REVIEW Lecture 11:

- **Finite Differences based Polynomial approximations**
  - Obtain polynomial (in general un-equally spaced), then differentiate as needed
    - Newton’s interpolating polynomial formulas
      
      \[ f(x) = f_0 + \frac{\Delta f_0}{h}(x - x_0) + \frac{\Delta^2 f_0}{2!h^2}(x - x_0)(x - x_1) + \ldots \]
      \[ + \frac{\Delta^n f_0}{n!h^n}(x - x_0)(x - x_1)\cdots(x - x_{n-1}) + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)\cdots(x - x_n) \]

  - Lagrange polynomial
    (Reformulation of Newton’s polynomial)
    \[ f(x) = \sum_{k=0}^{n} L_k(x) f(x_k) \quad \text{with} \quad L_k(x) = \prod_{j=0, j\neq k}^{n} \frac{x - x_j}{x_k - x_j} \]

  - Hermite Polynomials and Compact/Pade’s Difference schemes
    (Use the values of the function and its derivative(s) at nodes)
    \[ \sum_{i=-r}^{s} b_i \left( \frac{\partial^m u}{\partial x^m} \right)_{j+i} - \sum_{i=-p}^{q} a_i u_{j+i} = \tau_{\Delta x} \]

- **Finite Difference: Boundary conditions**
  - Different approx. at and near the boundary => impacts global order of accuracy and linear system to be solved
REVIEW Lecture 11:

• 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
FINITE DIFFERENCES – Outline for Today

• Finite-Differences on Non-Uniform Grids and Uniform Errors: 1-D
• Grid Refinement and Error Estimation
• Fourier Analysis and Error Analysis
  – Differentiation, definition and smoothness of solution for ≠ order of spatial operators
• Stability
  – Heuristic Method
  – Energy Method
• 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”.


Grid-Refinement and Error estimation

- We found that for a convergent scheme, the discretization error $\varepsilon$ is of the form: 
  $$\varepsilon = \alpha O(\Delta x^p) + R$$  
  (recall: $\phi = \hat{\phi} + \varepsilon$, $\mathcal{L}(\phi) = 0$, $\hat{\mathcal{L}}_{\Delta x}(\hat{\phi}) = 0$) 
  where $R$ is the remainder.

- The degree of accuracy and discretization error can be estimated between solutions obtained on systematically refined/coarsened grids.

  - True solution $u$ can be expressed either as: 
    $$u = u_{\Delta x} + \beta \Delta x^p + R$$  
    $$u = u_{2\Delta x} + \beta' (2\Delta x)^p + R'$$

  - Thus, the exponent $p$ can be estimated: 
    $$p \approx \log \left( \frac{u_{2\Delta x} - u_{4\Delta x}}{u_{\Delta x} - u_{2\Delta x}} \right) / \log 2$$
    (need to eliminate $u$ and then need 2 eqns. to eliminate both $\Delta x$ and $p$, hence $u_{4\Delta x}$)

- The discretization error on the grid $\Delta x$ can be estimated by: 
  $$\varepsilon_{\Delta x} \approx \frac{u_{\Delta x} - u_{2\Delta x}}{2^p - 1}$$

- Good idea: estimate $p$ to check code. Is it equal to what it is supposed to be?

- When solutions on several grids are available, an approximation of higher accuracy can be obtained from the remainder: Richardson Extrapolation!
Richardson Extrapolation: method to obtain a third improved estimate of an integral based on two other estimates

Consider:

\[ I = I(h) + E(h) \]

For two different grid space \( h_1 \) and \( h_2 \):

\[ I(h_1) + E(h_1) = I(h_2) + E(h_2) \]

\[ \Rightarrow E(h_1) \approx E(h_2) \left( \frac{h_1}{h_2} \right)^2 \]

\[ I(h_1) + E(h_2) \left( \frac{h_1}{h_2} \right)^2 \approx I(h_2) + E(h_2) \]

\[ E(h_2) \approx \frac{I(h_1) - I(h_2)}{1 - \left( \frac{h_1}{h_2} \right)^2} \]

Richardson Extrapolation:

\[ I = I(h_2) + \frac{I(h_2) - I(h_1)}{(h_1/h_2)^2 - 1} + O(h^4) \]

Example

Assume: \( h_2 = h_1/2 \)

\[ I = I(h_2) + \frac{I(h_2) - I(h_1)}{(2^2 - 1)} + O(h^4) \]

\[ = \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1) + O(h^4) \]

From two \( O(h^2) \), we get an \( O(h^4) \)!
Romberg’s Integration: Iterative application of Richardson’s extrapolation

Romberg Integration Algorithm, for any order $k$

$$I_{j,k} \approx \frac{4^{k-1}I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

For Order 2 (case of previous slide):

