

2.29 Numerical Fluid Mechanics Spring 2015 – Lecture 11

REVIEW Lecture 10:

- Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations
 - Parabolic PDEs
 - Elliptic PDEs
 - Hyperbolic PDEs

• Error Types and Discretization Properties: $\mathcal{L}(\phi) = 0$, $\hat{\mathcal{L}}_{\Delta x}(\hat{\phi}) = 0$

- Consistency:
- Truncation error:
- Error equation:
- Stability:
- Convergence:

 $\begin{aligned} \left| \mathcal{L}(\phi) - \hat{\mathcal{L}}_{\Delta x}(\phi) \right| &\to 0 \quad \text{when } \Delta x \to 0 \\ \tau_{\Delta x} &= \mathcal{L}(\phi) - \hat{\mathcal{L}}_{\Delta x}(\phi) \to O(\Delta x^{p}) \quad \text{for } \Delta x \to 0 \\ \tau_{\Delta x} &= \mathcal{L}(\phi) - \hat{\mathcal{L}}_{\Delta x}(\hat{\phi} + \varepsilon) = -\hat{\mathcal{L}}_{\Delta x}(\varepsilon) \quad \text{(for linear systems)} \\ \left\| \hat{\mathcal{L}}_{\Delta x}^{-1} \right\| &< \text{Const.} \quad \text{(for linear systems)} \\ \left\| \varepsilon \right\| &\leq \left\| \hat{\mathcal{L}}_{\Delta x}^{-1} \right\| \quad \left\| \tau_{\Delta x} \right\| \leq \alpha \ O(\Delta x^{p}) \end{aligned}$



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REVIEW Lecture 10, 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



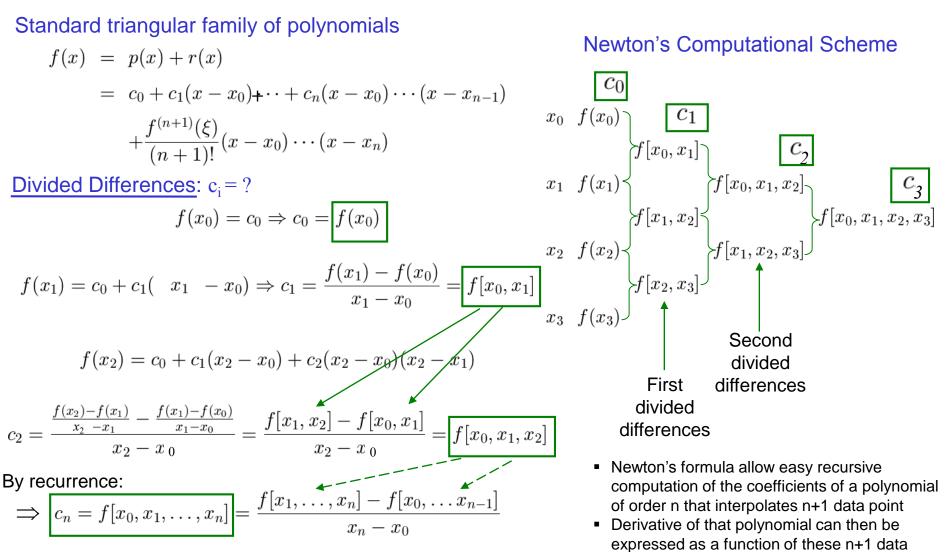
References and Reading Assignments

- Chapter 23 on "Numerical Differentiation" and Chapter 18 on "Interpolation" of "Chapra and Canale, Numerical Methods for Engineers, 2006/2010/2014."
- 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 using Polynomial approximations **Numerical Interpolation:** "Historical" Newton's Iteration Formula

