MAE 6220

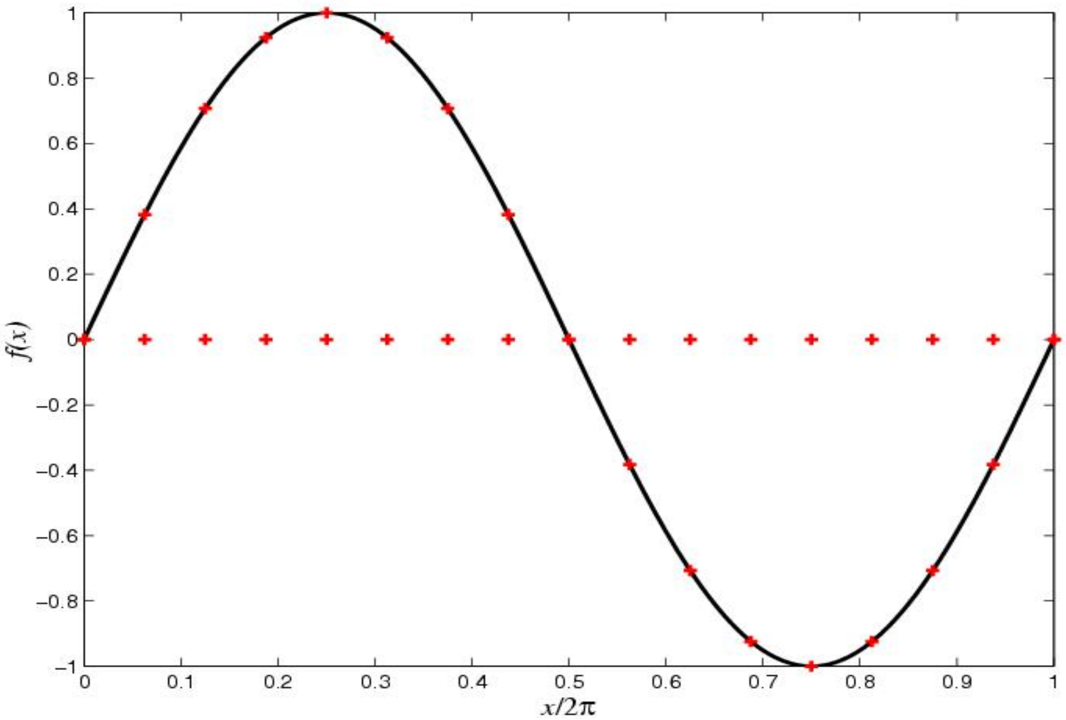
Applied Computational Fluid Dynamics

ELIAS BALARAS

Lecture 2

Accuracy of finite-difference schemes

- Consider a function only known at a set of uniformly distributed discrete points



Accuracy of finite-difference scheme

- Finite differences are obtained by removing the limit from the definition of a derivative:

$$\begin{aligned}
\frac{df_i}{dx} &= \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \\
&\simeq \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \\
&= \frac{f(x_{i+1}) - f(x_i)}{\Delta x} \\
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\end{aligned}$$

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Forward Finite-Difference Approximation

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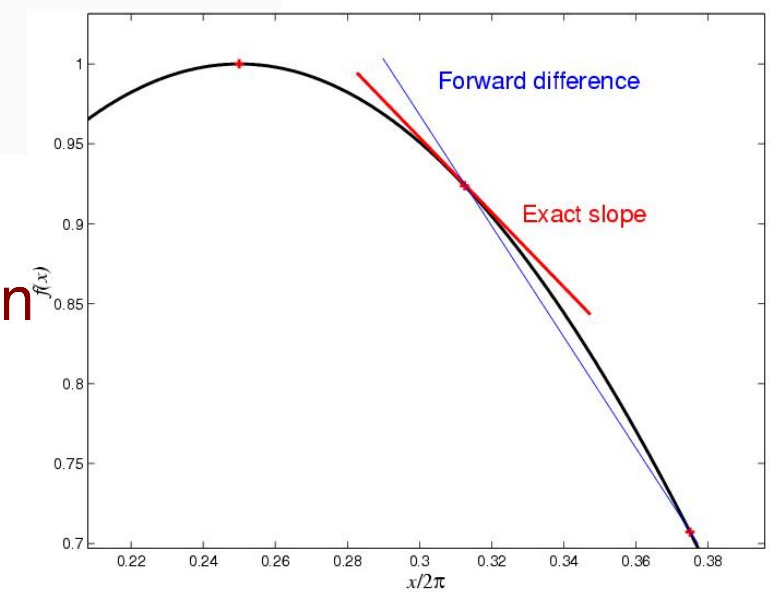
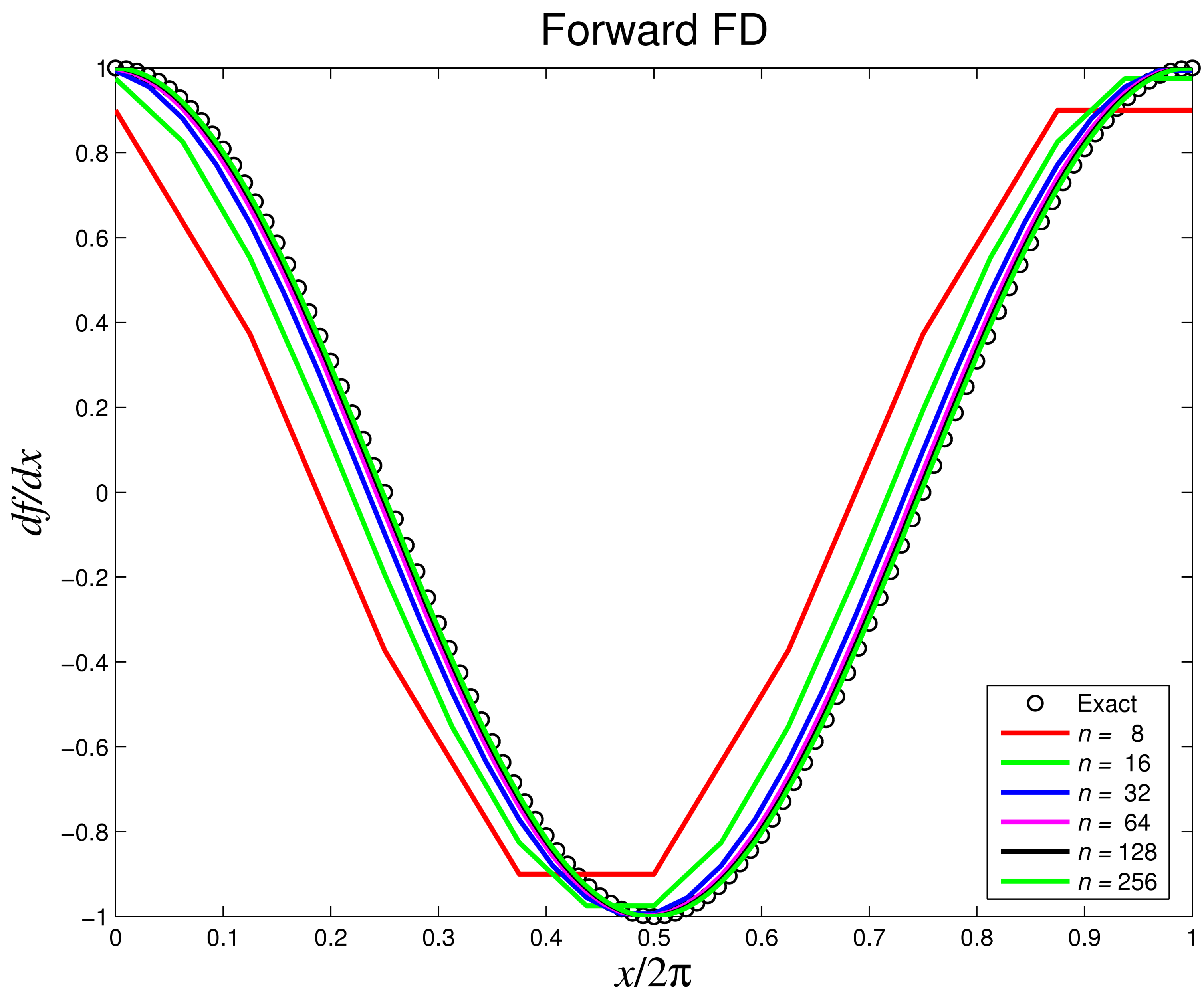
Forward Finite-Difference Approximation



