2.29 Numerical Fluid Mechanics
Fall 2011 – Lecture 15

REVIEW Lecture 14:

- Finite Difference: Boundary conditions
  - Different approx. at and near the boundary => impacts linear system to be solved
- Finite-Differences on Non-Uniform Grids and Uniform Errors: 1-D
  - If non-uniform grid is refined, error due to the 1st order term decreases faster than that of 2nd order term
  - Convergence becomes asymptotically 2nd order (1st order term cancels)
- Grid-Refinement and Error estimation
  - Estimation of the order of convergence and of the discretization error
  - Richardson's extrapolation and Iterative improvements using Roomberg's algorithm
- Fourier Analysis of canonical PDE
  - Generic PDE: $\frac{\partial f}{\partial t} = \frac{\partial^n f}{\partial x^n}$, with $f(x,t) = \sum_{k=-\infty}^{\infty} f_k(t)\, e^{ikx} \Rightarrow \frac{d\, f_k(t)}{dt} = (ik)^n\ f_k(t) = \sigma\, f_k(t) \quad \text{for} \ \ \sigma = (ik)^n$
  - Differentiation, definition and smoothness of solution for ≠ order n of spatial operators

Outline for TODAY (Lecture 15): FINITE DIFFERENCES, Cont'd

- Fourier Analysis and Error Analysis
- Stability
  - Heuristic Method
  - Energy Method
  - Von Neumann Method (Introduction): 1st order linear convection/wave eqn
- Hyperbolic PDEs and Stabilty
  - Example: 2nd order wave equation and waves on a string
    - Effective numerical wave numbers and dispersion
  - CFL condition:
    - Definition
    - Examples: 1st order linear convection/wave eqn, 2nd order wave eqn
    - Other FD schemes
  - Von Neumann examples: 1st order linear convection/wave eqn
  - Tables of schemes for 1st order linear convection/wave eqn

References and Reading Assignments

- Lapidus and Pinder, 1982: Numerical solutions of PDEs in Science and Engineering. Section 4.5 on “Stability”.
- Chapter 3 on “Finite Difference Methods” of “J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd edition, 2002”
- Chapter 3 on “Finite Difference Approximations” of “H. Lomax, T. H. Pulliam, D.W. Zingg, *Fundamentals of Computational Fluid Dynamics (Scientific Computation).* Springer, 2003”
- Chapter 29 and 30 on “Finite Difference: Elliptic and Parabolic equations” of “Chapra and Canale, Numerical Methods for Engineers, 2010/2006.”

Fourier Error Analysis: 1st derivatives

- In the decomposition: $$f(x,t) = \sum_{k=-\infty}^{\infty} f_k(t)\, e^{ikx}$$
  - All components are of the form: $f_k(t)\, e^{ikx}$
  - Exact 1st order spatial derivative: $$\frac{\partial f_k(t)\, e^{ikx}}{\partial x} = f_k(t)\, ik\, e^{ikx} = f_k(t)\, \left(ik\, e^{ikx}\right)$$
  - However, if we apply the centered finite-difference (2nd order accurate):

$$\left(\frac{\partial f}{\partial x}\right)_j = \frac{f_{j+1} - f_{j-1}}{2\Delta x} \Rightarrow$$

