Dispersion: $(1-\nu^2) = 0$.

3. **Beam-Warming:** $u_j^{n+1} = \mathbf{u_{j-1}^n}$. Dispersion: $(1-\nu)(2-\nu) = 0$.

Physical Explanation: The characteristic curve passing through (x_j, t^{n+1}) has equation $x(t) = x_j - a(t^{n+1} - t)$. At the previous time level t^n, this characteristic originates at:

$$x(t^n) = x_j - a\Delta t = x_j - \Delta x = x_{j-1} \tag{15}$$

When $\nu = 1$, the characteristic line connects grid point x_j at t^{n+1} **exactly to grid point** x_{j-1} **at** t^n. No spatial interpolation is required, so all numerical error vanishes identically!

6 Numerical Simulations: Smearing vs. Oscillations

To visually confirm these theoretical predictions, we simulate the advection of both a smooth Gaussian wave and a discontinuous step profile at CFL $\nu = 0.5$ using Julia.

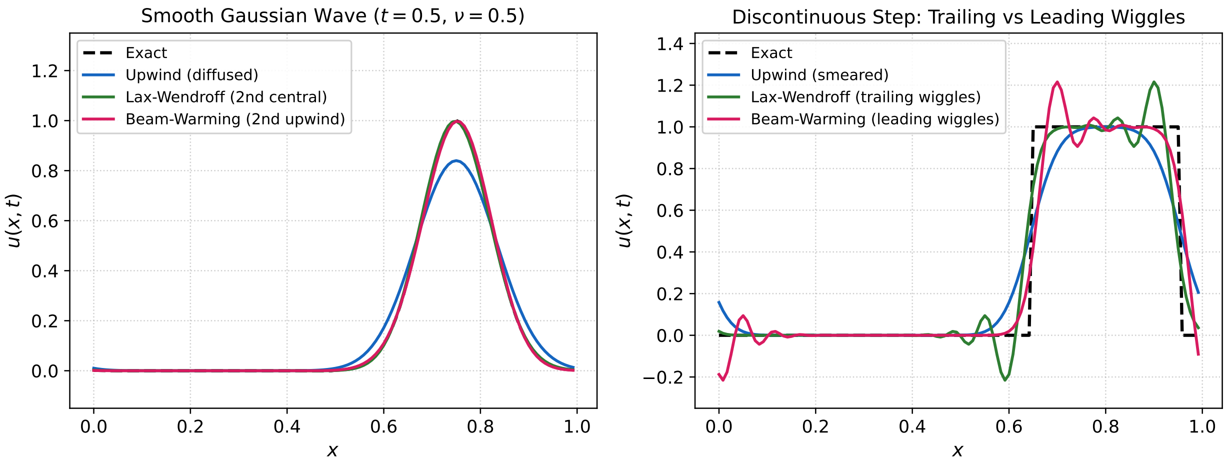

Figure 1: Advection simulation at $t = 0.5$ with CFL $\nu = 0.5$. Left: Smooth Gaussian pulse. First-order upwind severely diffuses the peak, while second-order schemes preserve the amplitude. Right: Discontinuous step. First-order upwind smears the jump. Lax-Wendroff produces **trailing oscillations** (behind the jump), while Beam-Warming produces **leading oscillations** (ahead of the jump). Generated with Julia.

From Figure 1, we observe:

1. **First-Order Upwind:** Completely free of oscillations, but broadens the pulse and degrades sharp corners due to $\mathcal{O}(\Delta x)$ artificial diffusion.

2. **Lax-Wendroff:** Keeps the jump sharp, but creates post-shock undershoots and overshoots ($u < 0$ and $u > 1$).

3. **Beam-Warming:** Keeps the jump sharp, but oscillations appear on the high-side ahead of the front.

7 Godunov's Barrier Theorem and the Road to High-Resolution CFD

The dilemma between artificial diffusion (first-order) and spurious oscillations (second-order) is governed by a famous impossibility theorem proven by Sergei Godunov in 1959:

Godunov's Barrier Theorem (1959)

Linear numerical schemes for solving partial differential equations cannot be simultaneously higher than first-order accurate and monotonicity-preserving (oscillation-free).

7.1 How Modern CFD Escapes Godunov's Barrier

Notice the precise wording of the theorem: it restricts **linear** schemes (schemes where the update coefficients are constants).

To overcome Godunov's barrier, modern computational fluid dynamics uses **non-linear schemes**, even for linear PDEs! The core strategy is **adaptive hybrid switching**:

- **In Smooth Flow Regions:** The algorithm uses a second-order scheme (Lax-Wendroff or Beam-Warming) to eliminate artificial diffusion and preserve waves.
- **Near Discontinuities or Shocks:** A local smoothness sensor detects steep gradients and automatically switches the scheme down to First-Order Upwind, injecting just enough numerical dissipation to suppress all oscillations.

This non-linear strategy forms the foundation of **Total Variation Diminishing (TVD) schemes** and **Flux Limiters**, which we will study in Module 4.

8 Exercises

Exercises for Lecture 8

E1. Modified Equation for Lax-Friedrichs: Starting from the Lax-Friedrichs difference equation:

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

use Taylor expansions and substitute time derivatives with spatial derivatives using $u_t = -au_x$ to derive its modified equation up to second order:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \frac{\Delta x^2}{2\Delta t}(1-\nu^2)\frac{\partial^2 u}{\partial x^2}$$

Explain why Lax-Friedrichs is far more diffusive than First-Order Upwind when $\nu \ll 1$.

E2. Beam-Warming Dispersion Derivation: Starting from equation (12), carry out the Taylor expansions up to third order and prove that the leading dispersive error coefficient is:

$$\beta_{\mathrm{BW}} = +\frac{a\Delta x^2}{6}(2 - 3\nu + \nu^2)$$

Confirm that $\beta_{\mathrm{BW}} = 0$ when $\nu = 1$ and $\nu = 2$.

E3. Wavenumber Phase Speed Analysis: Consider the modified equation $\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = -C\frac{\partial^3 u}{\partial x^3}$ with $C > 0$. Substitute a test wave $u(x,t) = e^{\mathrm{i}(kx-\omega t)}$ and show that the phase speed is:

$$c(k) = \frac{\omega}{k} = a - Ck^2$$

Explain why high wavenumbers (short wavelengths) travel slower than a, confirming why oscillations appear behind the shock wave.