Accuracy of finite-difference scheme



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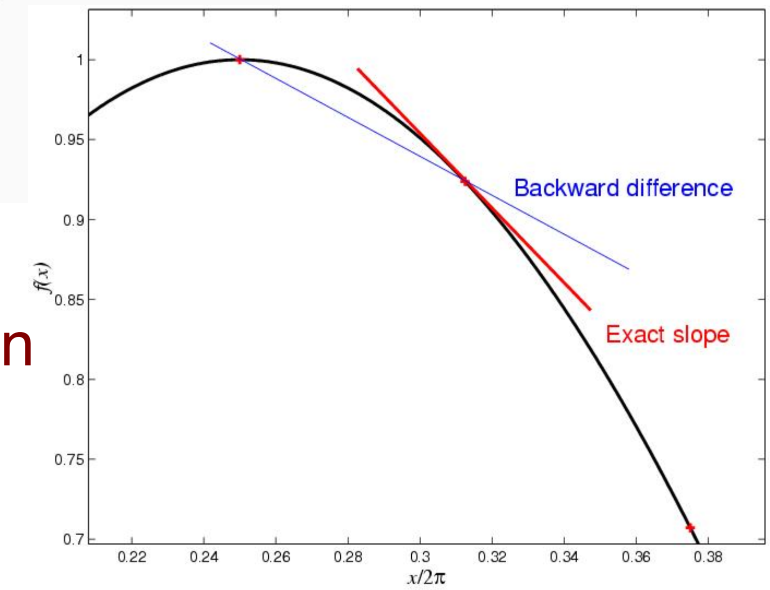
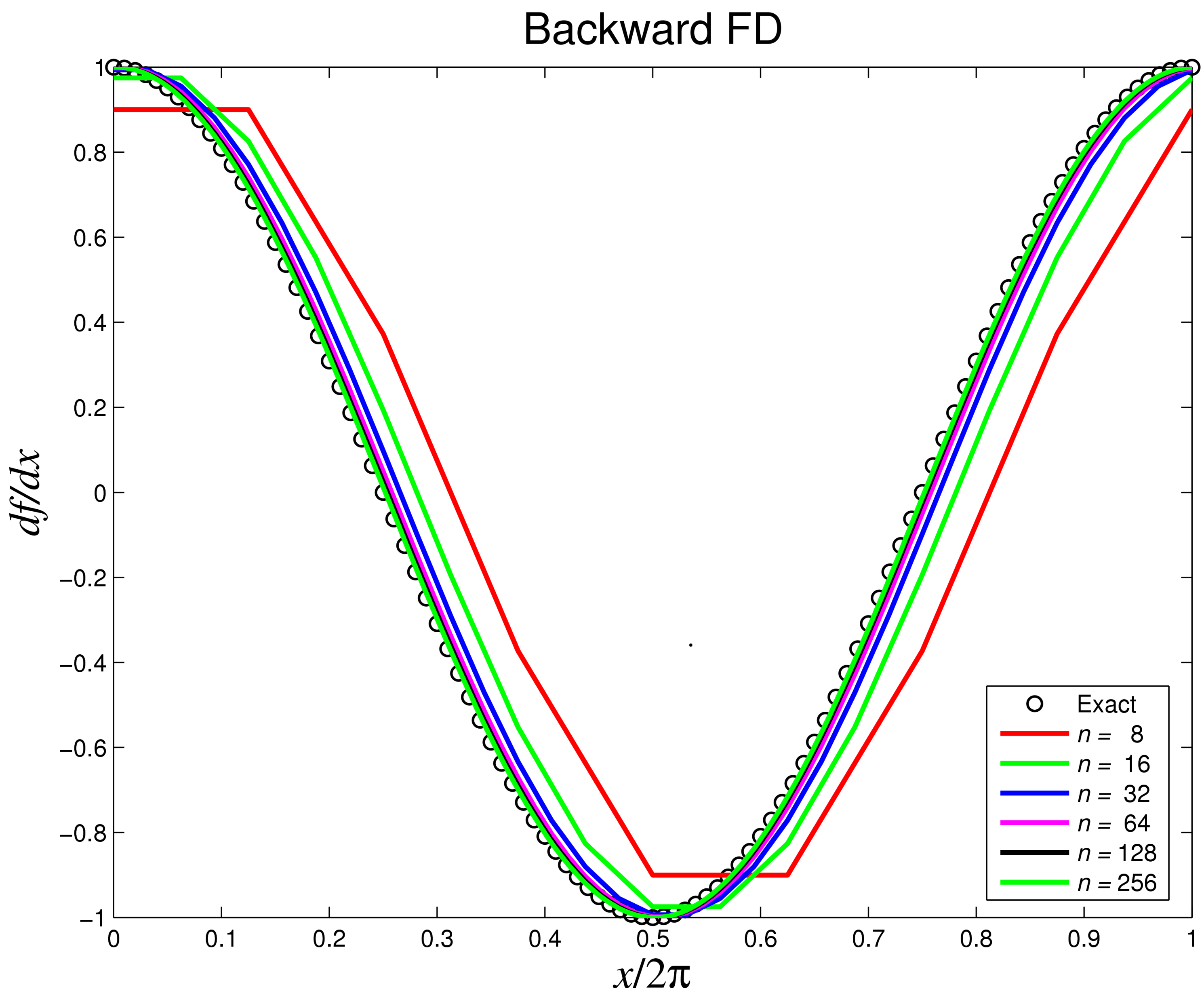
&= \frac{f(x_i) - f(x_{i-1})}{\Delta x} \\
&= \frac{f_i - f_{i-1}}{\Delta x}
\end{aligned}
$$

