Lecture 7: High Order Schemes

Part 1

Summary So Far

• Want to solve Navier-Stokes equations (any PDE).
• Use of simpler equation - Burgers equation
- has same features of N-S equations + has exact solutions.
• Approximated time and space derivatives by considering non-continuous discrete solution and Taylor expansions.
• The order of the terms neglected in the expansions determine the truncation error, and hence the order of accuracy of the scheme.
• Von-Neumann stability analysis used to give amplification factor and phase error information
• Stability analysis shows that schemes which violate physics of the flow, i.e. have incorrect signal propagation, are unstable.

Also shows that explicit schemes are only stable for $CFL = \frac{c\Delta t}{\Delta x} \leq 1$.

The numerical domain of dependence MUST contain the physical one.

The amplification factor, i.e. the effective damping, then depends on Δt and Δx. The higher order the scheme the smaller the amplification error. Normally $\lambda^2 = 1 - \mathrm{error}(\Delta x^p, \Delta t^q)$.

• Must have an 'upwind' scheme - where sign of the wavespeed determines which points are used in the finite-difference stencil.

However, 'non-upwind' or unstable schemes can be stabilised by adding an 'artificial viscosity' term (in the form $\alpha \frac{\partial^2 u}{\partial x^2}$) to damp the solution.

• Considered form of time-stepping scheme (steady/unsteady).

• Seen non-conservative form gives incorrect signal speed.

TODAY

• Higher-Order Schemes.

• Explicit Schemes for General Fluxes.

Higher-Order Schemes: Lax-Wendroff

The upwind scheme is only first-order accurate in space, and is too difusive. A higher-order scheme is required. A classic scheme in numerical analysis is that due to P.D. Lax and B. Wendroff, published in 1960. This is second-order in space and time. Consider again

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

We know

$$u_i^{n+1} = u_i^n + \Delta t \left.\frac{\partial u}{\partial t}\right|_i^n + \frac{1}{2}(\Delta t)^2 \left.\frac{\partial^2 u}{\partial t^2}\right|_i^n + O(\Delta t^3)$$

Previously the second difference was included in the truncation error; in the Lax-Wendroff method we use it, but second temporal difference is awkward.
So the first step is to formulate an expression for

$$\left.\frac{\partial^2 u}{\partial t^2}\right|_i^n$$

Step 1: Find expression for second temporal derivative

For the first temporal derivative, we rearrange our PDE:

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}$$

so

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

c is constant so

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

Then substitute for the first temporal derivative:

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

so we can say that:

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

Step 2: Taylor expansion in time now including second derivative term

Taylor expansion in time:

$$u_i^{n+1} = u_i^n + \Delta t \left.\frac{\partial u}{\partial t}\right|_i^n + \frac{1}{2}(\Delta t)^2 \left.\frac{\partial^2 u}{\partial t^2}\right|_i^n + O(\Delta t^3)$$

Substitute expressions for first and second derivatives

$$u_i^{n+1} = u_i^n + \Delta t \left.\left(-c\frac{\partial u}{\partial x}\right)\right|_i^n + \frac{1}{2}(\Delta t)^2 \left.\left(c^2\,\frac{\partial^2 u}{\partial x^2}\right)\right|_i^n + O(\Delta t^3)$$

or

$$u_i^{n+1} = u_i^n - c\Delta t \left.\frac{\partial u}{\partial x}\right|_i^n + \frac{1}{2}(\Delta t)^2 c^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_i^n + O(\Delta t^3)$$

We now have an expression for **the future solution** (u_i^{n+1}) in terms of the **first and second spatial derivatives**.

So the next step is to use finite difference formulae for the spatial terms.

Step 3: Finite differences for first and second spatial derivatives

Forward and backward Taylor expansions in space:

$$u_{i+1}^n = u_i^n + \Delta x \left.\frac{\partial u}{\partial x}\right|_i^n + \frac{1}{2}(\Delta x)^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_i^n + \frac{1}{6}(\Delta x)^3 \left.\frac{\partial^3 u}{\partial x^3}\right|_i^n + O(\Delta x^4)$$

$$u_{i-1}^n = u_i^n - \Delta x \left.\frac{\partial u}{\partial x}\right|_i^n + \frac{1}{2}(\Delta x)^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_i^n - \frac{1}{6}(\Delta x)^3 \left.\frac{\partial^3 u}{\partial x^3}\right|_i^n + O(\Delta x^4)$$

