### 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: $\mathcal{L}(\phi)=0, \quad \hat{\mathcal{L}}_{\Delta x}(\hat{\phi})=0$
- Consistency:

$$
\begin{aligned}
& \left|\mathcal{L}(\phi)-\hat{\mathcal{L}}_{\Delta x}(\phi)\right| \rightarrow 0 \text { when } \Delta x \rightarrow 0 \\
& \tau_{\Delta x}=\mathcal{L}(\phi)-\hat{\mathcal{L}}_{\Delta x}(\phi) \rightarrow O\left(\Delta x^{p}\right) \text { for } \Delta x \rightarrow 0
\end{aligned}
$$

- Truncation error:
- Error equation:
$\tau_{\Delta x}=\mathcal{L}(\phi)-\hat{\mathcal{L}}_{\Delta x}(\hat{\phi}+\varepsilon)=-\hat{\mathcal{L}}_{\Delta x}(\varepsilon)$ (for linear systems)
- Stability:
$\left\|\hat{\mathcal{L}}_{\Delta x}^{-1}\right\|<$ Const. (for linear systems)
- Convergence:
$\|\varepsilon\| \leq\left\|\hat{\mathcal{L}}_{\Delta x}^{-1}\right\|\left\|\tau_{\Delta x}\right\| \leq \alpha O\left(\Delta x^{p}\right)$


### 2.29 Numerical Fluid Mechanics Spring 2015 - Lecture 11

## 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 $a_{\mathrm{i}}$


## 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, $3^{\text {rd }}$ 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

$$
\begin{aligned}
f(x)= & p(x)+r(x) \\
= & c_{0}+c_{1}\left(x-x_{0}\right)+\cdots+c_{n}\left(x-x_{0}\right) \cdots\left(x-x_{n-1}\right) \\
& +\frac{f^{(n+1)}(\xi)}{(n+1)!}\left(x-x_{0}\right) \cdots\left(x-x_{n}\right)
\end{aligned}
$$

$$
\begin{aligned}
& \text { Divided Differences: } \mathrm{c}_{\mathrm{i}}=\text { ? } \\
& f\left(x_{0}\right)=c_{0} \Rightarrow c_{0}=f\left(x_{0}\right) \\
& f\left(x_{1}\right)=c_{0}+c_{1}\left(x_{1}-x_{0}\right) \Rightarrow c_{1}=\frac{f\left(x_{1}\right)-f\left(x_{0}\right)}{x_{1}-x_{0}}=f\left[x_{0}, x_{1}\right] \\
& f\left(x_{2}\right)=c_{0}+c_{1}\left(x_{2}-x_{0}\right)+c_{2}\left(x_{2}-x_{0}\right) \\
& c_{2}=\frac{\frac{f\left(x_{2}\right)-f\left(x_{1}\right)}{x_{2}-x_{1}}-\frac{f\left(x_{1}\right)-f\left(x_{0}\right)}{x_{1}-x_{0}}}{x_{2}-x_{0}}=\frac{f\left[x_{1}, x_{2}\right]-f\left[x_{0}, x_{1}\right]}{x_{2}-x_{0}}=f\left[x_{0}, x_{1}, x_{2}\right] \\
& \text { By recurrence: } \\
& \Rightarrow c_{n}=f\left[x_{0}, x_{1}, \ldots, x_{n}\right] \\
& \Rightarrow \frac{f\left[x_{1}, \ldots, x_{n}\right]-f\left[x_{0}, \ldots x_{n-1}\right]}{x_{n}-x_{0}}
\end{aligned}
$$

- Newton's formula allow easy recursive computation of the coefficients of a polynomial of order $n$ that interpolates $n+1$ data point
- Derivative of that polynomial can then be expressed as a function of these $n+1$ data points (in our case, unknown fct values)