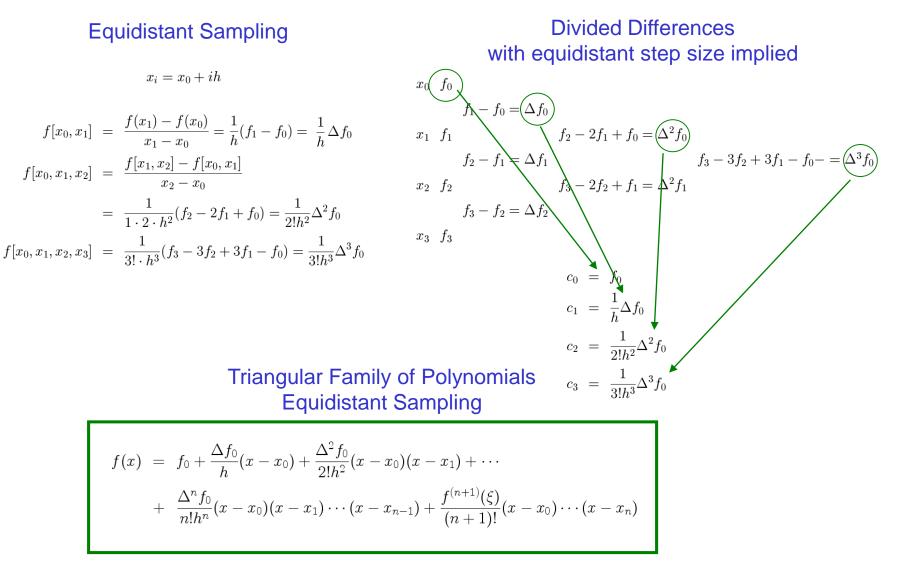
Standard triangular family of polynomials



points (in our case, unknown fct values)

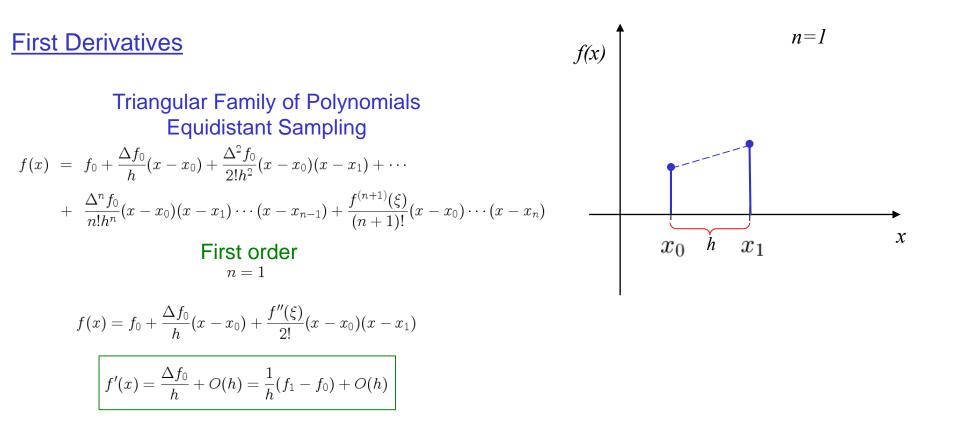


Finite Differences using Polynomial approximations Equidistant Newton's Interpolation





Numerical Differentiation using Newton's algorithm for equidistant sampling: 1st Order





Numerical Differentiation using Newton's algorithm for equidistant sampling: 2nd Order

Second order

n=2

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

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

$$f'(x_0) = \frac{f_1 - f_0}{h} - \frac{1}{2h} (f_2 - 2f_1 + f_0) + O(h^2)$$

$$= \frac{2f_1 - 2f_0 - f_2 + 2f_1 - f_0}{2h} + O(h^2)$$

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

$$= \frac{1}{2h} (f_2 - f_0) + O(h^2)$$
Central Difference
$$x_0 - h - x_1 - h - x_2 - x$$

Second Derivatives

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

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

I Difference

Numerical Fluid Mechanics



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

$$p(x) = \sum_{k=0}^{n} L_{k}(x) f(x_{k}) = \sum_{k=0}^{n} L_{k}(x) f_{k}$$

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

$$L_{k}(x_{i}) = \delta_{ki} = \begin{cases} 0 \quad k \neq i \\ 1 \quad k = i \end{cases}$$

$$L_{k}(x) = \prod_{j=0, j \neq k}^{n} \frac{x - x_{j}}{x_{k} - x_{j}}$$

$$I = \sum_{j=0, j \neq k}^{n} \frac{x - x_{j}}{x_{k} - x_{j}}$$

$$I = \sum_{j=0, j \neq k}^{n} \frac{x - x_{j}}{x_{k} - x_{j}}$$

$$I = \sum_{j=0, j \neq k}^{n} \frac{x - x_{j}}{x_{k} - x_{j}}$$

Important for numerical integration Nodal basis in FE



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
- Derivatives are then also unknowns