The **difference** between the two expansions gives the central difference approximation to the first derivative:

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

The **sum** of the two expansions gives a three-point second-order difference approximation to the second derivative:

$$u_{i+1}^n + u_{i-1}^n = 2u_i^n + 0 + (\Delta x)^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_i^n + 0 + O(\Delta x^4)$$

or

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

Finally substituting our spatial finite differences into our temporal expansions gives the Lax-Wendroff method:

$$u_i^{n+1} = u_i^n - c\frac{\Delta t}{2\Delta x}(u_{i+1}^n - u_{i-1}^n) + \frac{1}{2}\left(\frac{c\Delta t}{\Delta x}\right)^2 (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + O(\Delta x^2, \Delta t^2)$$

(Consider approximation of $\frac{\partial u}{\partial t}$ to obtain truncation error in t).
Hence, the Lax-Wendroff method is second-order accurate in both time and space $\rightarrow$ better than simple upwind scheme.

Stability Analysis

EXAMPLE PROBLEM: By considering Von-Neumann stability analysis, show that for the Lax-Wendroff method:

$$|\lambda|^2 = 1 - 4\nu^2(1-\nu^2)\sin^4(\frac{1}{2}k\Delta x)$$

(Start with $u_i^n = e^{I(ki\Delta x - kcn\Delta t)} = e^{Iki\Delta x}e^{-Ikcn\Delta t}$ and $u_i^{n+1} = \lambda u_i^n$).

This means again

$$\nu = \left|\frac{c\Delta t}{\Delta x}\right| \leq 1$$

The method is **consistent** and **stable**.

Stability Analysis

To tidy the algebra we can start from a point where the exponential in time has been divided through to gain the amplification factor. Increments of $i+1$ or $i-1$ are then just swapped for exponentials in Δx of appropriate sign.

$$\lambda = 1 - \nu \frac{e^{jk\Delta x} - e^{-jk\Delta x}}{2} + \nu^2 \frac{e^{jk\Delta x} + e^{-jk\Delta x} - 2}{2} \tag{1}$$

Noting that $\frac{e^{j\theta} - e^{-j\theta}}{2} = j\sin(\theta)$ and $\frac{e^{j\theta} + e^{-j\theta}}{2} = \cos(\theta)$

$$\lambda = 1 - \nu j \sin(k\Delta x) + \nu^2(\cos(k\Delta x) - 1) \tag{2}$$

$$\lambda^2 = (1 + \nu^2(\cos(k\Delta x) - 1))^2 + \nu^2(\sin^2(k\Delta x)) \tag{3}$$

$$\lambda^2 = (1 - \nu^2(1 - \cos(k\Delta x)))^2 + \nu^2(1 - \cos^2(k\Delta x)) \tag{4}$$

Frame Title

$$\lambda^2 = 1 - 2\nu^2(1 - \cos(k\Delta x)) + \nu^2(1 - \cos^2(k\Delta x)) + \nu^4(1 - \cos(k\Delta x))^2 \tag{5}$$

note that

$$\begin{aligned}
-2\nu^2(1 - \cos(k\Delta x)) + \nu^2(1 - \cos^2(\Delta x)) &= -2\nu^2 + 2\nu^2 \cos(\Delta x) + \nu^2 - \nu^2 \cos^2(\Delta x) \\
&= -\nu^2 + 2\nu^2 \cos(\Delta x) - \nu^2 \cos^2(\Delta x) \\
&= -(\nu - \nu \cos(\Delta x))^2
\end{aligned}$$

so have

$$\lambda^2 = 1 - \nu^2(1 - \cos(\Delta x))^2 + \nu^4(1 - \cos(k\Delta x))^2 \tag{6}$$

$$\lambda^2 = 1 - \nu^2(1 - \nu^2)(1 - \cos(k\Delta x))^2 \tag{7}$$

$$2\sin^2(\theta) = 1 - \cos(2\theta) \tag{8}$$

$$2\sin^2(k\Delta x/2) = 1 - \cos(k\Delta x) \tag{9}$$

$$\lambda^2 = 1 - 4\nu^2(1 - \nu^2)\sin^4\left(\frac{k\Delta x}{2}\right) \tag{10}$$

