2.29 Numerical Fluid Mechanics
Fall 2009 – Lecture 13

REVIEW Lecture 12:

- **Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations**
  - Parabolic PDEs
  - Elliptic PDEs
  - Hyperbolic PDEs
- **Error Types and Discretization Properties:** $L(\phi) = 0 , \quad \hat{L}_{\Delta x}(\hat{\phi}) = 0$
  - Consistency: $\left| L(\phi) - \hat{L}_{\Delta x}(\phi) \right| \rightarrow 0 \quad \text{when } \Delta x \rightarrow 0$
  - Truncation error: $\tau_{\Delta x} = L(\phi) - \hat{L}_{\Delta x}(\phi) \rightarrow O(\Delta x^p) \quad \text{for } \Delta x \rightarrow 0$
  - Error equation: $\tau_{\Delta x} = L(\phi) - \hat{L}_{\Delta x}(\hat{\phi} + \varepsilon) = -\hat{L}_{\Delta x}(\varepsilon)$ (for linear systems)
  - Stability: $\left\| \hat{L}_{\Delta x}^{-1} \right\| < \text{Const.}$ (for linear systems)
  - Convergence: $\left\| \varepsilon \right\| \leq \left\| \hat{L}_{\Delta x}^{-1} \right\| \left\| \tau_{\Delta x} \right\| \leq \alpha \, O(\Delta x^p)$

2.29 Numerical Fluid Mechanics
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REVIEW Lecture 12, Cont'd:

- Classification of PDEs and examples
- Error Types and Discretization Properties
- **Finite Differences based on Taylor Series Expansions**
  - Higher Order Accuracy Differences, with Examples
    - Incorporate more higher-order terms of the Taylor series expansion than strictly needed and express them as finite differences themselves (making them function of neighboring function values)
    - If these finite-differences are of sufficient accuracy, this pushes the remainder to higher order terms => increased order of accuracy of the FD method
    - General approximation:

$$\left(\frac{\partial^m u}{\partial x^m}\right)_j - \sum_{i=-r}^{s} a_i \, u_{j+i} = \tau_{\Delta x}$$

  - Taylor Tables or Method of Undetermined Coefficients (Polynomial Fitting)
    - Simply a more systematic way to solve for coefficients a_i

FINITE DIFFERENCES – Outline for Today

- Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations (Elliptic, Parabolic and Hyperbolic PDEs)
- **Error Types and Discretization Properties**
  - Consistency, Truncation error, Error equation, Stability, Convergence
- **Finite Differences based on Taylor Series Expansions**
  - Higher Order Accuracy Differences, with Example
  - Taylor Tables or Method of Undetermined Coefficients (Polynomial Fitting)
- **Polynomial approximations**
  - Newton's formulas
  - Lagrange polynomial and un-equally spaced differences
  - Hermite Polynomials and Compact/Pade's Difference schemes
  - Boundary conditions
  - Un-Equally spaced differences
  - Error Estimation: order of convergence, discretization error, Richardson's extrapolation, and iterative improvements using Roomberg's algorithm

References and Reading Assignments

- Part 8 (PT 8.1-2), Chapter 23 on “Numerical Differentiation” and Chapter 18 on “Interpolation” of “Chapra and Canale, Numerical Methods for Engineers, 2010/2006.”
- 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”

FINITE DIFFERENCES: Interpolation Formulas for Higher Order Accuracy

2nd approach: Generalize Taylor series using interpolation formulas

- Fit the unknown function solution of the (P)DE to an interpolation curve and differentiate the resulting curve. For example:
  - Fit a parabola to data at points $x_{i-1}, x_i, x_{i+1} \quad (\Delta x_i = x_i - x_{i-1})$, then differentiate to obtain:

$$f'(x_i) = \frac{f(x_{i+1})(\Delta x_i)^2 - f(x_{i-1})(\Delta x_{i+1})^2 + f(x_i)\left[(\Delta x_{i+1})^2 - (\Delta x_i)^2\right]}{\Delta x_{i+1}\, \Delta x_i\, (\Delta x_i + \Delta x_{i+1})}$$

  - This is a 2nd order approximation
  - For uniform spacing, reduces to centered difference seen before
  - In general, approximation of first derivative has truncation error of the order of the polynomial
- All types of polynomials or numerical differentiation methods can be used to derive such interpolations formulas
  - Polynomial fitting, Method of undetermined coefficients, Newton's interpolating polynomials, Lagrangian and Hermite Polynomials, etc

FINITE DIFFERENCES Higher Order Accuracy: Taylor Tables or Method of Undetermined Coefficients

Taylor Tables: Convenient way of forming linear combinations of Taylor Series on a term-by-term basis

The Taylor table for a centered three point Lagrangian approximation to a second derivative.