> First differences divided differences

## Finite Differences using Polynomial approximations Equidistant Newton's Interpolation

Equidistant Sampling

$$
x_{i}=x_{0}+i h
$$

$$
\begin{aligned}
f\left[x_{0}, x_{1}\right] & =\frac{f\left(x_{1}\right)-f\left(x_{0}\right)}{x_{1}-x_{0}}=\frac{1}{h}\left(f_{1}-f_{0}\right)=\frac{1}{h} \Delta f_{0} \\
f\left[x_{0}, x_{1}, x_{2}\right] & =\frac{f\left[x_{1}, x_{2}\right]-f\left[x_{0}, x_{1}\right]}{x_{2}-x_{0}} \\
& =\frac{1}{1 \cdot 2 \cdot h^{2}}\left(f_{2}-2 f_{1}+f_{0}\right)=\frac{1}{2!h^{2}} \Delta^{2} f_{0} \\
f\left[x_{0}, x_{1}, x_{2}, x_{3}\right] & =\frac{1}{3!\cdot h^{3}}\left(f_{3}-3 f_{2}+3 f_{1}-f_{0}\right)=\frac{1}{3!h^{3}} \Delta^{3} f_{0}
\end{aligned}
$$

Divided Differences with equidistant step size implied

Triangular Family of Polynomials

## Equidistant Sampling

$$
c_{3}=\frac{1}{3!h^{3}} \Delta^{3} f_{0}
$$

$$
\begin{aligned}
f(x) & =f_{0}+\frac{\Delta f_{0}}{h}\left(x-x_{0}\right)+\frac{\Delta^{2} f_{0}}{2!h^{2}}\left(x-x_{0}\right)\left(x-x_{1}\right)+\cdots \\
& +\frac{\Delta^{n} f_{0}}{n!h^{n}}\left(x-x_{0}\right)\left(x-x_{1}\right) \cdots\left(x-x_{n-1}\right)+\frac{f^{(n+1)}(\xi)}{(n+1)!}\left(x-x_{0}\right) \cdots\left(x-x_{n}\right)
\end{aligned}
$$

## Numerical Differentiation using Newton's algorithm for equidistant sampling: $1^{\text {st }}$ Order

First Derivatives



$$
\begin{gathered}
f(x)=f_{0}+\frac{\Delta f_{0}}{h}\left(x-x_{0}\right)+\frac{f^{\prime \prime}(\xi)}{2!}\left(x-x_{0}\right)\left(x-x_{1}\right) \\
f^{\prime}(x)=\frac{\Delta f_{0}}{h}+O(h)=\frac{1}{h}\left(f_{1}-f_{0}\right)+O(h)
\end{gathered}
$$

## Numerical Differentiation using Newton's algorithm for equidistant sampling: $2^{\text {nd }}$ Order

## Second order

$$
n=2
$$

$$
\begin{gathered}
f(x)=f_{0}+\frac{\Delta f_{0}}{h}\left(x-x_{0}\right)+\frac{\Delta^{2} f_{0}}{2!h^{2}}\left(x-x_{0}\right)\left(x-x_{1}\right)+\frac{f^{\prime \prime \prime}(\xi)}{3!}\left(x-x_{0}\right)\left(x-x_{1}\right)\left(x-x_{2}\right)+\cdots \\
f^{\prime}(x)=\frac{\Delta f_{0}}{h}+\frac{\Delta^{2} f_{0}}{2 h^{2}}\left(x-x_{0}\right)+\frac{\Delta^{2} f_{0}}{2 h^{2}}\left(x-x_{1}\right)+O\left(h^{2}\right)
\end{gathered}
$$

$$
f^{\prime}\left(x_{0}\right)=\frac{f_{1}-f_{0}}{h}-\frac{1}{2 h}\left(f_{2}-2 f_{1}+f_{0}\right)+O\left(h^{2}\right)
$$