$k = 2, j = 1$

$$I_{1,2} \approx \frac{4I_{2,1} - I_{1,1}}{3}$$

Increasing resolution

- a. 0.172800 → 1.367467 → 1.068800
- b. 0.172800 → 1.367467 → 1.640533 → 1.068800 → 1.623467 → 1.484800
- c. Increasing resolution
Romberg’s Differentiation:
Iterative application of Richardson’s extrapolation

‘Romberg’ Differentiation Algorithm, for any order $k$

$$D_{j,k} \sim \frac{4^{k-1}D_{j+1,k-1} - D_{j,k-1}}{4^{k-1} - 1}$$

For Order 2 (as previous slide, but for differentiation):

$k = 2, j = 1$

$$D_{1,2} \sim \frac{4D_{2,1} - D_{1,1}}{3}$$

Increasing resolution

<table>
<thead>
<tr>
<th>$j$</th>
<th>$D$</th>
<th>$k$</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.172800</td>
<td>1.367467</td>
<td>1</td>
<td>O($h^2$)</td>
</tr>
<tr>
<td>1.068800</td>
<td>1.068800</td>
<td>2</td>
<td>O($h^4$)</td>
</tr>
<tr>
<td>1.484800</td>
<td>1.640533</td>
<td>3</td>
<td>O($h^6$)</td>
</tr>
<tr>
<td>1.639467</td>
<td>1.640533</td>
<td>4</td>
<td>O($h^8$)</td>
</tr>
</tbody>
</table>
Fourier (Error) Analysis: Definitions

- Leading error terms and discretization error estimates can be complemented by a Fourier error analysis.

- Fourier decomposition:
  - Any arbitrary periodic function can be decomposed into its Fourier components:

\[
f(x) = \sum_{k=-\infty}^{\infty} f_k e^{ikx} \quad (k \text{ integer, wavenumber})
\]

\[
2\pi \int_0^{2\pi} e^{ikx} e^{-imx} = 2\pi \delta_{km} \quad (\text{orthogonality property})
\]

Using the orthog. property, taking the integral/FT of \(f(x)\):

\[
f_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx} \, dx
\]

- Note: rate at which \(|f_k|\) with \(|k|\) decays determine smoothness of \(f(x)\).

- Examples drawn in lecture: \(\sin(x)\), Gaussian \(\exp(-\pi x^2)\), multi-frequency functions, etc.
Fourier (Error) Analysis: Differentiations

• Consider the decompositions:

\[ f(x) = \sum_{k=-\infty}^{\infty} f_k e^{ikx} \quad \text{or} \quad f(x,t) = \sum_{k=-\infty}^{\infty} f_k(t) e^{ikx} \]

• Taking spatial derivatives gives:

\[ \frac{\partial^n f}{\partial x^n} = \sum_{k=-\infty}^{\infty} f_k(t) (ik)^n e^{ikx} \]

• Taking temporal derivatives gives:

\[ \frac{\partial^r f}{\partial t^r} = \sum_{k=-\infty}^{\infty} \frac{d^r f_k(t)}{dt^r} e^{ikx} \]

• Hence, in particular, for even or odd spatial derivatives:

\[ n = 2q \quad \Rightarrow \quad (ik)^n = (-1)^q k^{2q} \quad \text{(real)} \]

\[ n = 2q - 1 \quad \Rightarrow \quad (ik)^n = -i (-1)^q k^{2q-1} \quad \text{(imaginary)} \]
Fourier (Error) Analysis: Generic equation

- Consider the generic PDE:
  \[ \frac{\partial f}{\partial t} = \frac{\partial^n f}{\partial x^n} \]

- Fourier Analysis:
  \[ f(x,t) = \sum_{k=-\infty}^{\infty} f_k(t) e^{ikx} \]

- Hence:
  \[ \sum_{k=-\infty}^{\infty} \frac{d f_k(t)}{d t} e^{ikx} = \sum_{k=-\infty}^{\infty} f_k(t) (ik)^n e^{ikx} \]

- Thus:
  \[ \frac{d f_k(t)}{d t} = (ik)^n f_k(t) = \sigma f_k(t) \quad \text{for} \quad \sigma = (ik)^n \]

- And:
  \[ f_k(t) = f_k(0) e^{\sigma t}, \quad f(x,t) = \sum_{k=-\infty}^{\infty} f_k(0) e^{ikx+\sigma t} \]

  - “Phase speed”: \[ c = -\sigma / ik \]
Fourier (Error) Analysis:
Generic equation

- Generic PDE, FT:

\[ f(x,t) = \sum_{k=-\infty}^{\infty} f_k(0) e^{ikx+\sigma t} \]

\[ \frac{df_k(t)}{dt} = \sigma f_k(t) \quad \text{for} \quad \sigma = (ik)^n \]