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_j - \frac{1}{\Delta x^2}(a\,u_{j-1} + b\,u_j + c\,u_{j+1}) = ?$$

What we are looking for

Taylor series at:

		u_j	$\Delta x \left(\frac{\partial u}{\partial x}\right)_j$	$\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_j$	$\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3}\right)_j$	$\Delta x^4 \left(\frac{\partial^4 u}{\partial x^4}\right)_j$
	$\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_j$			1		
j-1	$-a \cdot u_{j-1}$	$-a$	$-a \cdot (\text{-}1) \cdot \frac{1}{1}$	$-a \cdot (\text{-}1)^2 \cdot \frac{1}{2}$	$-a \cdot (\text{-}1)^3 \cdot \frac{1}{6}$	$-a \cdot (\text{-}1)^4 \cdot \frac{1}{24}$
j	$-b \cdot u_j$	$-b$				
j+1	$-c \cdot u_{j+1}$	$-c$	$-c \cdot (1) \cdot \frac{1}{1}$	$-c \cdot (1)^2 \cdot \frac{1}{2}$	$-c \cdot (1)^3 \cdot \frac{1}{6}$	$-c \cdot (1)^4 \cdot \frac{1}{24}$

Sum each column starting from left, force the sums to zero and so choose a, b, c, etc

FINITE DIFFERENCES
Higher Order Accuracy: Taylor Tables Cont'd

The Taylor table for a centered three point Lagrangian approximation to a second derivative.

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_j - \frac{1}{\Delta x^2}\left(a\,u_{j-1} + b\,u_j + c\,u_{j+1}\right) = ?$$

Sum each column starting from left and force the sums to be zero by proper choice of a, b, c, etc:

$$\begin{bmatrix} -1 & -1 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -2 \end{bmatrix} \Rightarrow \begin{bmatrix} a & b & c \end{bmatrix} = \begin{bmatrix} 1 & -2 & 1 \end{bmatrix}$$

= Familiar 3-point central difference

Truncation error is first column in the table that does not vanish, here fifth column of table:

$$\tau_{\Delta x} = \frac{1}{\Delta x^2}\left[\frac{-a}{24} + \frac{-c}{24}\right]\Delta x^4 \left(\frac{\partial^4 u}{\partial x^4}\right)_j = -\frac{\Delta x^2}{12}\left(\frac{\partial^4 u}{\partial x^4}\right)_j$$

FINITE DIFFERENCES
Higher Order Accuracy: Taylor Tables Cont'd

The Taylor table for a backward three point Lagrangian approximation to a second derivative.

$$\left(\frac{\partial u}{\partial x}\right)_j - \frac{1}{\Delta x}(a_2 u_{j-2} + a_1 u_{j-1} + b\, u_j) = ?$$

	u_j	$\Delta x\left(\frac{\partial u}{\partial x}\right)_j$	$\Delta x^2\left(\frac{\partial^2 u}{\partial x^2}\right)_j$	$\Delta x^3\left(\frac{\partial^3 u}{\partial x^3}\right)_j$	$\Delta x^4\left(\frac{\partial^4 u}{\partial x^4}\right)_j$
$\Delta x\left(\frac{\partial u}{\partial x}\right)_j$		1			
$-a_2 \cdot u_{j-2}$	$-a_2$	$-a_2 \cdot (\text{-}2) \cdot \frac{1}{1}$	$-a_2 \cdot (\text{-}2)^2 \cdot \frac{1}{2}$	$-a_2 \cdot (\text{-}2)^3 \cdot \frac{1}{6}$	$-a_2 \cdot (\text{-}2)^4 \cdot \frac{1}{24}$
$-a_1 \cdot u_{j-1}$	$-a_1$	$-a_1 \cdot (\text{-}1) \cdot \frac{1}{1}$	$-a_1 \cdot (\text{-}1)^2 \cdot \frac{1}{2}$	$-a_1 \cdot (\text{-}1)^3 \cdot \frac{1}{6}$	$-a_1 \cdot (\text{-}1)^4 \cdot \frac{1}{24}$
$-b \cdot u_j$	$-b$				