$$
=\frac{2 f_{1}-2 f_{0}-f_{2}+2 f_{1}-f_{0}}{2 h}+O\left(h^{2}\right)
$$

$$
=\frac{1}{h}\left(-\frac{3}{2} f_{0}+2 f_{1}-\frac{1}{2} f_{2}\right)+O\left(h^{2}\right) \quad \text { Forward Difference }
$$

$$
f^{\prime}\left(x_{1}\right)=\frac{f_{1}-f_{0}}{h}+\frac{1}{2 h}\left(f_{2}-2 f_{1}+f_{0}\right)+O\left(h^{2}\right)
$$

$$
=\frac{1}{2 h}\left(f_{2}-f_{0}\right)+O\left(h^{2}\right)
$$

Central Difference


Second Derivatives

$$
\begin{array}{ll}
n=2 & f^{\prime \prime}\left(x_{0}\right)=\frac{\Delta^{2} f_{0}}{h^{2}}+O(h)=\frac{1}{h^{2}}\left(f_{0}-2 f_{1}+f_{2}\right)+O(h) \\
n=3 & f^{\prime \prime}\left(x_{1}\right)=\frac{1}{h^{2}}\left(f_{0}-2 f_{1}+f_{2}\right)+O\left(h^{2}\right)
\end{array}
$$

Forward Difference
Central Difference

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

$$
\begin{gathered}
p(x)=\sum_{k=0}^{n} L_{k}(x) f\left(x_{k}\right)=\sum_{k=0}^{n} L_{k}(x) f_{k} \\
L_{k}(x)=\sum_{i=0}^{n} \ell_{i k} x^{i} \\
L_{k}\left(x_{i}\right)=\delta_{k i}= \begin{cases}0 & k \neq i \\
1 & k=i\end{cases} \\
L_{k}(x)=\prod_{j=0, j \neq k}^{n} \frac{x-x_{j}}{x_{k}-x_{j}}
\end{gathered}
$$


Difficult to program
Difficult to estimate errors
Divisions are expensive

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

$$
\mathrm{d}\left(\frac{\partial \mathrm{u}}{\partial \mathrm{x}}\right)_{\mathrm{j}-1}+\left(\frac{\partial \mathrm{u}}{\partial \mathrm{x}}\right)_{\mathrm{j}}+\mathrm{e}\left(\frac{\partial \mathrm{u}}{\partial \mathrm{x}}\right)_{\mathrm{j}+1}-\frac{1}{\Delta \mathrm{x}}\left(\mathrm{au}_{\mathrm{j}-1}+\mathrm{bu}_{\mathrm{j}}+\mathrm{cu}_{\mathrm{j}+1}\right)=?
$$

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

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

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

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:

$$
\left[\begin{array}{ccccc}
-1 & -1 & -1 & 0 & 0 \\
1 & 0 & -1 & 1 & 1 \\
-1 & 0 & -1 & -2 & 2 \\
1 & 0 & -1 & 3 & 3 \\
-1 & 0 & -1 & -4 & 4
\end{array}\right]\left[\begin{array}{c}
a \\
b \\
c \\
d \\
e
\end{array}\right]=\left[\begin{array}{c}
0 \\
-1 \\
0 \\
0 \\
0
\end{array}\right] \Rightarrow\left[\begin{array}{lllll}
a & b & c & d & e
\end{array}\right]=\frac{1}{4}\left[\begin{array}{lllll}
-3 & 0 & 3 & 1 & 1
\end{array}\right]
$$

Truncation error is sum of the first column that does not vanish in the table, here $6^{\text {th }}$ column (divided by $\Delta x$ ):

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

## Compact / Pade' Difference Schemes: Examples

We can derive family of compact centered approximations for $\phi$ up to $6^{\text {th }}$ order using:

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

| Scheme | Truncation error | $\alpha$ | $\beta$ | $\gamma$ |
| :---: | :---: | :---: | :---: | :---: |
| 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 | $\frac{4(\Delta x)^{6}}{7!} \frac{\partial^{7} \phi}{\partial x^{7}}$ | $\frac{1}{3}$ | $\frac{14}{9}$ | $\frac{1}{9}$ |

Comments:

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

Image by MIT OpenCourseWare.