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

Table 3.3. Taylor table for central 3-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	$\Delta \mathbf{x} \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)_{\mathbf{j}}$	$\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2} \right)_j$	$\Delta x^3 \left(\frac{\partial^3 u}{\partial x^3} \right)_j$	$\Delta \mathbf{x}^{4} \left(\frac{\partial^{4} \mathbf{u}}{\partial \mathbf{x}^{4}} \right)_{\mathbf{j}}$	$\Delta x^{5} \left(\frac{\partial^{5} u}{\partial x^{5}} \right)_{j}$		
$\Delta x d \left(\frac{\partial u}{\partial x} \right)_{j-1}$	_	d	$d\cdot(-1)\cdot\frac{1}{1}$	$d \cdot (-1)^2 \cdot \frac{1}{2}$	$d \cdot (-1)^3 \cdot \frac{1}{6}$	$d \cdot (-1)^4 \cdot \frac{1}{24}$		
$\Delta \mathbf{x} \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} \right)_{\mathbf{j}}$	_	1	—	—	—	_		
$\Delta x e \left(\frac{\partial u}{\partial x} \right)_{j+1}$	_	е	$e \cdot (1) \cdot \frac{1}{1}$	$e \cdot (1)^2 \cdot \frac{1}{2}$	$e \cdot (1)^3 \cdot \frac{1}{6}$	$e \cdot (1)^4 \cdot \frac{1}{24}$		
-a · 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 ∙ u _j	-b	_	_	_	_	_		
-c • u _{j+1}	-с	$-c \cdot (1) \cdot \frac{1}{1}$	$-c \cdot (1)^2 \cdot \frac{1}{2}$	$-c \cdot (1)^3 \cdot \frac{1}{6}$	$-c \cdot (1)^4 \cdot \frac{1}{24}$	$-c \cdot (1)^5 \cdot \frac{1}{120}$		

Image by MIT OpenCourseWare.



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

Table 3.3. Taylor table for central 3-point Hermitian approximation to a first derivative

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

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

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

Truncation error is sum of the first column that does not vanish in the table, here 6th column (divided by Δx):

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

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THE TECHNOLOGY

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	$\frac{\left(\Delta x\right)^2}{3!} \frac{\partial^3 \phi}{\partial x^3}$	0	1	0
CDS-4	$\frac{13(\Delta x)^4}{3\cdot 3!} \frac{\partial^5 \phi}{\partial x^5}$	0	<u>4</u> 3	$-\frac{1}{3}$
Padé-4	$\frac{(\Delta x)^4}{5!} \frac{\partial^5 \phi}{\partial x^5}$	$\frac{1}{4}$	<u>3</u> 2	0
Padé-6	$4 \frac{(\Delta x)^6}{7!} \frac{\partial^7 \phi}{\partial x^7}$	$\frac{1}{3}$	<u>14</u> 9	$\frac{1}{9}$

Comments:

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

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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 still 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:
$$u(x = x_{bnd}, t) = u_{bnd}(t)$$
 (Dirichlet BCs)
ii) a gradient in a specific direction, e.g.: $\frac{\partial u}{\partial x}\Big|_{(x_{bnd}, t)} = \phi_{bnd}(t)$ (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: $\frac{\partial u}{\partial x}\Big|_{(x_{\text{bnd}},t)} = 0 \implies \frac{u_2 u_1}{x_2 x_1} \approx 0 \implies u_1 = u_2$
 - Parabolic fit to the bnd point and two inner points:

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

• Cubic fit to 4 nodes (3rd order difference): $\frac{\partial u}{\partial x}\Big|_{(x_{\text{bnd}},t)} \approx \frac{2u_4 - 9u_3 + 18u_2 - 11u_1}{6\Delta x} + O(\Delta x^3)$ 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 (embedded) approach and/or generalized inverse problem (using data in the interior)



Finite-Differences on Non-Uniform Grids: 1-D

 Truncation error depends not only on grid spacing but also on the derivatives of the variable

$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + \frac{\Delta x^3}{3!} f'''(x_i) + \dots + \frac{\Delta x^n}{n!} f^n(x_i) + R_n$$
$$R_n = \frac{\Delta x^{n+1}}{n+1!} f^{(n+1)}(\xi)$$