$\Rightarrow \; [a_2 \quad a_1 \quad b] = [1 \quad -4 \quad 3]/2$ and $\tau_{\Delta x} = \frac{1}{\Delta x}\left[\frac{8a_2}{6} + \frac{a_1}{6}\right]\Delta x^3\left(\frac{\partial^3 u}{\partial x^3}\right)_j = \frac{\Delta x^2}{3}\left(\frac{\partial^3 u}{\partial x^3}\right)_j$

(as in lecture 12)

Finite Differences using Polynomial approximations
Numerical Interpolation: Newton's Iteration Formula

Standard triangular family of polynomials

$$\begin{aligned} f(x) &= p(x) + r(x) \\ &= c_0 + c_1(x - x_0) + \cdots + c_n(x - x_0)\cdots(x - x_{n-1}) \\ &\quad + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)\cdots(x - x_n) \end{aligned}$$

Divided Differences

$$f(x_0) = c_0 \Rightarrow c_0 = \boxed{f(x_0)}$$

$$f(x_1) = c_0 + c_1(x_1 - x_0) \Rightarrow c_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \boxed{f[x_0, x_1]}$$

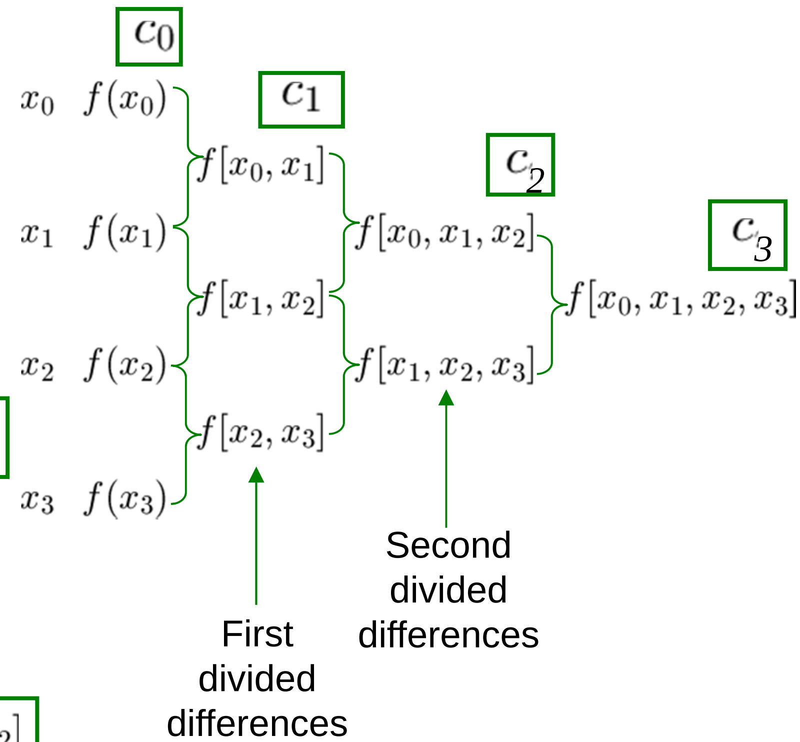
$$f(x_2) = c_0 + c_1(x_2 - x_0) + c_2(x_2 - x_0)(x_2 - x_1)$$

$$c_2 = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0} = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} = \boxed{f[x_0, x_1, x_2]}$$

By recurrence:

$$\Rightarrow \boxed{c_n = f[x_0, x_1, \ldots, x_n]} = \frac{f[x_1, \ldots, x_n] - f[x_0, \ldots x_{n-1}]}{x_n - x_0}$$

Newton's Computational Scheme



Finite Differences using Polynomial approximations
Equidistant Newton's Interpolation

Equidistant Sampling

$$x_i = x_0 + ih$$

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1}{h}(f_1 - f_0) = \frac{1}{h}\Delta f_0$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} = \frac{1}{1 \cdot 2 \cdot h^2}(f_2 - 2f_1 + f_0) = \frac{1}{2!h^2}\Delta^2 f_0$$

$$f[x_0, x_1, x_2, x_3] = \frac{1}{3! \cdot h^3}(f_3 - 3f_2 + 3f_1 - f_0) = \frac{1}{3!h^3}\Delta^3 f_0$$