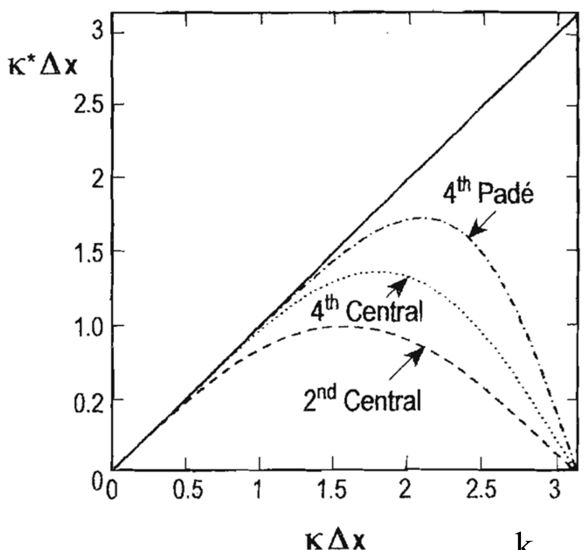
$$\left(\frac{\partial\, e^{ikx}}{\partial x}\right)_j = \frac{e^{ik(x_j+\Delta x)} - e^{ik(x_j-\Delta x)}}{2\Delta x} = \frac{\left(e^{ik\Delta x} - e^{-ik\Delta x}\right) e^{ikx_j}}{2\Delta x} = i\,\frac{\sin(k\Delta x)}{\Delta x}\, e^{ikx_j} = i\, k_{\mathrm{eff}}\, e^{ikx_j}$$

where $k_{\mathrm{eff}} = \dfrac{\sin(k\Delta x)}{\Delta x}$ (uniform grid resolution Δx)

  - k_{eff} = effective wavenumber
  - For low wavenumbers (smooth functions): $$k_{\mathrm{eff}} = \frac{\sin(k\Delta x)}{\Delta x} = k - \frac{k^3 \Delta x^2}{6} + \ldots$$
    - Shows the 2nd order nature of center-difference approx. (here, of k by k_{eff})

Fourier Error Analysis, Cont'd: Effective Wave numbers

- Different approximations $\left(\frac{\partial\, e^{ikx}}{\partial x}\right)_j$ have different effective wavenumbers
  - CDS, 2nd order: $k_{\text{eff}} = \frac{\sin(k\Delta x)}{\Delta x} = k - \frac{k^3 \Delta x^2}{6} + \ldots$
  - CDS, 4th order: $k_{\text{eff}} = \frac{\sin(k\Delta x)}{3\Delta x}\left(4 - \cos(k\Delta x)\right)$
  - Pade scheme, 4th order: $i\,k_{\text{eff}} = \frac{3i\,\sin(k\Delta x)}{\left(2+\cos(k\Delta x)\right)\Delta x}$



$k_{\max}\,\Delta x$

Fig. 3.4. Modified wavenumber for various schemes

Source: Lomax, H., T. Pulliam, and D. Zingg. *Fundamentals of Computational Fluid Dynamics*. Springer, 2001.

The fourth-order Padé scheme is given by

$$(\delta_x u)_{j-1} + 4(\delta_x u)_j + (\delta_x u)_{j+1} = \frac{3}{\Delta x}(u_{j+1} - u_{j-1}) .$$

The modified wavenumber for this scheme satisfies[6]

$$\mathrm{i}\kappa^* \mathrm{e}^{-\mathrm{i}\kappa\Delta x} + 4\mathrm{i}\kappa^* + \mathrm{i}\kappa^* \mathrm{e}^{\mathrm{i}\kappa\Delta x} = \frac{3}{\Delta x}(\mathrm{e}^{\mathrm{i}\kappa\Delta x} - \mathrm{e}^{-\mathrm{i}\kappa\Delta x}) ,$$

which gives

$$\mathrm{i}\kappa^* = \frac{3\mathrm{i}\sin\kappa\Delta x}{(2+\cos\kappa\Delta x)\Delta x} .$$

Note that k_{eff} is bounded: $0 \le k_{eff} \le k_{\max}$

$$k_{\max} = \frac{\pi}{\Delta x}$$

Fourier Error Analysis, Cont'd
Effective Wave Speeds

Different approximations $\left(\frac{\partial\, e^{ikx}}{\partial x}\right)_j$ also lead to different effective wave speeds:

- Consider linear convection equations: $\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0$
  - For the exact solution: $f(x,t) = \sum_{k=-\infty}^{\infty} f_k(0)\, e^{ikx+\sigma t} = \sum_{k=-\infty}^{\infty} f_k(0)\, e^{ik(x-ct)}$ (since $\sigma = -i\,k\,c$)
  - For the numerical sol.: if $f = f_k^{num.}(t)e^{ikx} \Rightarrow \frac{d\, f_k^{num.}}{dt} e^{ikx_j} = -f_k^{num.}(t)\, c \left(\frac{\partial\, e^{ikx}}{\partial x}\right)_j = -f_k^{num.}(t)\, c \left(i\, k_{\text{eff}}\, e^{ikx_j}\right)$

  which we can solve exactly (our interest here is only error due to spatial approx.)

$$\Rightarrow \quad f_k^{num.}(t) = f_k(0)e^{-ik_{\text{eff}}\,c\,t}$$

$$\Rightarrow f^{\,numerical}(x,t) = \sum_{k=-\infty}^{\infty} f_k\,(0)\, e^{ikx-ik_{\text{eff}}\,c\,t} = \sum_{k=-\infty}^{\infty} f_k\,(0)\, e^{ik(x-c_{\text{eff}}\,t)}$$

$$\Rightarrow \frac{c_{eff}}{c} = \frac{\sigma_{eff}}{\sigma} = \frac{k_{eff}}{k} \quad (\text{defining } \sigma_{\text{eff}} = -i\,k_{\text{eff}}\,c = -i\,k\,c_{\text{eff}}$$

  - Often, $c_{\text{eff}}/\,c < 1$ => numerical solution is too slow.
  - Since c_{eff} is a function of the effective wavenumber,

  the scheme is dispersive (even though the PDE is not)

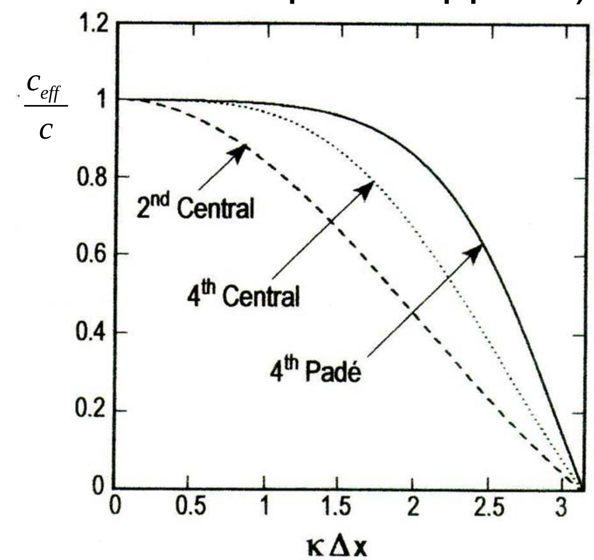


Fig. 3.5. Numerical phase speed for various schemes

Source: Lomax, H., T. Pulliam, and D. Zingg. *Fundamentals of Computational Fluid Dynamics*. Springer, 2001.

Evaluation of the Stability of a FD Scheme

Recall: $\tau_{\Delta x} = L(\phi) - \hat{L}_{\Delta x}(\hat{\phi} + \varepsilon) = -\hat{L}_{\Delta x}(\varepsilon)$ Stability: $\left\| \hat{L}_{\Delta x}^{-1} \right\| < \text{Const.}$ (for linear systems)

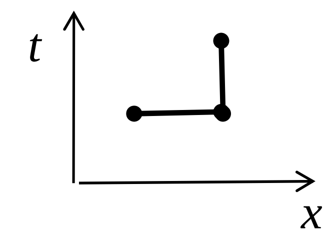
- Heuristic stability:
  - Stability is defined with reference to an error (e.g. round-off) made in the calculation, which is damped (stability) or grows (instability)
  - Heuristic Procedure: Try it out
    - Introduce an isolated error and observed how the error behaves
    - Requires an exhaustive search to ensure full stability, hence mainly informational approach
- Energy Method
  - Basic idea:
    - Find a quantity, L_2 norm e.g. $\sum_j \left(\phi_j^n\right)^2$
    - Shows that it remains bounded for all n
  - Less used than Von Neumann method, but can be applied to nonlinear equations and to non-periodic BCs
- Von Neumann method (Fourier Analysis method)

