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 $1^{\text{st}}$ order term decreases faster than that of $2^{\text{nd}}$ order term
  - Convergence becomes asymptotically $2^{\text{nd}}$ order ($1^{\text{st}}$ 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 $f(x,t) = \sum_{k=-\infty}^{\infty} f_k(t) e^{ikx}$ \(\Rightarrow\) $\frac{df_k(t)}{dt} = (ik)^n f_k(t) = \sigma f_k(t)$ for $\sigma = (ik)^n$
  - Differentiation, definition and smoothness of solution for $n$ order 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 Stability
  – 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”.


Fourier Error Analysis: 1\textsuperscript{st} 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 1\textsuperscript{st} 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 (2\textsuperscript{nd} order accurate):
    \[ \left( \frac{\partial f}{\partial x} \right)_j = \frac{f_{j+1} - f_{j-1}}{2\Delta x} \Rightarrow \]
    \[ \left( \frac{\partial e^{ikx}}{\partial x} \right)_j = \frac{e^{ik(x_j+\Delta x)} - e^{ik(x_j-\Delta x)}}{2\Delta x} = \frac{\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)e^{ikx}}{2\Delta x} = i \frac{\sin(k\Delta x)}{\Delta x} e^{ikx} = i k_{eff} e^{ikx} \]

    where \( k_{eff} = \frac{\sin(k\Delta x)}{\Delta x} \) (uniform grid resolution \( \Delta x \))

    - \( k_{eff} = \) effective wavenumber

    - For low wavenumbers (smooth functions):
      \[ k_{eff} = \frac{\sin(k\Delta x)}{\Delta x} = k - \frac{k^3\Delta x^2}{6} + ... \]

    - Shows the 2\textsuperscript{nd} 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, 2\textsuperscript{nd} order:
  \[
  k_{\text{eff}} = \frac{\sin(k\Delta x)}{\Delta x} = k - \frac{k^3\Delta x^2}{6} + ...
  \]

- CDS, 4\textsuperscript{th} order:
  \[
  k_{\text{eff}} = \frac{\sin(k\Delta x)}{3\Delta x} (4 - \cos(k\Delta x))
  \]

- Pade scheme, 4\textsuperscript{th} order:
  \[
  ik_{\text{eff}} = \frac{3i\sin(k\Delta x)}{(2 + \cos(k\Delta x))\Delta x}
  \]

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

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

which gives

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

Note that \( k_{\text{eff}} \) is bounded: 
\[
0 \leq k_{\text{eff}} \leq k_{\max}
\]

\[
k_{\max} = \frac{\pi}{\Delta x}
\]
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 \( \sigma = -ikc \))

  - For the numerical sol.: if \( f = f_{num}^k(t)e^{ikx} \Rightarrow d f_{num}^k(t)/dt e^{ikx} = -f_{num}^k(t) c \left( \frac{\partial e^{ikx}}{\partial x} \right)_j = -f_{num}^k(t) c \left( i k_{eff} e^{ikx} \right) \)

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

  \[
  \Rightarrow f_{num}^k(t) = f_k(0)e^{-i k_{eff} c t}
  \]

  \[
  \Rightarrow f_{numerical}(x,t) = \sum_{k=-\infty}^{\infty} f_k(0) e^{ikx-i k_{eff} c t} = \sum_{k=-\infty}^{\infty} f_k(0) e^{ik(x-c_{eff} t)}
  \]

  \[
  \Rightarrow \frac{c_{eff}}{c} = \frac{\sigma_{eff}}{\sigma} = \frac{k_{eff}}{k} \quad \text{(defining } \sigma_{eff} = -i k_{eff} c = -i k c_{eff} \text{)}
  \]

  - Often, \( c_{eff}/c < 1 \Rightarrow \text{numerical solution is too slow.} \)

  - Since \( c_{eff} \) is a function of the effective wavenumber, the scheme is dispersive (even though the PDE is not)
Evaluation of the Stability of a FD Scheme

Recall: \( \tau_{\Delta x} = L (\phi) - \hat{L}_{\Delta x}(\hat{\phi} + \epsilon) = -\hat{L}_{\Delta x}(\epsilon) \)

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. \( \sum_j (\phi_j^n)^2 \)
    • 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:

\[
\frac{\partial \phi}{\partial t} + c \frac{\partial \phi}{\partial x} = 0
\]

• A possible FD formula (“upwind” scheme for \( c > 0 \)):

\[
\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0
\]

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

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

Evaluation of the Stability of a FD Scheme
Energy Method Example

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: $\varepsilon_\beta(t) e^{i\beta x} \approx e^{\gamma t} e^{i\beta x}$ where $\gamma$ is in general complex and function of $\beta$: $\gamma = \gamma(\beta)$
- Strict Stability: for the error not to grow in time, $|e^{\gamma t}| \leq 1 \ \forall \gamma$
  - in other words, for $t = n\Delta t$, the condition for strict stability can be written: $|e^{\gamma \Delta t}| \leq 1$ or for $\xi = e^{\gamma \Delta t}$, $|\xi| \leq 1$

Norm of amplification factor $\xi$ 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:

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

- 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 \( \xi = e^{i\Delta t} \) is then obtained by multiplying \( \xi \) 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 \( \frac{e^{i\beta \Delta x} + e^{-i\beta \Delta x}}{2} = \cos(\beta \Delta x) \) and \( 1 - \cos(\beta \Delta x) = 2\sin^2\left(\frac{\beta \Delta x}{2}\right) \) \( \Rightarrow \)

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

- Thus, the strict von Neumann stability criterion gives

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

Since \( \sin^2\left(\frac{\beta \Delta x}{2}\right) \geq 0 \quad \forall \beta \quad \left(1 - \cos(\beta \Delta x)\right) \geq 0 \quad \forall \beta \)

we obtain the same result as for the energy method:

\[
|\xi| \leq 1 \quad \Leftrightarrow \quad \mu(1 - \mu) \geq 0 \quad \Leftrightarrow \quad 0 \leq c\frac{\Delta t}{\Delta x} \leq 1 \quad (\mu = c\frac{\Delta t}{\Delta x})
\]

Equivalent to the CFL condition
Partial Differential Equations

Hyperbolic PDE: \( B^2 - 4AC > 0 \)

Examples:

1. \( \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \)  
   Wave equation, 2\(^{nd}\) order

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

3. \( \frac{\partial u}{\partial t} + (U \cdot \nabla) u = g \)  
   Unsteady (linearized) inviscid convection
   (Wave equation first order)

4. \( (U \cdot \nabla) u = g \)  
   Steady (linearized) inviscid convection

- Allows non-smooth solutions
- Information travels along characteristics, e.g.:
  - For (3) above: \( \frac{dx_c}{dt} = U(x_c(t)) \)
  - For (4), along streamlines: \( \frac{dx_c}{ds} = U \)
- Domain of dependence of \( u(x, T) \) = “characteristic path”
  - e.g., for (3), it is: \( x_c(t) \) for \( 0 < t < T \)
- Finite Differences, Finite Volumes and Finite Elements
Partial Differential Equations
Hyperbolic PDE

Waves on a String

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

Initial Conditions

\[ u(x,0) = f(x), \quad 0 \leq x \leq L \]
\[ u_t(x,0) = g(x), \quad 0 < x < L \]

Boundary Conditions

\[ u(0,t) = 0, \quad 0 < t < \infty \]
\[ u(L,t) = 0, \quad 0 < t < \infty \]

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
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