Divided Differences
Equidistant Step size Implied

x_0	f_0			
		$f_1 - f_0 = \Delta f_0$		
x_1	f_1		$f_2 - 2f_1 + f_0 = \Delta^2 f_0$	
		$f_2 - f_1 = \Delta f_1$		$f_3 - 3f_2 + 3f_1 - f_0 - = \Delta^3 f_0$
x_2	f_2		$f_3 - 2f_2 + f_1 = \Delta^2 f_1$	
		$f_3 - f_2 = \Delta f_2$		
x_3	f_3			

$$c_0 = f_0$$

$$c_1 = \frac{1}{h}\Delta f_0$$

$$c_2 = \frac{1}{2!h^2}\Delta^2 f_0$$

$$c_3 = \frac{1}{3!h^3}\Delta^3 f_0$$

Triangular Family of Polynomials
Equidistant Sampling

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

Numerical Differentiation using Newton's algorithm for equidistant sampling

Triangular Family of Polynomials Equidistant Sampling

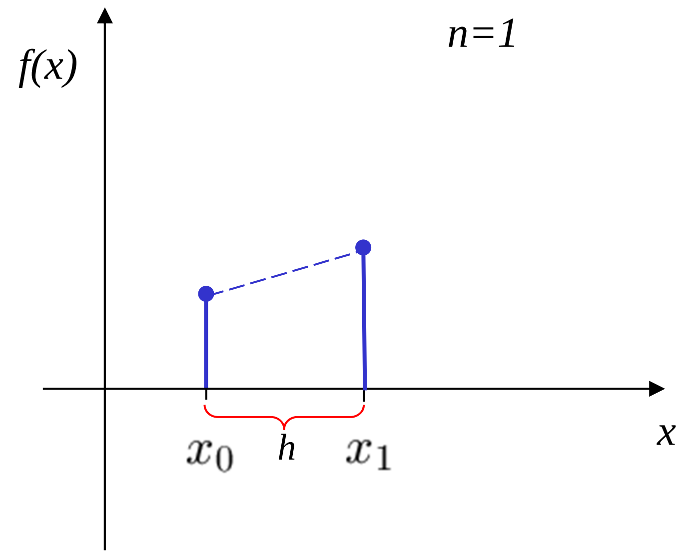
$$f(x) = f_0 + \frac{\Delta f_0}{h}(x-x_0) + \frac{\Delta^2 f_0}{2!h^2}(x-x_0)(x-x_1) + \cdots$$
$$+ \frac{\Delta^n f_0}{n!h^n}(x-x_0)(x-x_1)\cdots(x-x_{n-1}) + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)\cdots(x-x_n)$$

First order

$$n = 1$$

$$f(x) = f_0 + \frac{\Delta f_0}{h}(x-x_0) + \frac{f''(\xi)}{2!}(x-x_0)(x-x_1)$$

$$f'(x) = \frac{\Delta f_0}{h} + O(h) = \frac{1}{h}(f_1 - f_0) + O(h)$$



Numerical Differentiation using Newton's algorithm for equidistant sampling, Cont'd

Second order

$$n = 2$$

$$f(x) = f_0 + \frac{\Delta f_0}{h}(x-x_0) + \frac{\Delta^2 f_0}{2!h^2}(x-x_0)(x-x_1) + \frac{f'''(\xi)}{3!}(x-x_0)(x-x_1)(x-x_2) + \cdots$$

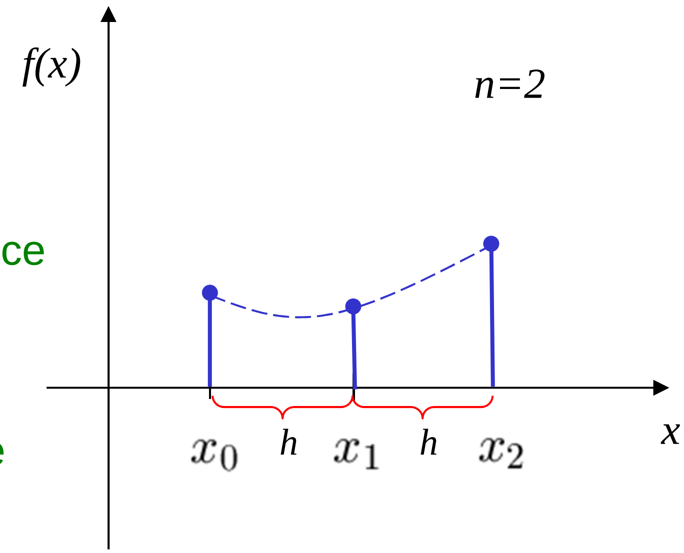
$$f'(x) = \frac{\Delta f_0}{h} + \frac{\Delta^2 f_0}{2h^2}(x-x_0) + \frac{\Delta^2 f_0}{2h^2}(x-x_1) + O(h^2)$$