Backward Finite-difference Approximation



Accuracy of finite-difference scheme



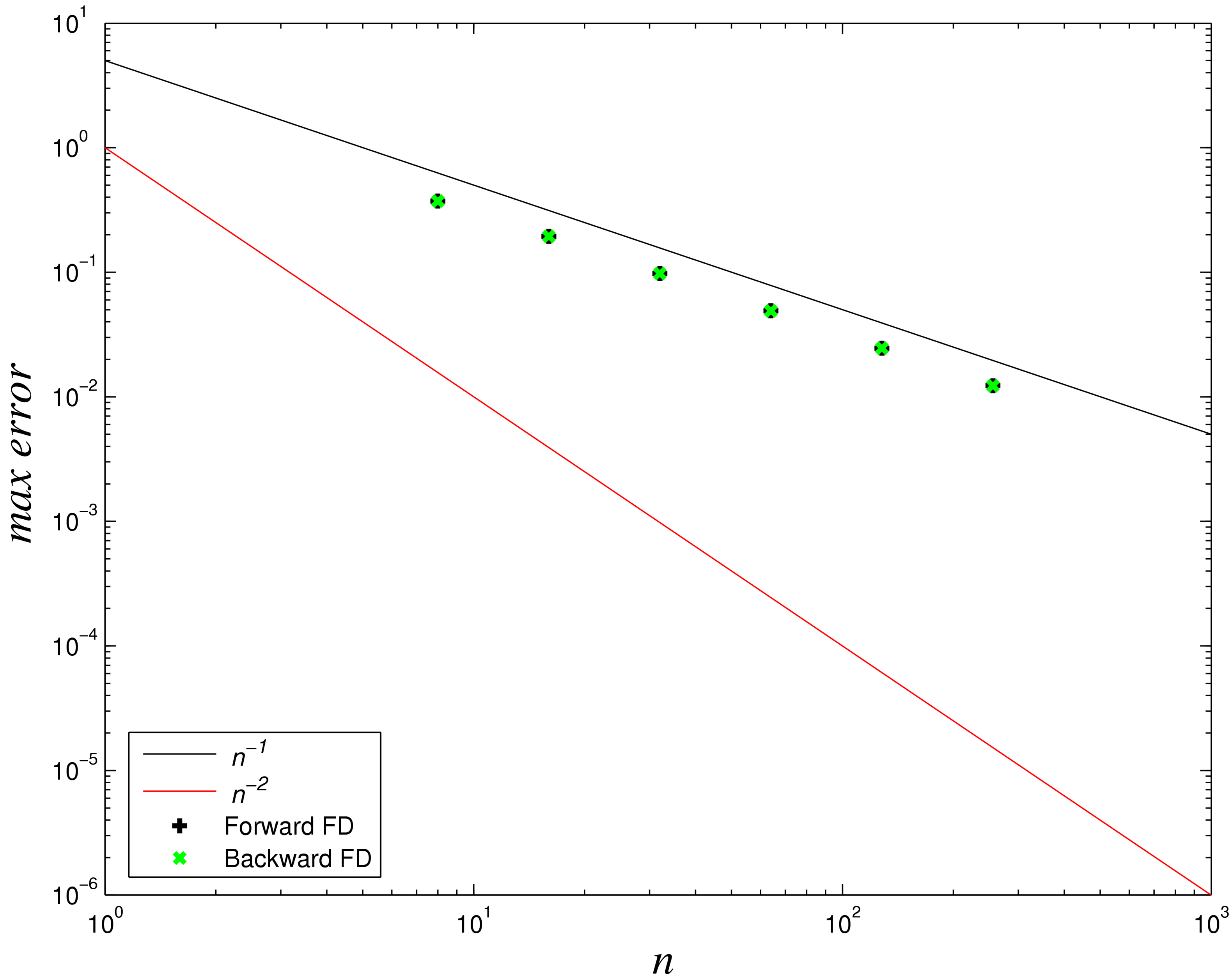
Accuracy of finite-difference scheme

- Define an error norm:

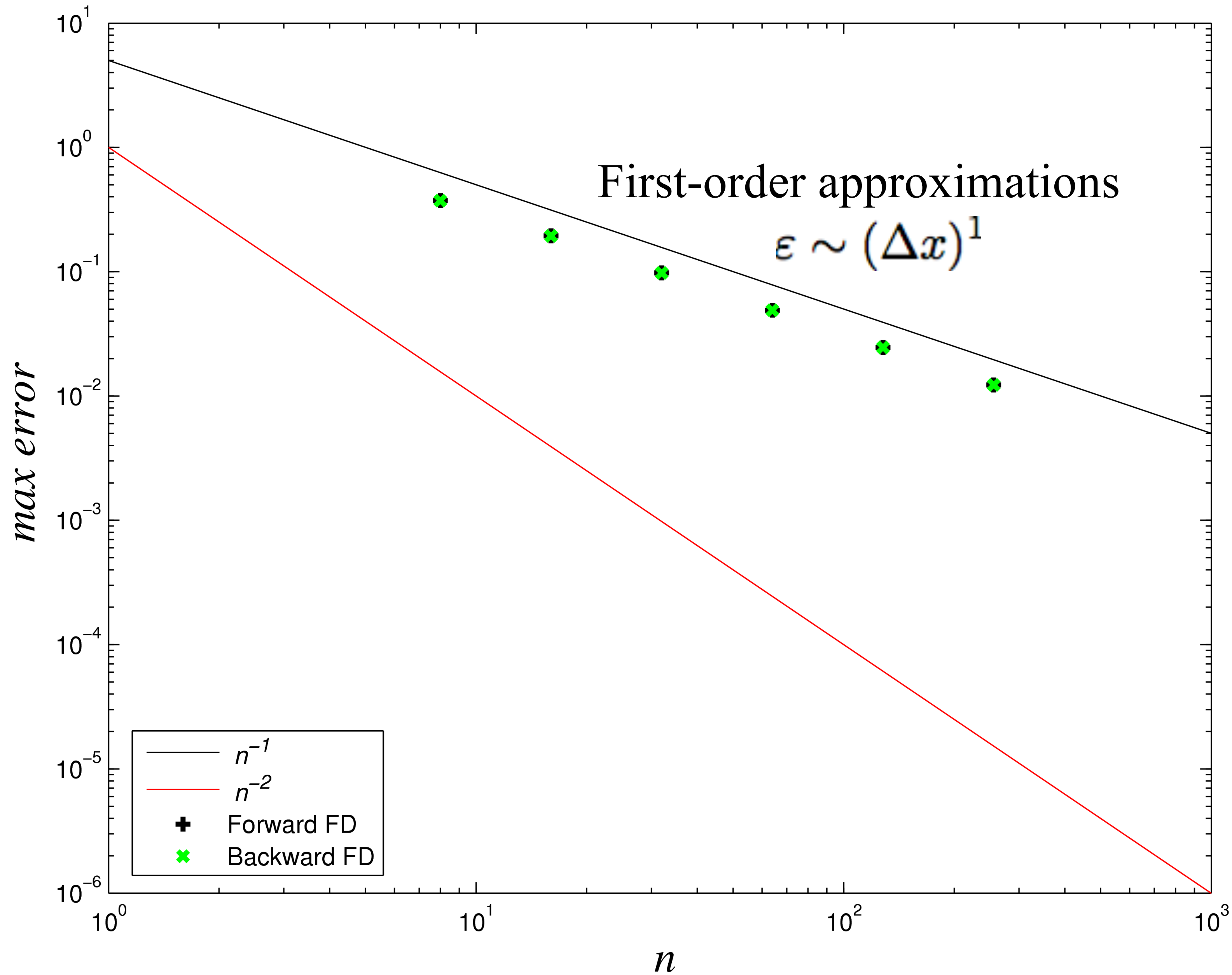
$$\varepsilon = \max\left(\left|\frac{df}{dx} - \frac{\delta f}{\delta x}\right|\right)$$

- Evaluate as the grid is refined (number of points is increased).

Accuracy of finite-difference scheme



Accuracy of finite-difference scheme

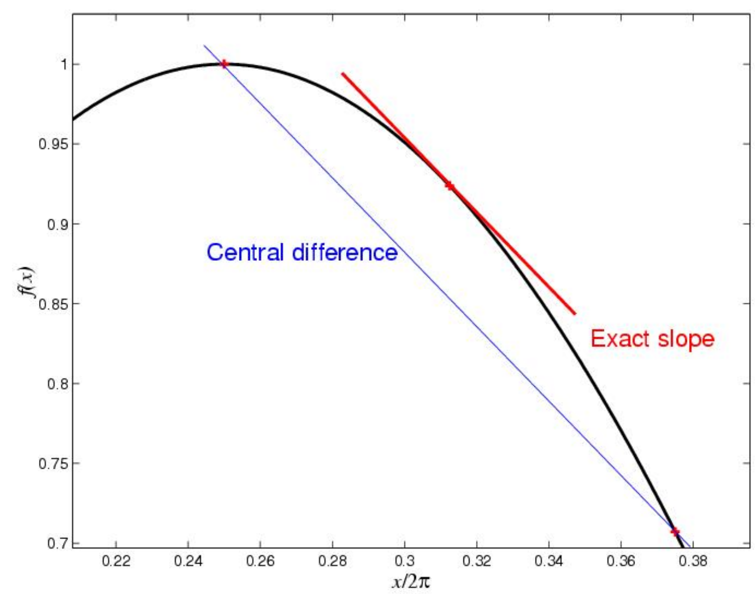


Accuracy of finite-difference scheme

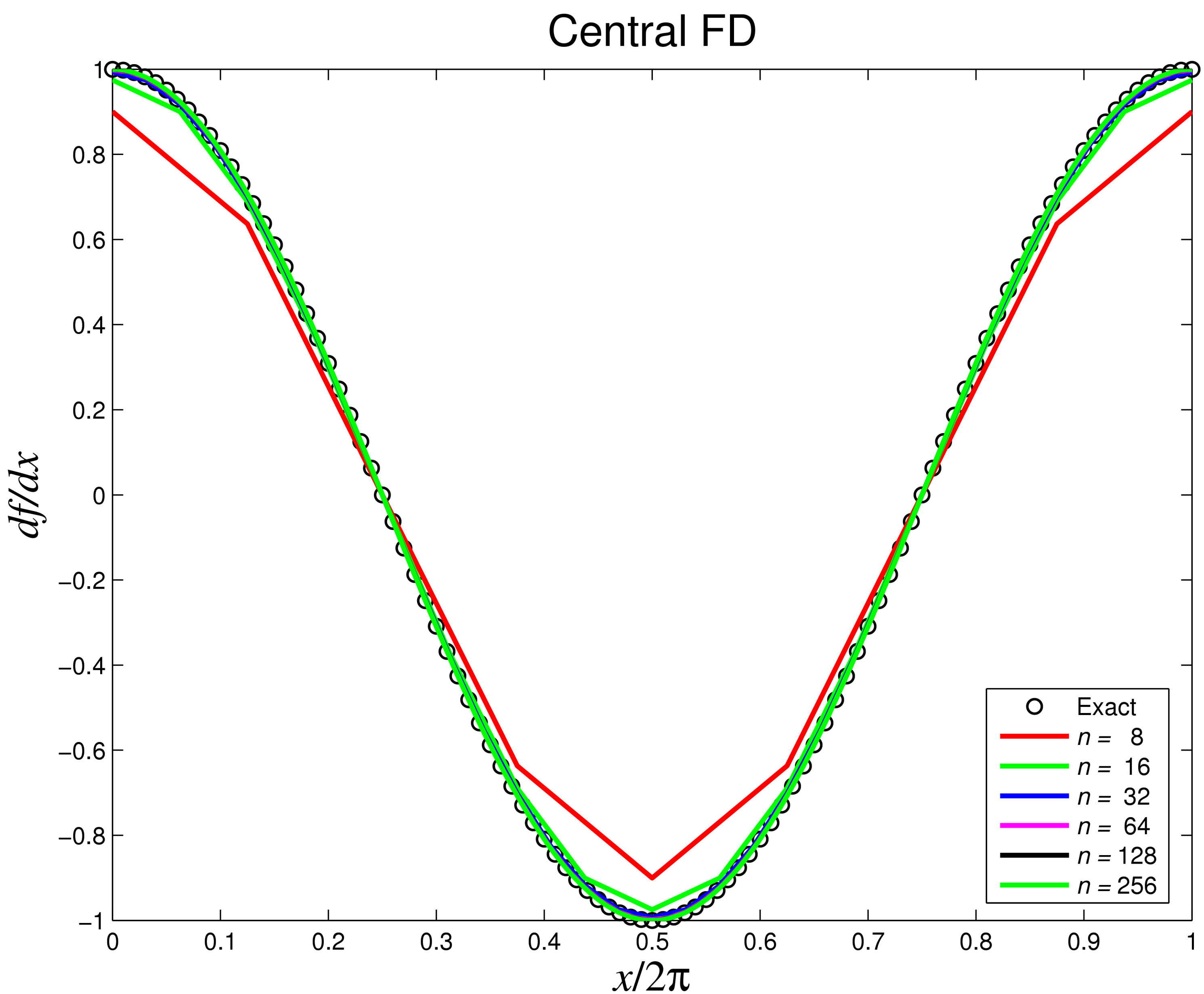
- Taking the average of the two:

$$\begin{aligned}\frac{df_i}{dx} &\simeq \frac{1}{2}\left(\frac{f_{i+1}-f_i}{\Delta x}+\frac{f_i-f_{i-1}}{\Delta x}\right)\\ &= \frac{f_{i+1}-f_{i-1}}{2\Delta x}\end{aligned}$$

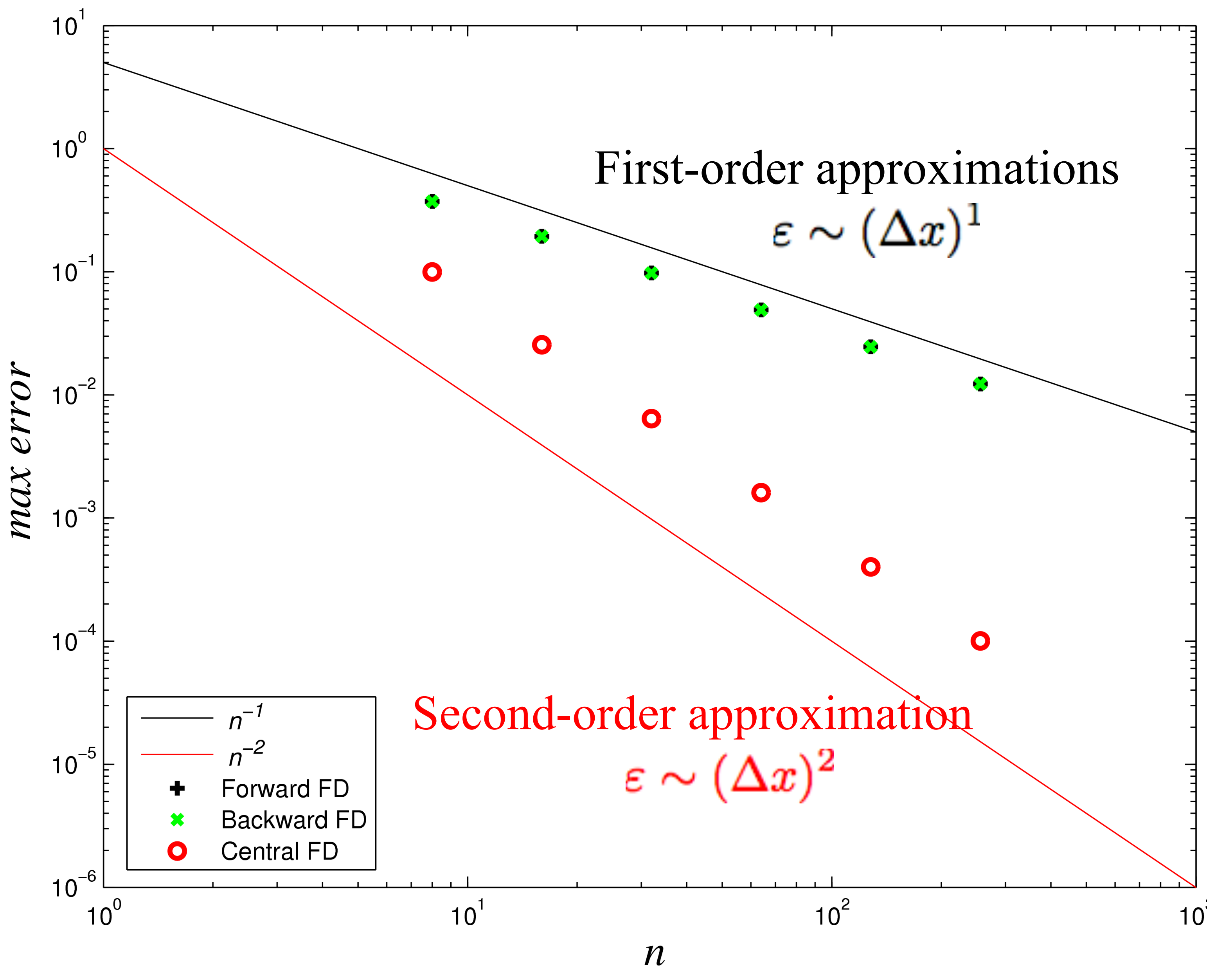
Central Finite-Difference Approximation



Accuracy of finite-difference scheme

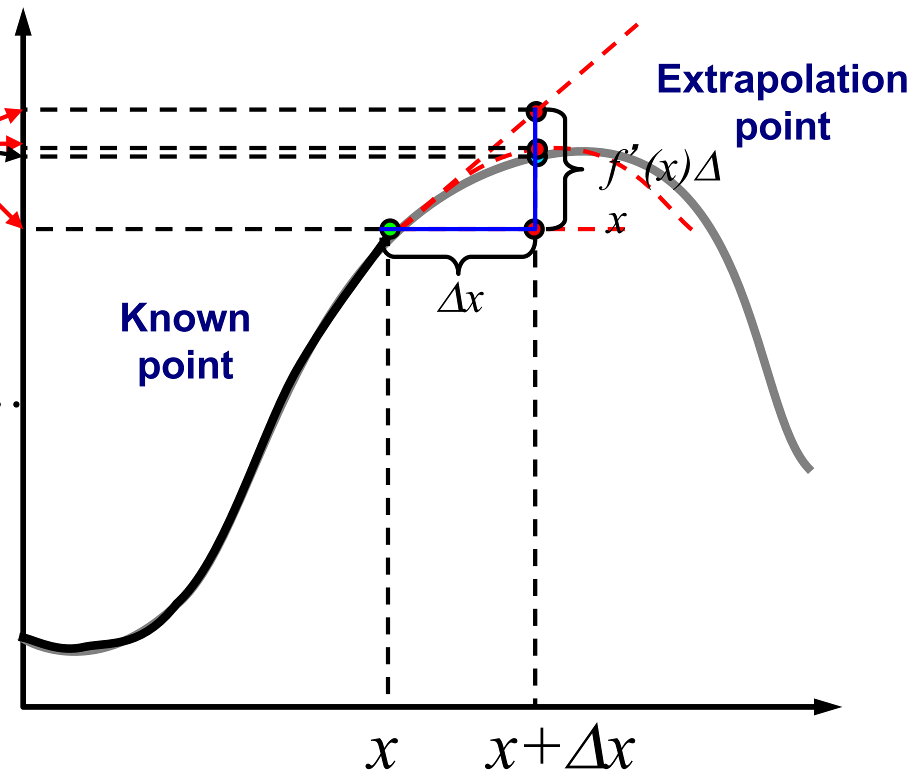


Accuracy of finite-difference scheme



Taylor series - review

- Taylor series:
  - *Method to extrapolate function value at positions where f is unknown, using known values of f and its derivatives*
  - *How?*
    - Start simple and improve:



$$f(x+\Delta x) \cong f(x) + \left.\frac{df}{dx}\right|_x \Delta x + \left.\frac{d^2 f}{dx^2}\right|_x \frac{\Delta x^2}{2} + \cdots$$

Accuracy of finite-difference schemes

- Given any finite-difference approximation of a derivative, its order of accuracy can be calculated by using Taylor series.

$$
\begin{aligned}
\phi_{j+1} &= \phi_j + \phi_j' h + \frac{h^2}{2!}\phi_j'' + \frac{h^3}{3!}\phi_j''' + o(h^4) \\
\phi_{j-1} &= \phi_j - \phi_j' h + \frac{h^2}{2!}\phi_j'' - \frac{h^3}{3!}\phi_j''' + o(h^4)
\end{aligned}
$$

$$
\frac{\delta_c \phi}{\delta x} = \frac{\phi_{j+1} - \phi_{j-1}}{2h} = \phi_j' + \frac{h^2}{3!}\phi_j'''
$$

Accuracy of finite-difference schemes

- One can use Taylor series to construct a finite-difference scheme of any order of accuracy.
- Example: three-point forward ($j+2$, $j+1$ and j) 2nd-order approximation to $\delta\phi/\delta x$:

$$
\begin{aligned}
\phi_{j+2} &= \phi_j + \phi_j' 2h + \frac{4h^2}{2!}\phi_j'' + \frac{8h^3}{3!}\phi_j''' + o(h^4) \\
\phi_{j+1} &= \phi_j + \phi_j' h + \frac{h^2}{2!}\phi_j'' + \frac{h^3}{3!}\phi_j''' + o(h^4) \\
\phi_j &= \phi_j
\end{aligned}
$$

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\phi_j &= \phi_j \\
\frac{\delta\phi}{\delta x} &= \alpha\phi_{j+2} + \beta\phi_{j+1} + \gamma\phi_j
\end{aligned}