- Uniform error distribution can not be achieved on a uniform grid => non-uniform grids
 - Use smaller (larger) Δx in regions where derivatives of the function are large (small) => uniform discretization error
 - However, in some approximation (centered-differences), specific terms cancel only when the spacing is uniform
- Example: Lets define $\Delta x_{i+1} = x_{i+1} x_i$, $\Delta x_i = x_i x_{i-1}$ and write the Taylor series at x_i :

$$f(x) = f(x_i) + (x - x_i)f'(x_i) + \frac{(x - x_i)^2}{2!}f''(x_i) + \frac{(x - x_i)^3}{3!}f'''(x_i) + \dots + \frac{(x - x_i)^n}{n!}f^n(x_i) + R_n$$

$$R_{n} = \frac{(x - x_{i})^{n+1}}{n+1!} f^{(n+1)}(\xi)$$
 Numerica



Non-Uniform Grids Example: 1-D Central-difference

- Evaluate f(x) at x_{i+1} and x_{i-1} , subtract results, lead to central-difference $f(x_{i+1}) = f(x_i) + \Delta x_{i+1} f'(x_i) + \frac{\Delta x_{i+1}^2}{2!} f''(x_i) + \frac{\Delta x_{i+1}^3}{3!} f'''(x_i) + \dots + \frac{\Delta x_{i+1}^n}{n!} f^n(x_i) + R_n$ $- \frac{f(x_{i-1}) = f(x_i) - \Delta x_i f'(x_i) + \frac{\Delta x_i^2}{2!} f''(x_i) - \frac{\Delta x_i^3}{3!} f'''(x_i) + \dots + \frac{(-\Delta x_i)^n}{n!} f^n(x_i) + R_n}{f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} - \frac{\Delta x_{i+1}^2 - \Delta x_i^2}{2!} f''(x_i) - \frac{\Delta x_{i+1}^3 + \Delta x_i^3}{3!} f'''(x_i) + \dots + R_n}$ $(\Delta x_{i+1} + \Delta x_i = x_{i+1} - x_{i-1})$ $= \text{Truncation error } \tau_{\Delta x}$
- For a non-uniform mesh, the leading truncation term is $O(\Delta x)$
 - -The more non-uniform the mesh, the larger the 1st term in truncation error
 - If the grid contracts/expands with a constant factor r_e :

$$\Delta x_{i+1} = r_e \ \Delta x_i$$

- -Leading truncation error term is : $\tau_{\Delta x}^{r_e} \approx \frac{(1-r_e) \Delta x_i}{2} f''(x_i)$
- If r_e is close to one, the first-order truncation error remains small: this is good for handling any types of unknown function f(x)



Non-Uniform Grids Example: 1-D Central-difference

- What also matters is: "rate of error reduction as grid is refined"!
- Consider case where refinement is done by adding more grid points but keeping a constant ratio of spacing (geometric progression), i.e.

$$\Delta x_{i+1}^{2h} = r_{e,2h} \Delta x_i^{2h}$$

$$\Delta x_{i+1} = r_{e,h} \Delta x_i$$

$$i - 1 \qquad i \qquad i + 1 \qquad i + 2 \qquad \text{Grid } 2h$$

$$i - 2 \qquad i - 1 \qquad i \qquad i + 1 \qquad i + 2 \qquad \text{Grid } h$$

Fig. 3.3. Refinement of a non-uniform grid which expands by a constant factor r_e

- For coarse grid pts to be collocated with fine-grid pts: $(r_{e,h})^2 = r_{e,2h}$
- The ratio of the two truncation errors at a common point is then:

 $R \approx \frac{\frac{(1 - r_{e,2h}) \Delta x_i^{2h}}{2} f''(x_i)}{\frac{(1 - r_{e,h}) \Delta x_i^{h}}{2} f''(x_i)} \quad \text{which is } \boxed{R \approx \frac{(1 + r_{e,h})^2}{r_{e,h}}} \text{ since } \Delta x_i^{2h} = \Delta x_i + \Delta x_{i-1} = (r_{e,h} + 1) \Delta x_{i-1}$

- The factor R = 4 if $r_e = 1$ (uniform grid). R is actually minimum at $r_e = 1$.

– When $r_e > 1$ (expending grid) or $r_e < 1$ (contracting grid), the factor R > 4



Non-Uniform Grids Example: 1-D Central-difference Conclusions

- When a non-uniform "geometric progression" grid is refined, error due to the 1st order term decreases faster than that of 2nd order term !
- Since $(r_{e,h})^2 = r_{e,2h}$, we have $r_{e,h} \rightarrow 1$ as the grid is refined. Hence, convergence becomes asymptotically 2nd order (1st order term cancels)
- Non-uniform grids are thus useful, if one can reduce Δx in regions where derivatives of the unknown solution are large
 - Automated means of adapting the grid to the solution (as it evolves)
 - However, automated grid adaptation schemes are more challenging in higher dimensions and for multivariate (e.g. physics-biology-acoustics) or multiscale problems
- (Adaptive) Grid generation still an area of active research in CFD
- Conclusions also valid for higher dimensions and for other methods (finite elements, etc)

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