$$\begin{aligned} f'(x_0) &= \frac{f_1 - f_0}{h} - \frac{1}{2h}(f_2 - 2f_1 + f_0) + O(h^2) \\ &= \frac{2f_1 - 2f_0 - f_2 + 2f_1 - f_0}{2h} + O(h^2) \\ &= \boxed{\frac{1}{h}(-\frac{3}{2}f_0 + 2f_1 - \frac{1}{2}f_2) + O(h^2)} \end{aligned}$$

Forward Difference

$$\begin{aligned} f'(x_1) &= \frac{f_1 - f_0}{h} + \frac{1}{2h}(f_2 - 2f_1 + f_0) + O(h^2) \\ &= \boxed{\frac{1}{2h}(f_2 - f_0) + O(h^2)} \end{aligned}$$

Central Difference



Second Derivatives

n=2 $\quad f''(x_0) = \frac{\Delta^2 f_0}{h^2} + O(h) = \boxed{\frac{1}{h^2}(f_0 - 2f_1 + f_2) + O(h)}$ Forward Difference

n=3 $\quad f''(x_1) = \boxed{\frac{1}{h^2}(f_0 - 2f_1 + f_2) + O(h^2)}$ Central Difference

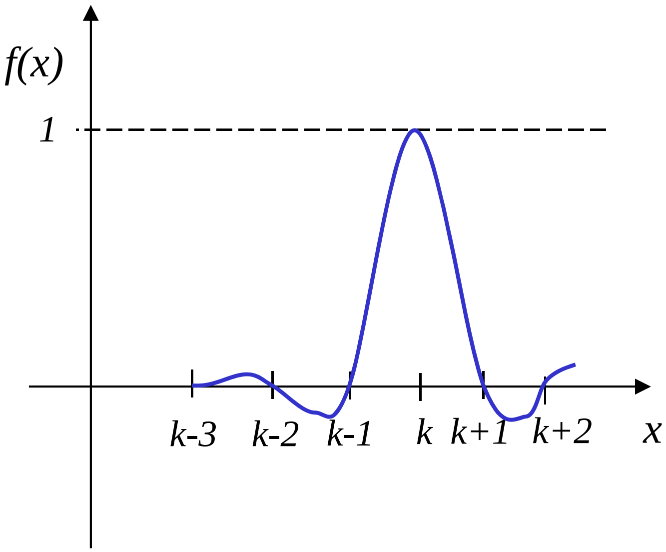
Finite Differences using Polynomial approximations Numerical Interpolation: Lagrange Polynomials (Reformulation of Newton's polynomial)

$$p(x) = \sum_{k=0}^{n} L_k(x) f(x_k) = \sum_{k=0}^{n} L_k(x) f_k$$

$$L_k(x) = \sum_{i=0}^{n} \ell_{ik} x^i$$

$$L_k(x_i) = \delta_{ki} = \begin{cases} 0 & k \neq i \\ 1 & k = i \end{cases}$$

$$L_k(x) = \prod_{j=0, j\neq k}^{n} \frac{x - x_j}{x_k - x_j}$$



Difficult to program
Difficult to estimate errors
Divisions are expensive

Important for numerical integration

Hermite Interpolation Polynomials and Compact / Pade' Difference Schemes

- Use the values of the function and its derivative(s) at given points k
  - For example, for values of the function and of its first derivatives at pts k

$$u(x) = \sum_{k=1}^{n} a_k(x)\, u_k + \sum_{k=1}^{m} b_k(x) \left(\frac{\partial u}{\partial x} \right)_k$$

- General form for implicit/explicit schemes (here focusing on space)

$$\sum_{i=-r}^{s} b_i \left(\frac{\partial^m u}{\partial x^m} \right)_{j+i} - \sum_{i=-p}^{q} a_i \, u_{j+i} = \tau_{\Delta x}$$

  - Generalizes the Lagrangian approach by using Hermitian interpolation
- Leads to the "Compact difference schemes" or " Pade' schemes "
- Are implemented by the use of efficient banded solvers