## Higher-Order Finite Difference Schemes <br> 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: $u\left(x=x_{\text {bnd }}, t\right)=u_{\text {bnd }}(t)$
(Dirichlet BCs)
ii) a gradient in a specific direction, e.g.: $\left.\frac{\partial u}{\partial x}\right|_{\left(x_{\text {bnd }}, t\right)}=\phi_{\text {bnd }}(\mathrm{t}) \quad$ (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,
- $1^{\text {st }}$ order forward-difference: $\left.\quad \frac{\partial u}{\partial x}\right|_{\left(x_{\text {ond }}, t\right)}=0 \Rightarrow \frac{u_{2}-u_{1}}{x_{2}-x_{1}} \approx 0 \Rightarrow u_{1}=u_{2}$
- Parabolic fit to the bnd point and two inner points:
$\left.\frac{\partial u}{\partial x}\right|_{\left(x_{\text {mad }}, t\right)} \approx \frac{-u_{3}\left(x_{2}-x_{1}\right)^{2}+u_{2}\left(x_{3}-x_{1}\right)^{2}-u_{1}\left[\left(x_{3}-x_{1}\right)^{2}-\left(x_{2}-x_{1}\right)^{2}\right]}{\left(x_{2}-x_{1}\right)\left(x_{3}-x_{1}\right)\left(x_{3}-x_{2}\right)} \quad\left(\approx \frac{-u_{3}+4 u_{2}-3 u_{1}}{2 \Delta x}\right.$ for equidistant nodes $)$
- Cubic fit to 4 nodes ( $3^{\text {rd }}$ order difference): $\left.\frac{\partial u}{\partial x}\right|_{\left(x_{\text {bnd }, t)}\right.} \approx \frac{2 u_{4}-9 u_{3}+18 u_{2}-11 u_{1}}{6 \Delta x}+O\left(\Delta x^{3}\right)$ for equidistant nodes
- Compact schemes, cubic fit to 4 pts: $\quad u_{\left(x_{\text {nnd }}, t\right)}=u_{1} \approx \frac{18 u_{2}-9 u_{3}+2 u_{4}}{11}-\frac{6 \Delta x}{11}\left(\frac{\partial u}{\partial x}\right)_{1}$ 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

$$
\begin{aligned}
& f\left(x_{i+1}\right)=f\left(x_{i}\right)+\Delta x f^{\prime}\left(x_{i}\right)+\frac{\Delta x^{2}}{2!} f^{\prime \prime}\left(x_{i}\right)+\frac{\Delta x^{3}}{3!} f^{\prime \prime \prime}\left(x_{i}\right)+\ldots+\frac{\Delta x^{n}}{n!} f^{n}\left(x_{i}\right)+R_{n} \\
& R_{n}=\frac{\Delta x^{n+1}}{n+1!} f^{(n+1)}(\xi)
\end{aligned}
$$

- Uniform error distribution can not be achieved on a uniform grid => non-uniform grids
- Use smaller (larger) $\Delta x$ 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 $\underline{\Delta x_{i+1}=x_{i+1}-x_{i}, \Delta x_{i}=x_{i}-x_{i-1}}$ and write the Taylor series at $x_{i}$ :

$$
\begin{aligned}
& f(x)=f\left(x_{i}\right)+\left(x-x_{i}\right) f^{\prime}\left(x_{i}\right)+\frac{\left(x-x_{i}\right)^{2}}{2!} f^{\prime \prime}\left(x_{i}\right)+\frac{\left(x-x_{i}\right)^{3}}{3!} f^{\prime \prime \prime}\left(x_{i}\right)+\ldots+\frac{\left(x-x_{i}\right)^{n}}{n!} f^{n}\left(x_{i}\right)+R_{n} \\
& R_{n}=\frac{\left(x-x_{i}\right)^{n+1}}{n+1!} f^{(n+1)}(\xi) \quad \quad \text { PFJL Lecture 11, } 17
\end{aligned}
$$