Numerical Example

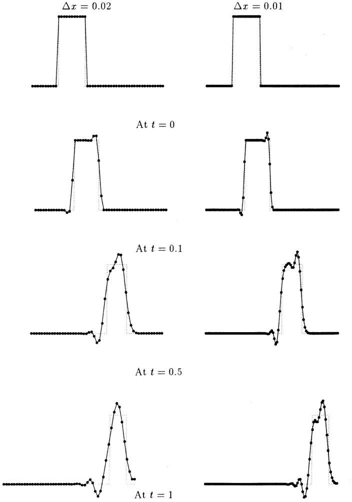
Consider again square pulse initial conditions for non-linear wave equation (wave speed not constant) now computed with Lax-Wendroff.

$$u_t + c(x,t)u_x = 0$$

$$c(x,t) = \frac{1+x^2}{1+2xt+2x^2+x^4}$$

$$u(x,0) = \begin{cases} 1.0 & 0.2 \le x \le 0.4 \\ 0.0 & \text{otherwise} \end{cases}$$

For all points $\Delta t = \Delta x$, and so $\nu = \frac{c\Delta t}{\Delta x}$ is variable.



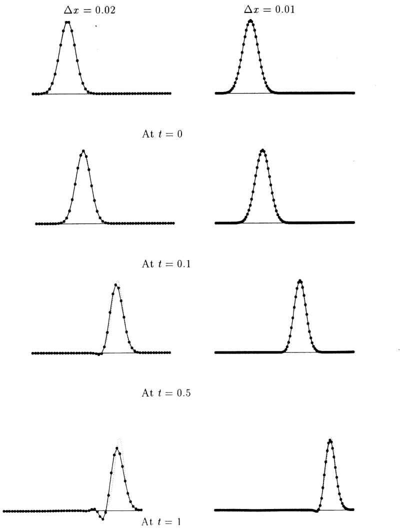
Lax-Wendroff scheme updates each point with a weighted value of three points, two weights are positive, one negative. Hence, solution can contain oscillations with internal maxima and minima.
Now consider smoother initial conditions.

$$u_t + c(x,t)u_x = 0$$

$$c(x,t) = \frac{1+x^2}{1+2xt+2x^2+x^4}$$

$$u(x,0) = \exp\left[-10(4x-1)^2\right]$$

For all points $\Delta t = \Delta x$, and so $\nu = \frac{c\Delta t}{\Delta x}$ is variable.



Lecture 7: High Order Schemes

Part 2

Explicit Methods for General Fluxes

So far we have only considered schemes for linear equations, i.e. constant wavespeeds. The non-linear Burgers equation results in a FDA scheme for the first order upwind scheme

$$\frac{\partial u}{\partial t} + \frac{\partial(\frac{1}{2}u^2)}{\partial x} = 0$$

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

where the 'effective wavespeed' term is clear. Non-linear equations are normally written

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0$$

which result in a first-order upwind scheme of the form

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}\left(F(u_i^n) - F(u_{i-1}^n)\right)$$

which is written as

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}\left(F_i^n - F_{i-1}^n\right)$$

However, the Lax-Wendroff scheme for non-linear equations becomes more complex.

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0$$

We know as before

$$u_i^{n+1} = u_i^n + \Delta t \left.\frac{\partial u}{\partial t}\right|_i^n + \frac{1}{2}(\Delta t)^2 \left.\frac{\partial^2 u}{\partial t^2}\right|_i^n + O(\Delta t^3)$$

and so again

$$\left.\frac{\partial u}{\partial t}\right|_i^n = -\left.\frac{\partial F(u)}{\partial x}\right|_i^n = -\frac{\left(F_{i+1}^n - F_{i-1}^n\right)}{2\Delta x} + O(\Delta x^2)$$

But the second order term causes the problem.

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

But

$$\frac{\partial F(u)}{\partial t} = \frac{\partial F(u)}{\partial u}\frac{\partial u}{\partial t} = -\frac{\partial F(u)}{\partial u}\frac{\partial F(u)}{\partial x}$$

so

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial}{\partial x}\left[-\frac{\partial F(u)}{\partial u}\frac{\partial F(u)}{\partial x}\right] = \frac{\partial}{\partial x}\left[\frac{\partial F(u)}{\partial u}\frac{\partial F(u)}{\partial x}\right]$$

The spatial derivatives do not cause any problems, but the $\frac{\partial F(u)}{\partial u}$ is complex to compute, and also it is not clear exactly where it should be evaluated. This then also has to be differentiated. This term is known as the Jacobian. For a system of N equations, it is an N x N matrix.