FINITE DIFFERENCES: Higher Order Accuracy
Taylor Tables for Pade' schemes

Taylor table for a central three point Hermitian approximation to a first derivative.

$$d\left(\frac{\partial u}{\partial x}\right)_{j-1} + \left(\frac{\partial u}{\partial x}\right)_{j} + e\left(\frac{\partial u}{\partial x}\right)_{j+1} - \frac{1}{\Delta x}\left(au_{j-1} + bu_j + cu_{j+1}\right) = ?$$

—	u_j	$\Delta x\left(\frac{\partial u}{\partial x}\right)_j$	$\Delta x^2\left(\frac{\partial^2 u}{\partial x^2}\right)_j$	$\Delta x^3\left(\frac{\partial^3 u}{\partial x^3}\right)_j$	$\Delta x^4\left(\frac{\partial^4 u}{\partial x^4}\right)_j$	$\Delta x^5\left(\frac{\partial^5 u}{\partial x^5}\right)_j$
$\Delta x d\left(\frac{\partial u}{\partial x}\right)_{j-1}$	—	d	$d\cdot(-1)\cdot\frac{1}{1}$	$d\cdot(-1)^2\cdot\frac{1}{2}$	$d\cdot(-1)^3\cdot\frac{1}{6}$	$d\cdot(-1)^4\cdot\frac{1}{24}$
$\Delta x\left(\frac{\partial u}{\partial x}\right)_{j}$	—	1	—	—	—	—
$\Delta x e\left(\frac{\partial u}{\partial x}\right)_{j+1}$	—	e	$e\cdot(1)\cdot\frac{1}{1}$	$e\cdot(1)^2\cdot\frac{1}{2}$	$e\cdot(1)^3\cdot\frac{1}{6}$	$e\cdot(1)^4\cdot\frac{1}{24}$
$-a\cdot u_{j-1}$	-a	$-a\cdot(-1)\cdot\frac{1}{1}$	$-a\cdot(-1)^2\cdot\frac{1}{2}$	$-a\cdot(-1)^3\cdot\frac{1}{6}$	$-a\cdot(-1)^4\cdot\frac{1}{24}$	$-a\cdot(-1)^5\cdot\frac{1}{120}$
$-b\cdot u_j$	-b	—	—	—	—	—
$-c\cdot u_{j+1}$	-c	$-c\cdot(1)\cdot\frac{1}{1}$	$-c\cdot(1)^2\cdot\frac{1}{2}$	$-c\cdot(1)^3\cdot\frac{1}{6}$	$-c\cdot(1)^4\cdot\frac{1}{24}$	$-c\cdot(1)^5\cdot\frac{1}{120}$

FINITE DIFFERENCES: Higher Order Accuracy
Taylor Tables for Pade' schemes, Cont'd

Taylor table for a central three point Hermitian approximation to a first derivative.

$$d\left(\frac{\partial u}{\partial x}\right)_{j-1} + \left(\frac{\partial u}{\partial x}\right)_{j} + e\left(\frac{\partial u}{\partial x}\right)_{j+1} - \frac{1}{\Delta x}\left(au_{j-1} + bu_{j} + cu_{j+1}\right) = ?$$

Image by MIT OpenCourseWare.

Sum each column starting from left and force the sums to be zero by proper choice of a, b, c, etc:

$$\begin{bmatrix} -1 & -1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 1 & 1 \\ -1 & 0 & -1 & 2 & 2 \\ 1 & 0 & -1 & 3 & 2 \\ -1 & 0 & -1 & -4 & 4 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \\ e \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} a & b & c & d & e \end{bmatrix} = \frac{1}{4}\begin{bmatrix} -3 & 0 & 3 & 1 & 1 \end{bmatrix}$$

Truncation error is first column in the table that does not vanish, here sixth column:

$$\tau_{\Delta x} = \frac{\Delta x^4}{120}\left(\frac{\partial^5 u}{\partial x^5}\right)_j$$

Compact / Pade' Difference Schemes: Examples

We can derive family of compact centered approximations for ϕ up to 6th order using:

$$\alpha\left(\frac{\partial\phi}{\partial x}\right)_{i+1} + \left(\frac{\partial\phi}{\partial x}\right)_{i} + \alpha\left(\frac{\partial\phi}{\partial x}\right)_{i-1} = \beta\,\frac{\phi_{i+1}-\phi_{i-1}}{2\Delta x} + \gamma\,\frac{\phi_{i+2}-\phi_{i-2}}{4\Delta x}$$

