2.29 Numerical Fluid Mechanics
Spring 2015 – **Lecture 12**

REVIEW Lecture 11:

- **Finite Differences based Polynomial approximations**
  - Obtain polynomial (in general un-equally spaced), then differentiate as needed
    - Newton's interpolating polynomial formulas

Triangular Family of Polynomials (case of Equidistant Sampling, similar if not equidistant)

$$\begin{aligned} f(x) &= f_0 + \frac{\Delta f_0}{h}(x-x_0) + \frac{\Delta^2 f_0}{2!h^2}(x-x_0)(x-x_1) + \cdots \\ &+ \frac{\Delta^n f_0}{n!h^n}(x-x_0)(x-x_1)\cdots(x-x_{n-1}) + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)\cdots(x-x_n) \end{aligned}$$

- 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

2.29 Numerical Fluid Mechanics
Spring 2015 – **Lecture 12**

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^{st} order term decreases faster than that of 2^{nd} order term
  - Convergence becomes asymptotically 2^{nd} order (1^{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
  - 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”.
- 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, 2014/2010/2006.”

Grid-Refinement and Error estimation

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

  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: $\begin{cases} u = u_{\Delta x} + \beta\ \Delta x^p + R \\ u = u_{2\Delta x} + \beta'\,(2\Delta x)^p + R' \end{cases}$
  - Thus, the exponent p can be estimated: $p \approx \log\left(\dfrac{u_{2\Delta x} - u_{4\Delta x}}{u_{\Delta x} - u_{2\Delta x}}\right) \Big/ \log 2$

  (need to eliminate u and then need 2 eqns. to eliminate both Δx and p, hence $u_{4\Delta x}$)

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

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 h1 and h2:

$$I(h_1) + E(h_1) = I(h_2) + E(h_2)$$

Trapezoidal Rule:

$$E(h) = -\frac{b-a}{12} h^2 \bar{f}''$$

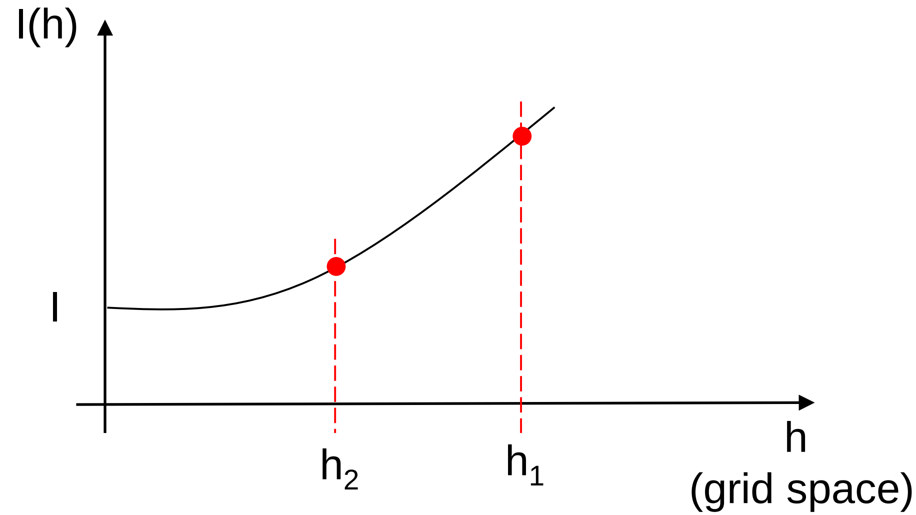
$$\Rightarrow E(h_1) \approx E(h_2) \left(\frac{h_1}{h_2}\right)^2$$

$$I(h_1) + E(h_2) \left(\frac{h_1}{h_2}\right)^2 \simeq I(h_2) + E(h_2)$$

$$E(h_2) \simeq \frac{I(h_1) - I(h_2)}{1 - (h_1/h_2)^2}$$

Richardson Extrapolation:

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



Example

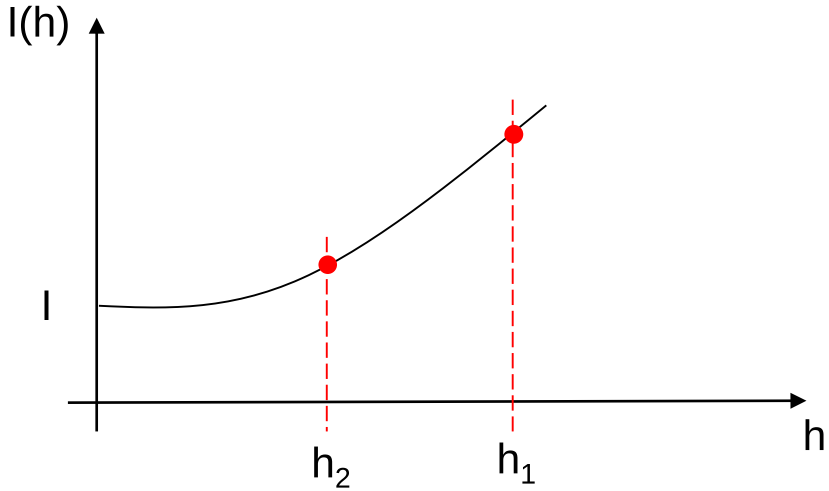
Assume: $h_2 = h_1/2$

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

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

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*

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

For Order 2 (case of previous slide):

$$k = 2, j = 1$$

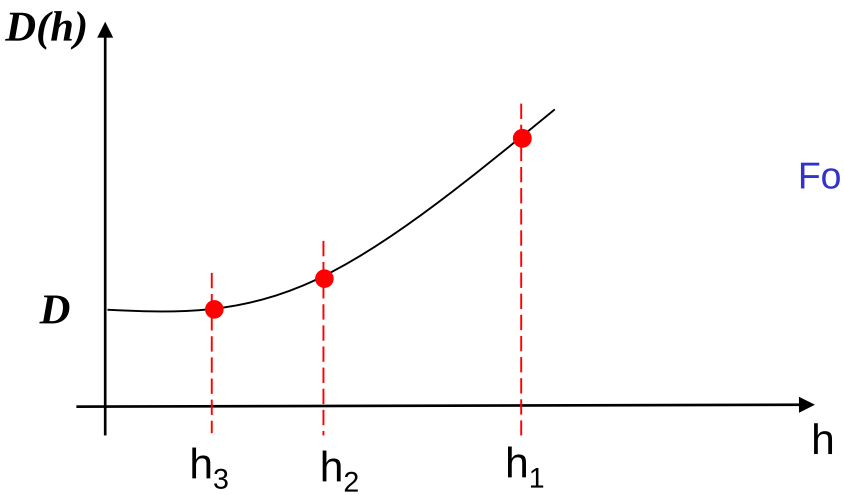
$$I_{1,2} \simeq \frac{4 I_{2,1} - I_{1,1}}{3}$$

k → Increasing order

j ↓ Increasing resolution

	1: $O(h^2)$	2: $O(h^4)$	3: $O(h^6)$	4: $O(h^8)$
a.	0.172800	1.367467		
	1.068800			
b,.	0.172800	1.367467	1.640533	
	1.068800	1.623467		
	1.484800			
c.	0.172800	1.367467	1.640533	1.640533
	1.068800	1.623467	1.640533	
	1.484800	1.639467		
	1.600800			

Romberg's Differentiation:
Iterative application of Richardson's extrapolation



'Romberg' Differentiation Algorithm, for any order *k*

$$\boldsymbol{D}_{j,k} \simeq \frac{4^{k-1}\boldsymbol{D}_{j+1,k-1} - \boldsymbol{D}_{j,k-1}}{4^{k-1}-1}$$

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

$$k = 2, j = 1$$

$$\boldsymbol{D}_{1,2} \simeq \frac{4\boldsymbol{D}_{2,1} - \boldsymbol{D}_{1,1}}{3}$$

k → Increasing order

j ↓ Increasing resolution

	1: O(h^2)	2: O(h^4)	3: O(h^6)	4: O(h^8)
a.	0.172800	1.367467		
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	1.600800			

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:

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

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

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:

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

- Taking spatial derivatives gives: $\dfrac{\partial^n f}{\partial x^n} = \sum_{k=-\infty}^{\infty} f_k(t) \; (ik)^n \; e^{ikx}$

- Taking temporal derivatives gives: $\dfrac{\partial^r f}{\partial t^r} = \sum_{k=-\infty}^{\infty} \dfrac{d^r f_k(t)}{dt^r} \; e^{ikx}$

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

$$n = 2q \qquad \Rightarrow \qquad (ik)^n = (-1)^q \, k^{2q} \qquad \text{(real)}$$

$$n = 2q-1 \qquad \Rightarrow \qquad (ik)^n = -i \, (-1)^q \, k^{2q-1} \qquad \text{(imaginary)}$$

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: $$\frac{d\, f_k(t)}{d\,t} = (ik)^n\; f_k(t) = \sigma f_k(t) \qquad \text{for } \; \sigma = (ik)^n$$
- And: $$f_k(t) = f_k(0)\; e^{\sigma t}, \qquad f(x,t) = \sum_{k=-\infty}^{\infty} f_k(0)\, e^{ikx+\sigma t}$$
  - "Phase speed": $c = -\sigma / ik$