Example Jacobian: 1D Euler

We are normally concerned with systems of equations, for example the Euler or Navier-Stokes equations. For a system of N equations, the Jacobian is an N x N matrix. 1-D Euler equations are

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (P + \rho u^2)}{\partial x} = 0$$

$$\frac{\partial E}{\partial t} + \frac{\partial (P + E)u}{\partial x} = 0$$

where,

$$E = \frac{P}{\gamma - 1} + \frac{1}{2}\rho u^2$$

These three equations are written as

$$\frac{\partial \underline{\mathbf{U}}}{\partial t} + \frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial x} = 0$$

where $\underline{\mathbf{U}}$ is the vector of conserved variables, and $\underline{\mathbf{F}}$ is the flux vector,

$$\underline{\mathbf{U}} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix} = \begin{bmatrix} \rho \\ m \\ E \end{bmatrix} \qquad \underline{\mathbf{F}} = \begin{bmatrix} \rho u \\ P + \rho u^2 \\ (P+E)u \end{bmatrix}$$

In this case the Jacobian would be (Not examinable)

$$\frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial \underline{\mathbf{U}}} = \mathbf{J} = \begin{bmatrix} | & | & | \\ \frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial \rho} & \frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial m} & \frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial E} \\ | & | & | \end{bmatrix} = \begin{bmatrix} 0, & 1, & 0 \\ \frac{(\gamma-3)u^2}{2}, & -(\gamma-3)u, & (\gamma-1) \\ \frac{-\gamma E u}{\rho} + (\gamma-1)u^3, & \frac{\gamma E}{\rho} - \frac{3(\gamma-1)u^2}{2}, & \gamma u \end{bmatrix}$$

Not examinable - how to derive that - noting $p = \rho RT = \rho R \frac{e}{C_v} = (\gamma - 1)(E - \frac{1}{2}\rho u^2)$ where $\frac{R}{C_v} = \gamma - 1$

$$\underline{\mathbf{F}} = \left[\begin{array}{c} \rho u \\ P + \rho u^2 \\ (P + E)u \end{array} \right] = \left[\begin{array}{c} m \\ (\gamma - 1)(E - \frac{1}{2}\frac{m^2}{\rho}) + \frac{m^2}{\rho} \\ ((\gamma - 1)(E - \frac{1}{2}\frac{m^2}{\rho}) + E)\frac{m}{\rho} \end{array} \right]$$

Then differentiate each entry in this vector with respect to ρ, m, E in turn to fill out matrix entries.

MacCormack's Method

A simpler higher-order scheme is MacCormack's method. This is also second-order accurate in time and space.
To solve

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0$$

MacCormack's scheme is a two-stage scheme, known as a 'predictor-corrector' method.
1) Predictor stage

$$u_i^{\overline{n+1}} = u_i^n - \frac{\Delta t}{\Delta x}\left(F_i^n - F_{i-1}^n\right)$$

2) Corrector stage

$$u_i^{n+1} = \frac{1}{2}\left(u_i^n + u_i^{\overline{n+1}}\right) - \frac{\Delta t}{2\Delta x}\left(F_{i+1}^{\overline{n+1}} - F_i^{\overline{n+1}}\right)$$

In the above

$$F_{i+1}^{\overline{n+1}} = F(u_{i+1}^{\overline{n+1}}) \text{ etc.}$$

By considering initially $F(u) = cu$ where c is constant, i.e. the linear wave equation, we can show that:

1) MacCormack's method is

   i) Second-order accurate in time and space, i.e. the truncation error is $O(\Delta x^2, \Delta t^2)$,

   ii) Stable for $CFL < 1$,

   iii) Consistent,

2) MacCormacks scheme is identical to the Lax-Wendroff method, but is much simpler to code, as the Jacobian is not required.

A Note on Wavespeeds

For a scalar equation

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0$$

we have used the chain-rule to expand the spatial gradient

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial u}\frac{\partial u}{\partial x} = 0$$

and the $\frac{\partial F(u)}{\partial u}$ term is the wavespeed. However, as we have seen, for a discrete numerical approximation to this, we must be careful how we evaluate the wavespeed term.

For example,

$$F(u) = \frac{1}{2}u^2, \quad \Rightarrow \frac{\partial F(u)}{\partial u} = u.$$

u is the wavespeed.