Evaluation of the Stability of a FD Scheme

Energy Method Example

- Consider again: $\dfrac{\partial \phi}{\partial t} + c\dfrac{\partial \phi}{\partial x} = 0$
- A possible FD formula ("upwind" scheme for c>0): $\dfrac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\dfrac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$

$(t = n\Delta t, x = j\Delta x)$ which can be rewritten:



$$\phi_j^{n+1} = (1-\mu)\,\phi_j^n + \mu\,\phi_{j-1}^n = 0 \quad \text{with} \quad \mu = \frac{c\,\Delta t}{\Delta x}$$

For the rest of this derivation, please see equations 2.18 through 2.22 in Durran, D. *Numerical Methods for Wave Equations in Geophysical Fluid Dynamics*. Springer, 1998. ISBN: 9780387983769.

Evaluation of the Stability of a FD Scheme

Energy Method Example

For the rest of this derivation, please see equations 2.18 through 2.22 in Durran, D. *Numerical Methods for Wave Equations in Geophysical Fluid Dynamics*. Springer, 1998. ISBN: 9780387983769.

Von Neumann Stability

- Widely used procedure
- Assumes initial error can be represented as a Fourier Series and considers growth or decay of these errors
- In theoretical sense, applies only to periodic BC problems and to linear problems
  - Superposition of Fourier modes can then be used
- Again, use, $f(x,t) = \sum_{k=-\infty}^{\infty} f_k(t)\, e^{ikx}$ but for the error: $\varepsilon(x,t) = \sum_{\beta=-\infty}^{\infty} \varepsilon_\beta(t)\, e^{i\beta x}$
- Being interested in error growth/decay, consider only one mode:

$$\varepsilon_\beta(t)\, e^{i\beta x} \approx e^{\gamma t}\, e^{i\beta x} \quad \text{where } \gamma \text{ is in general complex and function of } \beta: \ \gamma = \gamma(\beta)$$

- Strict Stability: for the error not to grow in time, $\left| e^{\gamma t} \right| \leq 1 \quad \forall \gamma$
  - in other words, for $t = n\Delta t$, the condition for strict stability can be written:

$$\left| e^{\gamma \Delta t} \right| \leq 1 \quad \text{or for } \xi = e^{\gamma \Delta t}, \quad \left| \xi \right| \leq 1$$

von Neumann condition

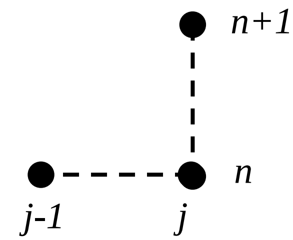
Norm of amplification factor ξ smaller than 1

Evaluation of the Stability of a FD Scheme
Von Neumann Example

- Consider again: $$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = 0$$
- A possible FD formula ("upwind" scheme) $$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$

  $(t = n\Delta t,\ \ x = j\Delta x)$ which can be rewritten:

$$\phi_j^{n+1} = (1-\mu)\,\phi_j^n + \mu\,\phi_{j-1}^n \quad \text{with} \quad \mu = \frac{c\,\Delta t}{\Delta x}$$



- Consider the Fourier error decomposition (one mode) and discretize it:

$$\varepsilon(x,t) = \varepsilon_\beta(t)\,e^{i\beta x} = e^{\gamma t}e^{i\beta x} \Rightarrow \varepsilon_j^n = e^{\gamma n\Delta t}e^{i\beta j\Delta x}$$

- Insert it in the FD scheme, assuming the error mode satisfies the FD:

$$\varepsilon_j^{n+1} = (1-\mu)\,\varepsilon_j^n + \mu\,\varepsilon_{j-1}^n \quad \Rightarrow \quad e^{\gamma(n+1)\Delta t}e^{i\beta j\Delta x} = (1-\mu)\,e^{\gamma n\Delta t}e^{i\beta j\Delta x} + \mu\,e^{\gamma n\Delta t}e^{i\beta(j-1)\Delta x}$$