Scheme	Truncation error	α	β	γ
CDS-2	$\frac{(\Delta x)^2}{3!}\frac{\partial^3\phi}{\partial x^3}$	0	1	0
CDS-4	$\frac{13(\Delta x)^4}{3\cdot 3!}\frac{\partial^5\phi}{\partial x^5}$	0	$\frac{4}{3}$	$-\frac{1}{3}$
Padé-4	$\frac{(\Delta x)^4}{5!}\frac{\partial^5\phi}{\partial x^5}$	$\frac{1}{4}$	$\frac{3}{2}$	0
Padé-6	$\frac{4(\Delta x)^6}{7!}\frac{\partial^7\phi}{\partial x^7}$	$\frac{1}{3}$	$\frac{14}{9}$	$\frac{1}{9}$

Image by MIT OpenCourseWare.

Comments:

- Pade' schemes use fewer computational nodes and thus are more compact than CDS
- Can be advantageous (more banded systems!)

Higher-Order Finite Difference Schemes Considerations

- Retaining more terms in Taylor Series or in polynomial approximations allows to obtain FD schemes of increased order of accuracy
- However, higher-order approximations involve more nodes, hence more complex system of equations to solve and more complex treatment of boundary condition schemes
- Results shown for one variable valid for mixed derivatives
- To approximate other terms that are not differentiated: reaction terms, etc
  - Values at the center node is normally all that is needed
  - However, for strongly nonlinear terms, care is needed (see later)
- Boundary conditions must be discretized

Finite Difference Schemes: Implementation of Boundary conditions

- For unique solutions, information is needed at boundaries
- Generally, one is given either:

i) the variable: $u\,(x = x_{\text{bnd}}, t) = u_{\text{bnd}}(t)$ (Dirichlet BCs)

ii) a gradient in a specific direction, e.g.: $\left.\frac{\partial u}{\partial x}\right|_{(x_{\text{bnd}}, t)} = \phi_{\text{bnd}}(\text{t})$ (Neumann BCs)

iii) a linear combination of the two quantities (Robin BCs)

- Straightforward cases:
  - If value is known, nothing special needed (one doesn't solve for the BC)
  - If derivatives are specified, for first-order schemes, this is also straightforward to treat

Finite Difference Schemes: Implementation of Boundary conditions, Cont'd

- Harder cases: when higher-order approximations are used
  - At and near the boundary: nodes outside of domain would be needed
- Remedy: use different approximations at and near the boundary
  - Either, approximations of lower order are used
  - Or, approximations go deeper in the interior and are one-sided. For example,
    - 1st order forward-difference: $\left.\frac{\partial u}{\partial x}\right|_{(x_{\text{bnd}},t)} = 0 \;\Rightarrow\; \frac{u_2 - u_1}{x_2 - x_1} \approx 0 \;\Rightarrow u_2 = u_1$
    - Parabolic fit to the bnd point and two inner points:

$$\left.\frac{\partial u}{\partial x}\right|_{(x_{\text{bnd}},t)} \approx \frac{-u_3(x_2-x_1)^2 + u_2(x_3-x_1)^2 - u_1\left[(x_3-x_1)^2 - (x_2-x_1)^2\right]}{(x_2-x_1)(x_3-x_1)(x_3-x_2)} \qquad \left(\approx \frac{-u_3 + 4\,u_2 - 3u_1}{2\Delta x} \text{ for equidistant nodes}\right)$$

    - Cubic fit to 4 nodes (3rd order difference): $\left.\frac{\partial u}{\partial x}\right|_{(x_{\text{bnd}},t)} \approx \frac{2u_4 - 9u_3 + 18u_2 - 11u_1}{6\Delta x} + O(\Delta x^3)$ for equidistant nodes
    - Compact schemes, cubic fit to 4 pts: $u_{(x_{bnd},t)} = u_1 \approx \frac{18u_2 - 9u_3 + 2u_4}{11} - \frac{6\Delta x}{11}\left(\frac{\partial u}{\partial x}\right)_1$ for equidistant nodes

- In Open-boundary systems, boundary problem is not well posed =>
  - Separate treatment for inflow/outflow points, multi-scale approach and/or generalized inverse problem (using data in the interior)

2.29 Numerical Fluid Mechanics
Fall 2011