For a system of equations

$$\frac{\partial \underline{\mathbf{U}}}{\partial t} + \frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial x} = 0$$

Same chain rule expansion

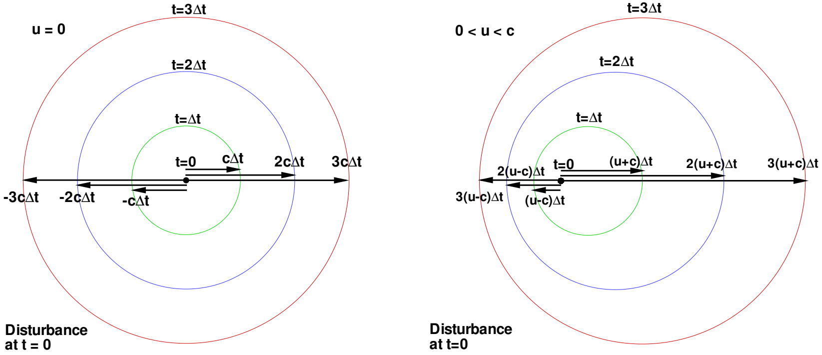
$$\frac{\partial \underline{\mathbf{U}}}{\partial t} + \frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial \underline{\mathbf{U}}} \frac{\partial \underline{\mathbf{U}}}{\partial x} = 0$$

The $\frac{\partial \underline{\mathbf{F}}(\underline{\mathbf{U}})}{\partial \underline{\mathbf{U}}}$ is now a matrix Jacobian, $\mathbf{J}$. For example, the 1-D Euler equations result in a 3×3 matrix. So how do we get wavespeeds from a matrix. In fact they are the eigenvalues of the Jacobian matrix.

$$|\mathbf{J} - \lambda \mathbf{I}| = 0 \quad \Rightarrow \lambda_{1,2,3} = u - \sqrt{\frac{\gamma P}{\rho}}, u, u + \sqrt{\frac{\gamma P}{\rho}}$$

(NOTE: λ here is NOT same as λ used for amplitude factor.)

Hence, the speed of sound in a fluid must be $c = \sqrt{\frac{\gamma P}{\rho}}$. From a fluid mechanics argument, this can be derived, but it was a mathematician that first showed this.



What does this mean for the time step ? The CFL condition for a scalar equation is

$$CFL = \frac{c\Delta t}{\Delta x} \leq 1 \quad \text{where } c \text{ is the wavespeed}$$

which means we have the time step limit $\Delta t \leq \frac{\Delta x}{c}$. When we have multiple wavespeeds, each one effectively has its own maximum time step, but the stability limit comes from ensuring the numerical domain of dependence (Δx in 1-D) contains the physical one ($c\Delta t$ for a simple scalar equation), and so for multiple wavespeeds we must ensure Δx contains the maximum wave propagation distance, and so we get, in general

$$CFL = \frac{\mathrm{MAX(wavespeed)}\Delta t}{\Delta x} \leq 1$$

For the 1-D Euler equations, if $u > 0$ the $u + c$ characteristic is the largest wavespeed. If $u < 0$ the $u - c$ characteristic is the largest wavespeed. Hence,

$$CFL = \frac{(|u| + c)\Delta t}{\Delta x} \leq 1 \quad \Rightarrow \; \Delta t \leq \frac{\Delta x}{|u| + c}$$

Summary

- For $CFL < 1$ first-order spatial schemes are too difussive.
- Derived a second-order accurate spatial scheme, the Lax-Wendroff method. The amplitude error is now of order Δx^4 compared to Δx^2 for the first-order upwind scheme.
- Higher order schemes do preserve amplitude better than first-order, but suffer from oscillations at large gradients.
- The second-order accurate spatial scheme due to Lax-Wendroff is awkward for general equations. Need a Jacobian, and the derivative of this $\Rightarrow$ MacCormack's method is also a second-order accurate spatial scheme, but is simpler to code than the Lax-Wendroff method. It is a two stage approach.
- The Jacobian is useful, and will be used later. From it, we can obtain the wavespeeds for a system of equations. A mathematician did this before a fluid dynamicist derived acoustic speed.
- For a system of equations, we must ensure all waves satisfy the CFL condition, and so we must use the maximum wavespeed to evaluate the allowable Δt.

NEXT LECTURE: Look at the alternative to explicit schemes.