- Cancel the common term (which is $\varepsilon_j^n = e^{\gamma n\Delta t}e^{i\beta j\Delta x}$) and obtain:

$$e^{\gamma\Delta t} = (1-\mu) + \mu\,e^{-i\beta\Delta x}$$

Evaluation of the Stability of a FD Scheme
von Neumann Example

- The magnitude of $\xi = e^{\gamma \Delta t}$ is then obtained by multiplying ξ with its complex conjugate:

$$|\xi|^2 = \left((1-\mu) + \mu\, e^{-i\beta\Delta x}\right)\left((1-\mu) + \mu\, e^{i\beta\Delta x}\right) = 1 - 2\mu(1-\mu)\left(1 - \frac{e^{i\beta\Delta x} + e^{-i\beta\Delta x}}{2}\right)$$

Since $\dfrac{e^{i\beta\Delta x} + e^{-i\beta\Delta x}}{2} = \cos(\beta\Delta x) \quad \text{and} \quad 1 - \cos(\beta\Delta x) = 2\sin^2(\dfrac{\beta\Delta x}{2}) \quad \Rightarrow$

$$|\xi|^2 = 1 - 2\mu(1-\mu)\left(1 - \cos(\beta\Delta x)\right) = 1 - 4\mu(1-\mu)\sin^2(\frac{\beta\Delta x}{2})$$

- Thus, the strict von Neumann stability criterion gives

$$|\xi| \le 1 \quad \Leftrightarrow \quad \left|1 - 4\mu(1-\mu)\sin^2(\frac{\beta\Delta x}{2})\right| \le 1$$

Since $\sin^2(\dfrac{\beta\Delta x}{2}) \ge 0 \quad \forall\beta \qquad \left(\left(1 - \cos(\beta\Delta x)\right) \ge 0 \quad \forall\beta\right)$

we obtain the same result as for the energy method:

$$|\xi| \le 1 \quad \Leftrightarrow \quad \mu(1-\mu) \ge 0 \quad \Leftrightarrow \quad \boxed{0 \le \frac{c\,\Delta t}{\Delta x} \le 1} \qquad (\mu = \frac{c\,\Delta t}{\Delta x})$$

Equivalent to the CFL condition

(from Lecture 12)

Partial Differential Equations
Hyperbolic PDE: $B^2 - 4AC > 0$

Examples:

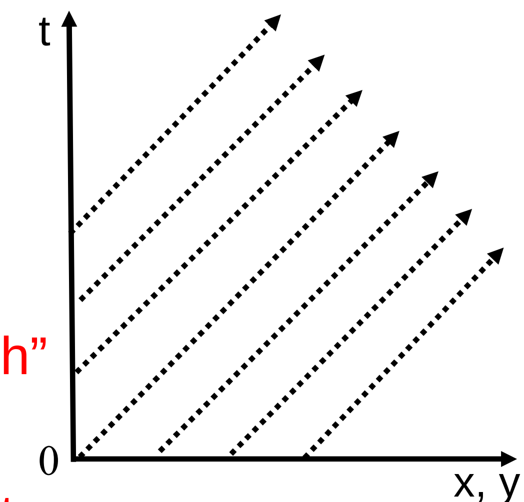
(1) $\dfrac{\partial^2 u}{\partial t^2} = c^2 \dfrac{\partial^2 u}{\partial x^2}$ ← Wave equation, 2^{nd} order

(2) $\dfrac{\partial u}{\partial t} \pm c \dfrac{\partial u}{\partial x} = 0$ ← Sommerfeld Wave/radiation equation, 1^{st} order

(3) $\dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{U} \cdot \nabla)\, \mathbf{u} = \mathbf{g}$ ← Unsteady (linearized) inviscid convection (Wave equation first order)

(4) $(\mathbf{U} \cdot \nabla)\, \mathbf{u} = \mathbf{g}$ ← Steady (linearized) inviscid convection