## 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

$$
\begin{array}{r}
f\left(x_{i+1}\right)=f\left(x_{i}\right)+\Delta x_{i+1} f^{\prime}\left(x_{i}\right)+\frac{\Delta x_{i+1}^{2}}{2!} f^{\prime \prime}\left(x_{i}\right)+\frac{\Delta x_{i+1}^{3}}{3!} f^{\prime \prime \prime}\left(x_{i}\right)+\ldots+\frac{\Delta x_{i+1}^{n}}{n!} f^{n}\left(x_{i}\right)+R_{n} \\
-\frac{f\left(x_{i-1}\right)=f\left(x_{i}\right)-\Delta x_{i} f^{\prime}\left(x_{i}\right)+\frac{\Delta x_{i}^{2}}{2!} f^{\prime \prime}\left(x_{i}\right)-\frac{\Delta x_{i}^{3}}{3!} f^{\prime \prime \prime}\left(x_{i}\right)+\ldots+\frac{\left(-\Delta x_{i}\right)^{n}}{n!} f^{n}\left(x_{i}\right)+R_{n}}{f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i-1}\right)}{x_{i+1}-x_{i-1}}-\underbrace{\frac{\Delta x_{i+1}^{2}-\Delta x_{i}^{2}}{2!\left(x_{i+1}-x_{i-1}\right)} f^{\prime \prime}\left(x_{i}\right)-\frac{\Delta x_{i+1}^{3}+\Delta x_{i}^{3}}{3!\left(x_{i+1}-x_{i-1}\right)} f^{\prime \prime \prime}\left(x_{i}\right)+\ldots+R_{n}}_{=\text {Truncation error } \tau_{\Delta x}}} \\
\left(\Delta x_{i+1}+\Delta x_{i}=x_{i+1}-x_{i-1}\right) \quad
\end{array}
$$

- For a non-uniform mesh, the leading truncation term is $O(\Delta x)$
- The more non-uniform the mesh, the larger the $1^{\text {st }}$ 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 : $\tau_{\Delta x}^{r_{e}} \approx \frac{\left(1-r_{e}\right) \Delta x_{i}}{2} f^{\prime \prime}\left(x_{i}\right)$
- 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.


Fig. 3.3. Refinement of a non-uniform grid which expands by a constant factor $r_{\mathrm{e}}$

- For coarse grid pts to be collocated with fine-grid pts: $\underline{\left(r_{e, h}\right)^{2}=r_{e, 2 h}}$
- The ratio of the two truncation errors at a common point is then:
$R \approx \frac{\frac{\left(1-r_{e, 2 h}\right) \Delta x_{i}^{2 h}}{2} f^{\prime \prime}\left(x_{i}\right)}{\frac{\left(1-r_{e, h}\right) \Delta x_{i}^{h}}{2} f^{\prime \prime}\left(x_{i}\right)}$ which is $R$

$$
R \approx \frac{\left(1+r_{e, h}\right)^{2}}{r_{e, h}} \text { since } \frac{\Delta x_{i}^{2 h}=\Delta x_{i}+\Delta x_{i-1}=\left(r_{e, h}+1\right) \Delta x_{i-1}}{}
$$

-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 $1^{\text {st }}$ order term decreases faster than that of $2^{\text {nd }}$ order term!
- Since $\left(r_{e, h}\right)^{2}=r_{e, 2 h}$, we have $r_{e, h} \rightarrow 1$ as the grid is refined. Hence, convergence becomes asymptotically $2^{\text {nd }}$ order ( $1^{\text {st }}$ order term cancels)
- Non-uniform grids are thus useful, if one can reduce $\Delta x$ 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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### 2.29 Numerical Fluid Mechanics

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