$$

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\phi_j &= \phi_j \\
\frac{\delta\phi}{\delta x} &= \alpha\phi_{j+2} + \beta\phi_{j+1} + \gamma\phi_j \\
&= (\alpha+\beta+\gamma)\phi_j + (2\alpha+\beta)h\phi_j' \\
&\quad +(4\alpha+\beta)\frac{h^2}{2}\phi_j'' + (8\alpha+\beta)\frac{h^3}{6}\phi_j''' + o(h^4)
\end{aligned}
$$

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\phi_j &= \phi_j \\
\frac{\delta\phi}{\delta x} &= \alpha\phi_{j+2} + \beta\phi_{j+1} + \gamma\phi_j \\
&= \underbrace{(\alpha+\beta+\gamma)}_{=0}\phi_j + \underbrace{(2\alpha+\beta)h}_{=1}\phi_j' \\
&+ \underbrace{(4\alpha+\beta)}_{=0}\frac{h^2}{2}\phi_j'' + (8\alpha+\beta)\frac{h^3}{6}\phi_j''' + o(h^4)
\end{aligned}
$$

Accuracy of finite-difference schemes

- One can use Taylor series to construct a finite-difference scheme of any order of accuracy.
- Example: three-point forward ($j+2$, $j+1$ and j) 2nd-order approximation to $\delta\phi/\delta x$:

$$\alpha = -\frac{1}{2h}; \qquad \beta = \frac{4}{2h}; \qquad \gamma = -\frac{3}{2h}$$

$$\begin{aligned}\frac{\delta\phi}{\delta x} &= \alpha\phi_{j+2} + \beta\phi_{j+1} + \gamma\phi_j \\ &= \frac{-\phi_{j+2} + 4\phi_{j+1} - 3\phi_j}{2h} - \frac{2h^2}{3}\phi_j''' + o(h^3)\end{aligned}$$

Accuracy of finite-difference schemes

- Commonly used schemes for the first derivative:

$$
\begin{aligned}
\phi_j' &= \frac{\phi_j - \phi_{j-1}}{h} + o(h) && \text{1st-order backwards}\\
&= \frac{\phi_{j+1} - \phi_j}{h} + o(h) && \text{1st-order forwards}\\
&= \frac{\phi_{j+1} - \phi_{j-1}}{2h} + o(h^2) && \text{2nd-order central}\\
&= \frac{3\phi_j - 4\phi_{j-1} + \phi_{j-2}}{2h} + o(h^2) && \text{2nd-order backwards}\\
&= \frac{-3\phi_j + 4\phi_{j+1} - \phi_{j+2}}{2h} + o(h^2) && \text{2nd-order forwards}\\
&= \frac{-\phi_{j+2} + 8\phi_{j+1} - 8\phi_{j-1} + \phi_{j-2}}{12h} + o(h^4) && \text{4th-order central}
\end{aligned}
$$