- Allows non-smooth solutions
- Information travels along characteristics, e.g.:
  - For (3) above: $\dfrac{d\,\mathbf{x_c}}{dt} = \mathbf{U}(\mathbf{x_c}(t))$
  - For (4), along streamlines: $\dfrac{d\,\mathbf{x_c}}{ds} = \mathbf{U}$
- Domain of dependence of $\mathbf{u}(\mathbf{x},T)$ = "characteristic path"
  - e.g., for (3), it is: $\mathbf{x_c}(t)$ for $0 < t < T$
- Finite Differences, Finite Volumes and Finite Elements



Partial Differential Equations
Hyperbolic PDE

Waves on a String

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2} \qquad 0 < x < L, \quad 0 < t < \infty$$

Initial Conditions

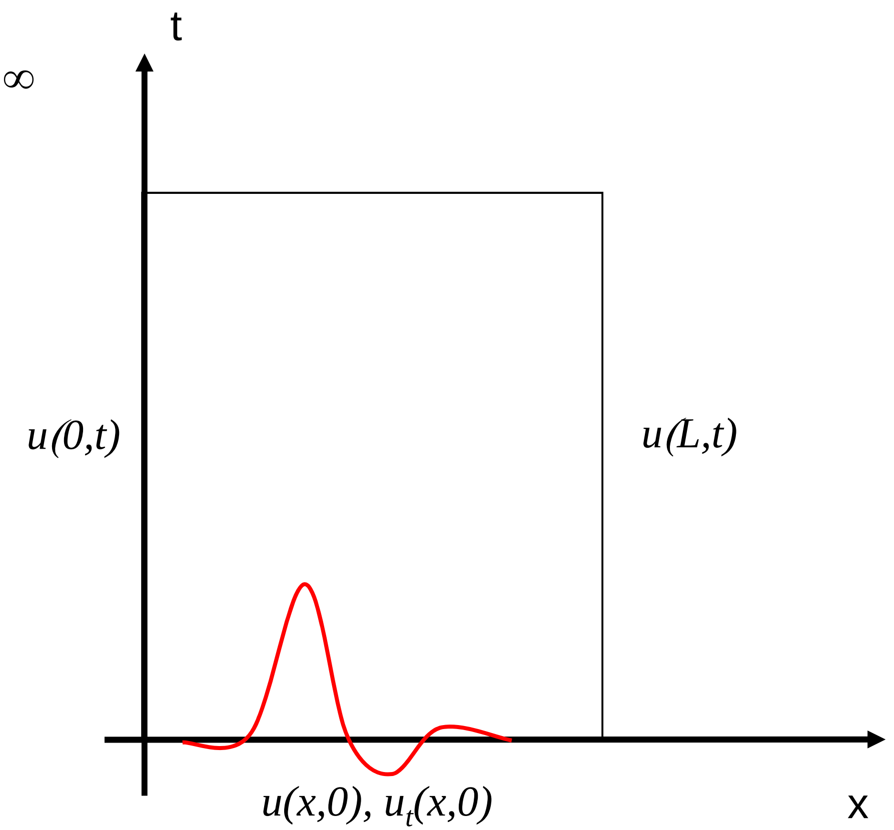
$$\begin{aligned} u(x,0) &= f(x), \ \ 0 \le x \le L \\ u_t(x,0) &= g(x), \ \ 0 < x < L \end{aligned}$$

Boundary Conditions

$$\begin{aligned} u(0,t) &= 0, \ , \ 0 < t < \infty \\ u(L,t) &= 0, \ , \ 0 < t < \infty \end{aligned}$$

Wave Solutions

$$u = \begin{cases} F(x-ct) & \text{Forward propagating wave} \\ G(x+ct) & \text{Backward propagating wave} \end{cases}$$



Typically Initial Value Problems in Time, Boundary Value Problems in Space
Time-Marching Solutions: Explicit Schemes Generally Stable

2.29 Numerical Fluid Mechanics
Fall 2011