- Hence:

\[ n = 2q \quad \Rightarrow \quad (ik)^n = (-1)^q k^{2q} \quad \text{(real)} \]

\[ n = 2q - 1 \quad \Rightarrow \quad (ik)^n = -i (-1)^q k^{2q-1} \quad \text{(imaginary)} \]

- Hence:

\[ n = 1 \quad \frac{\partial f}{\partial t} = \frac{\partial f}{\partial x} \quad \sigma = ik \quad \text{Propagation:} \quad c = -\sigma / ik = -1, \quad \text{No dispersion} \]

\[ n = 2 \quad \frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2} \quad \sigma = -k^2 \quad \text{Decay} \]

\[ n = 3 \quad \frac{\partial f}{\partial t} = \frac{\partial^3 f}{\partial x^3} \quad \sigma = -ik^3 \quad \text{Propagation:} \quad c = -\sigma / ik = +k^2, \quad \text{With dispersion} \]

\[ n = 4 \quad \frac{\partial f}{\partial t} = \pm \frac{\partial^4 f}{\partial x^4} \quad \sigma = \pm k^4 \quad +: \text{(Fast) Growth}, \quad -: \text{(Fast) Decay} \]

- Etc
Fourier Error Analysis: 1\textsuperscript{st} derivatives $\frac{\partial f}{\partial x}$

- 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: $\frac{\partial f_k(t) e^{ikx}}{\partial x} = f_k(t) ik e^{ikx} = f_k(t) (ik e^{ikx})$

- However, if we apply the centered finite-difference (2\textsuperscript{nd} order accurate):

\[
\left( \frac{\partial f}{\partial x} \right)_j = \frac{f_{j+1} - f_{j-1}}{2\Delta x} \Rightarrow \\
\left( \frac{\partial e^{ikx}}{\partial x} \right)_j = \frac{e^{ik(x_j+\Delta x)} - e^{ik(x_j-\Delta x)}}{2\Delta x} = \frac{\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)e^{ikx_j}}{2\Delta x} = i \frac{\sin(k\Delta x)}{\Delta x} e^{ikx_j} = i k_{\text{eff}} e^{ikx_j}
\]

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

  - $k_{\text{eff}} =$ effective wavenumber

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

  - Shows the 2\textsuperscript{nd} order nature of center-difference approx. (here, of $k$ by $k_{\text{eff}}$)
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\(^{nd}\) order: 
  \( k_{\text{eff}} = \frac{\sin(k\Delta x)}{\Delta x} = k - \frac{k^3 \Delta x^2}{6} + ... \)

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

- Pade scheme, 4\(^{th}\) order:
  \( \kappa \Delta x \)

\[
\sin(kx) + 3i \sin(k\Delta x) \\
\frac{2 + \cos(k\Delta x)}{\Delta x}
\]

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:

\[
0 \leq k_{\text{eff}} \leq k_{\text{max}}
\]

\[
k_{\text{max}} = \frac{\pi}{\Delta x}
\]
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 \( f = f_{k,\text{num.}}(t)e^{ikx} \Rightarrow \frac{d}{dt}f_{k,\text{num.}}(t)e^{ikx} = -f_{k,\text{num.}}(t) c \left( \frac{\partial e^{ikx}}{\partial x} \right)_j = -f_{k,\text{num.}}(t) c (i k_{\text{eff}} e^{ikx_j}) \)

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

\[
\Rightarrow f_{k,\text{num.}}(t) = f_k(0)e^{-ik_{\text{eff}} ct}
\]

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

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

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

- Since \( c_{\text{eff}} \) is a function of the effective wavenumber the scheme is dispersive (even though the PDE is not)

\[\text{Fig. 3.5. Numerical phase speed for various schemes}\]

© Springer. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.
Evaluation of the Stability of a FD Scheme: Three main approaches

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

Stability: \( \left\| \hat{\mathcal{L}}_{\Delta x}^{-1} \right\| < \text{Const.} \) (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 observe 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. \( \sum_j (\phi_j^\prime)^2 \)
    - 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:

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

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, 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: The error will not grow in time if \( |e^{\gamma t}| \leq 1 \quad \forall \gamma \)
  - in other words, for \( t = n\Delta t \), the condition for strict stability can be written:
    \[ |e^{\gamma n\Delta t}| \leq 1 \quad \text{or for} \quad \xi = e^{\gamma n\Delta t}, \quad |\xi| \leq 1 \quad \text{von Neumann condition} \]

Norm of amplification factor \( \xi \) smaller or equal to \( 1 \)
2.29 Numerical Fluid Mechanics
Spring 2015

For information about citing these materials or our Terms of Use, visit: http://ocw.mit.edu/terms.