Accuracy of finite-difference schemes

- Commonly used schemes for the second derivative:

$$\phi_j'' = \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2} + o(h^2)$$

2nd-order central

$$= \frac{\phi_j - 2\phi_{j-1} + \phi_{j-2}}{h^2} + o(h)$$

1st-order backwards

$$= \frac{\phi_j - 2\phi_{j+1} + \phi_{j+2}}{h^2} + o(h)$$

1st-order forwards

Accuracy of finite-difference schemes

- If a stencil with n points is used to calculate a finite-difference approximation for a derivative, at most one can obtain an approximation of order n-1.
- More accurate approximations (for a given stencil) can be obtained by expanding both the function and its derivatives in Taylor series.

$$
\begin{array}{lclllll}
\alpha_1\phi_{j+1} & = & \alpha_1 \;[& \phi_j & +\phi'_j h & +\phi''_j h^2/2! & +\phi'''_j h^3/3! \\
 & & & +\phi^{iv}_j h^4/4! & +\phi^{v}_j h^5/5! & +o(h^6) &] \\
\alpha_2\phi_j & = & \alpha_2 \;[& \phi_j & & & \\
\alpha_3\phi_{j-1} & = & \alpha_3 \;[& \phi_j & -\phi'_j h & +\phi''_j h^2/2! & -\phi'''_j h^3/3! \\
 & & & +\phi^{iv}_j h^4/4! & -\phi^{v}_j h^5/5! & +o(h^6) &] \\
\beta_1 h\phi'_{j+1} & = & \beta_1 h \;[& & \phi'_j & +\phi''_j h & +\phi'''_j h^2/2! \\
 & & & +\phi^{iv}_j h^3/3! & +\phi^{v}_j h^4/4! & +o(h^5) &] \\
\beta_3 h\phi'_{j-1} & = & \beta_3 h \;[& & \phi'_j & -\phi''_j h & +\phi'''_j h^2/2! \\
 & & & -\phi^{iv}_j h^3/3! & +\phi^{v}_j h^4/4! & +o(h^5) &].
\end{array}
$$

Accuracy of finite-difference schemes

$$
\begin{aligned}
\alpha_1\phi_{j+1} &+ \alpha_2\phi_j + \alpha_3\phi_{j-1} + \beta_1 h\phi'_{j+1} + \beta_3 h\phi'_{j-1} \\
&= (\alpha_1 + \alpha_2 + \alpha_3)\,\phi_j \\
&+ (\alpha_1 - \alpha_3 + \beta_1 + \beta_3)\,\phi'_j h \\
&+ (\alpha_1 + \alpha_3 + 2\beta_1 - 2\beta_3)\,\phi''_j h^2/2! \\
&+ (\alpha_1 - \alpha_3 + 3\beta_1 + 3\beta_3)\,\phi'''_j h^3/3! \\
&+ (\alpha_1 + \alpha_3 + 4\beta_1 - 4\beta_3)\,\phi^{iv}_j h^4/4! \\
&+ (\alpha_1 - \alpha_3 + 5\beta_1 + 5\beta_3)\,\phi^{v}_j h^5/5! + o(h^6).
\end{aligned}
$$

Accuracy of finite-difference schemes

$$
\begin{aligned}
\alpha_1\phi_{j+1} &+ \alpha_2\phi_j + \alpha_3\phi_{j-1} + \beta_1 h\phi'_{j+1} + \beta_3 h\phi'_{j-1} \\
&= \underbrace{(\alpha_1 + \alpha_2 + \alpha_3)}_{=0}\,\phi_j \\
&+ \underbrace{(\alpha_1 - \alpha_3 + \beta_1 + \beta_3)}_{=1}\,\phi'_j h \\
&+ \underbrace{(\alpha_1 + \alpha_3 + 2\beta_1 - 2\beta_3)}_{=0}\,\phi''_j h^2/2! \\
&+ \underbrace{(\alpha_1 - \alpha_3 + 3\beta_1 + 3\beta_3)}_{=0}\,\phi'''_j h^3/3! \\
&+ \underbrace{(\alpha_1 + \alpha_3 + 4\beta_1 - 4\beta_3)}_{=0}\,\phi^{iv}_j h^4/4! \\
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\end{aligned}
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Accuracy of finite-difference schemes

$$
\begin{aligned}
\alpha_1\phi_{j+1} \; + \; & \alpha_2\phi_j + \alpha_3\phi_{j-1} + \beta_1 h\phi'_{j+1} + \beta_3 h\phi'_{j-1} \\
= \; & \underbrace{\boxed{(\alpha_1+\alpha_2+\alpha_3)}}_{=0}\,\phi_j \\
+ \; & \underbrace{\boxed{(\alpha_1-\alpha_3+\beta_1+\beta_3)}}_{=1}\,\phi'_j h \\
+ \; & \underbrace{\boxed{(\alpha_1+\alpha_3+2\beta_1-2\beta_3)}}_{=0}\,\phi''_j h^2/2! \\
+ \; & \underbrace{\boxed{(\alpha_1-\alpha_3+3\beta_1+3\beta_3)}}_{=0}\,\phi'''_j h^3/3! \\
+ \; & \underbrace{\boxed{(\alpha_1+\alpha_3+4\beta_1-4\beta_3)}}_{=0}\,\phi^{iv}_j h^4/4! \\
+ \; & (\alpha_1-\alpha_3+5\beta_1+5\beta_3)\,\phi^{v}_j h^5/5! + o(h^6).
\end{aligned}
$$