Fourier (Error) Analysis: Generic equation

- Generic PDE, FT:

$$\frac{d\, f_k(t)}{d\,t} = \sigma f_k(t) \qquad \text{for} \quad \sigma = (ik)^n$$

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

$$n = 2q \qquad \Rightarrow \quad (ik)^n = (-1)^q\, k^{2q} \qquad \text{(real)}$$

$$n = 2q-1 \qquad \Rightarrow \quad (ik)^n = -i\,(-1)^q\, k^{2q-1} \qquad \text{(imaginary)}$$

- Hence:

$n=1$	$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x}$	$\sigma = ik$	Propagation: $c = -\sigma / ik = -1$, No dispersion
$n=2$	$\frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2}$	$\sigma = -k^2$	Decay
$n=3$	$\frac{\partial f}{\partial t} = \frac{\partial^3 f}{\partial x^3}$	$\sigma = -ik^3$	Propagation: $c = -\sigma / ik = +k^2$, With dispersion
$n=4$	$\frac{\partial f}{\partial t} = \pm \frac{\partial^4 f}{\partial x^4}$	$\sigma = \pm k^4$	$+$: (Fast) Growth, $-$: (Fast) Decay

- Etc

Fourier Error Analysis: 1st 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 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):

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

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

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

  - k_{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 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: $i\,k_{\text{eff}} = \frac{3i\,\sin(k\Delta x)}{\left(2 + \cos(k\Delta x)\right)\Delta x}$

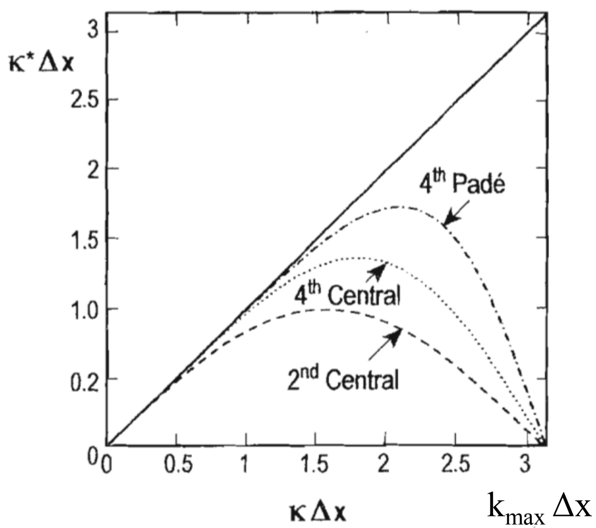


Fig. 3.4. Modified wavenumber for various schemes

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]

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

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: $0 \le k_{eff} \le k_{\max}$

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

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

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.)

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

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

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

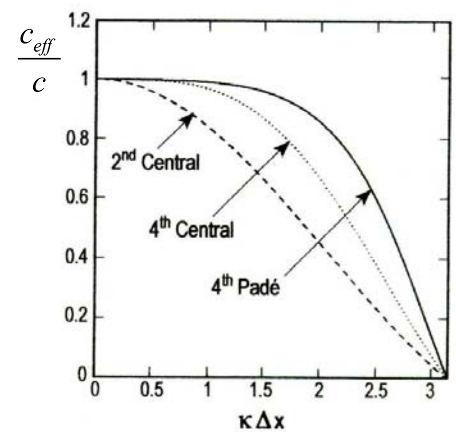


Fig. 3.5. Numerical phase speed for various schemes

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

- 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)

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)

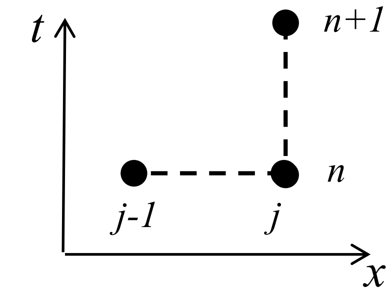
- Heuristic stability:
  - Stability is defined with reference to an error (e.g. round-off) made in the calculation, which is damped (stability) or grows (instability)
  - Heuristic Procedure: Try it out
    - Introduce an isolated error and observe how the error behaves
    - Requires an exhaustive search to ensure full stability, hence mainly informational approach
- Energy Method
  - Basic idea:
    - Find a quantity, L_2 norm e.g. $\sum_j \left(\phi_j^n\right)^2$
    - 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: $$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = 0$$
- 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:

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



Derivation removed due to copyright restrictions. 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

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:

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

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

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

von Neumann condition

Norm of amplification factor ξ smaller or equal to1