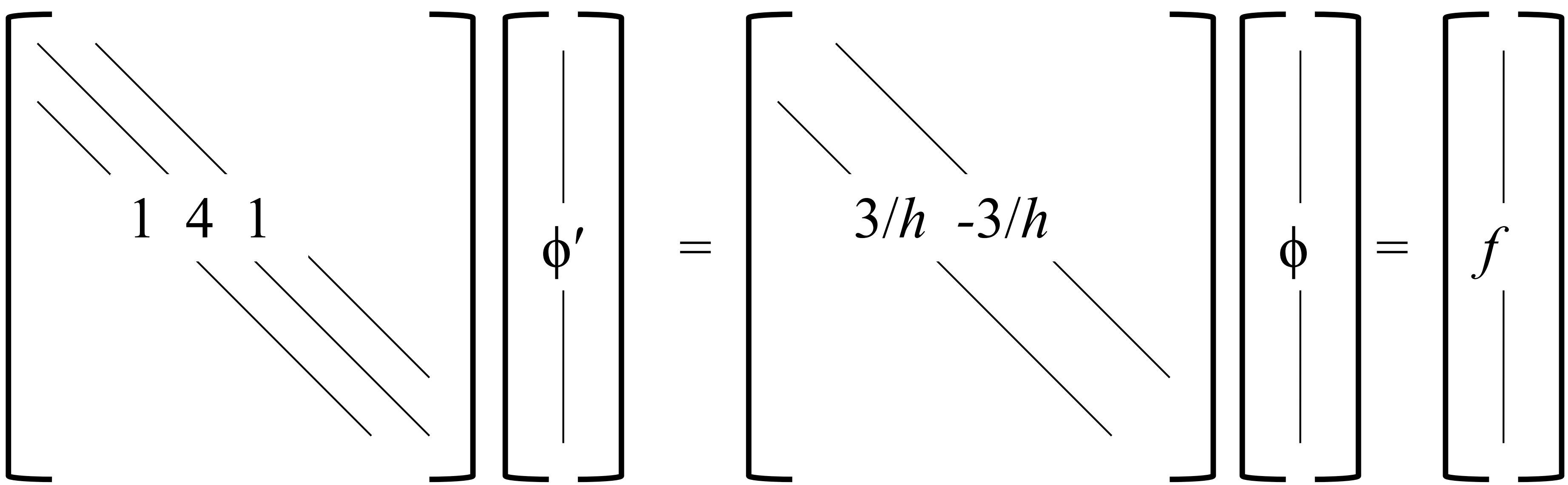
$$\alpha_1 = -\alpha_3 = 3/4; \qquad \alpha_2 = 0; \qquad \beta_1 = \beta_3 = -1/4.$$

$$\phi'_{j-1} + 4\phi'_j + \phi'_{j+1} = \frac{3}{h}\left(\phi_{j+1} - \phi_{j-1}\right) + o(h^4).$$

Accuracy of finite-difference schemes

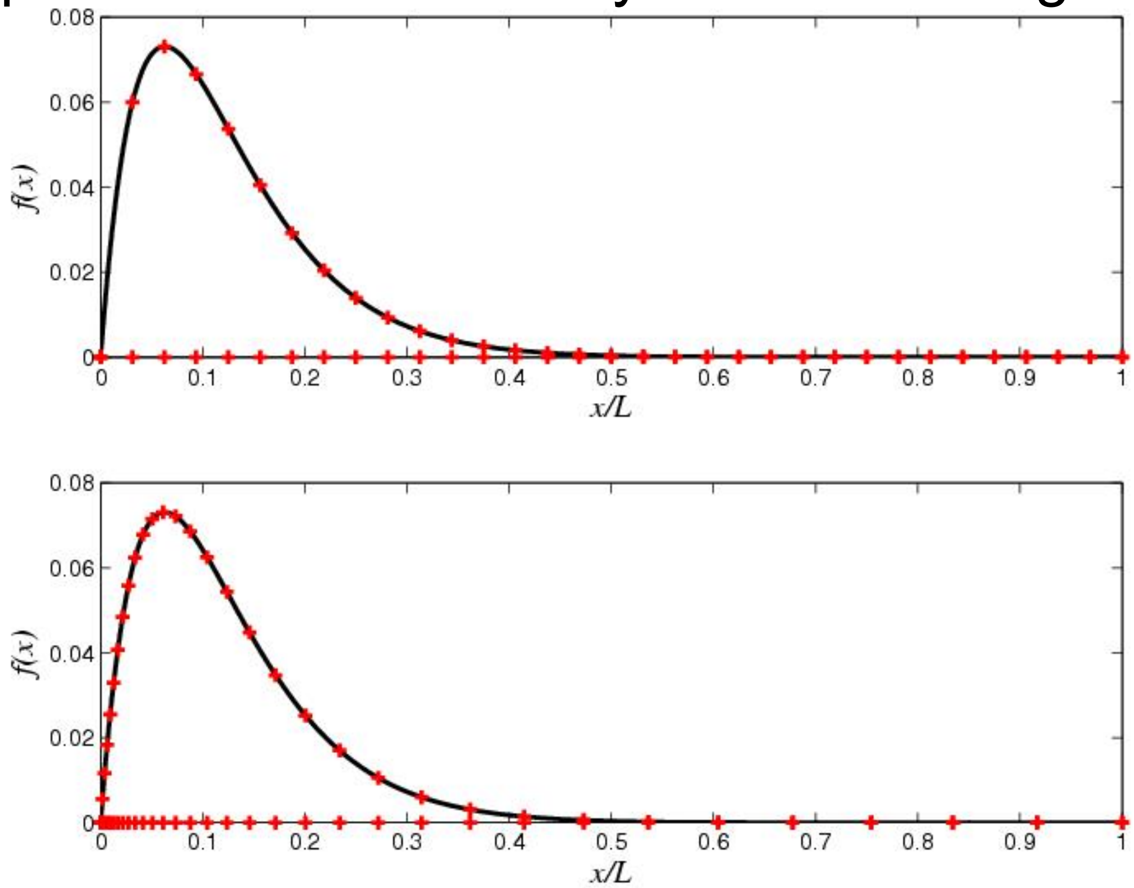
$$\phi'_{j-1} + 4\phi'_j + \phi'_{j+1} = \frac{3}{h}\left(\phi_{j+1} - \phi_{j-1}\right) + o(h^4).$$

- The evaluation of the derivative requires matrix inversion (tridiagonal in this case)



Non-uniform grids

- Sometime the function has sharp gradients confined to a small region of the domain:
- In such cases a uniform mesh may be inconvenient, since the number of points is determined by the minimum grid spacing.



Non-uniform grids

- Nominally 1st-order; 2nd-order on smooth grids

$$\frac{\delta\phi_j}{\delta x} = \frac{\phi_+ - \phi_-}{h_+ + h_-} = \phi_j' + \frac{h_+ - h_-}{2}\phi'' + o(h^2)$$

- 2nd-order

$$\frac{\delta\phi_j}{\delta x} = \frac{1}{h_+ + h_-}\left[\frac{h_-}{h_+}\phi_+ - \left(\frac{h_-}{h_+} - \frac{h_+}{h_-}\right)\phi - \frac{h_+}{h_-}\phi_-\right] = \phi_j' + o(h^2)$$

Grid types

- Hyperbolic tangent

$$x_j = L\left[1 + \frac{\tanh(\eta_j \tanh a)}{a}\right]; \qquad \eta_j = -1 + \frac{j-1}{N};$$

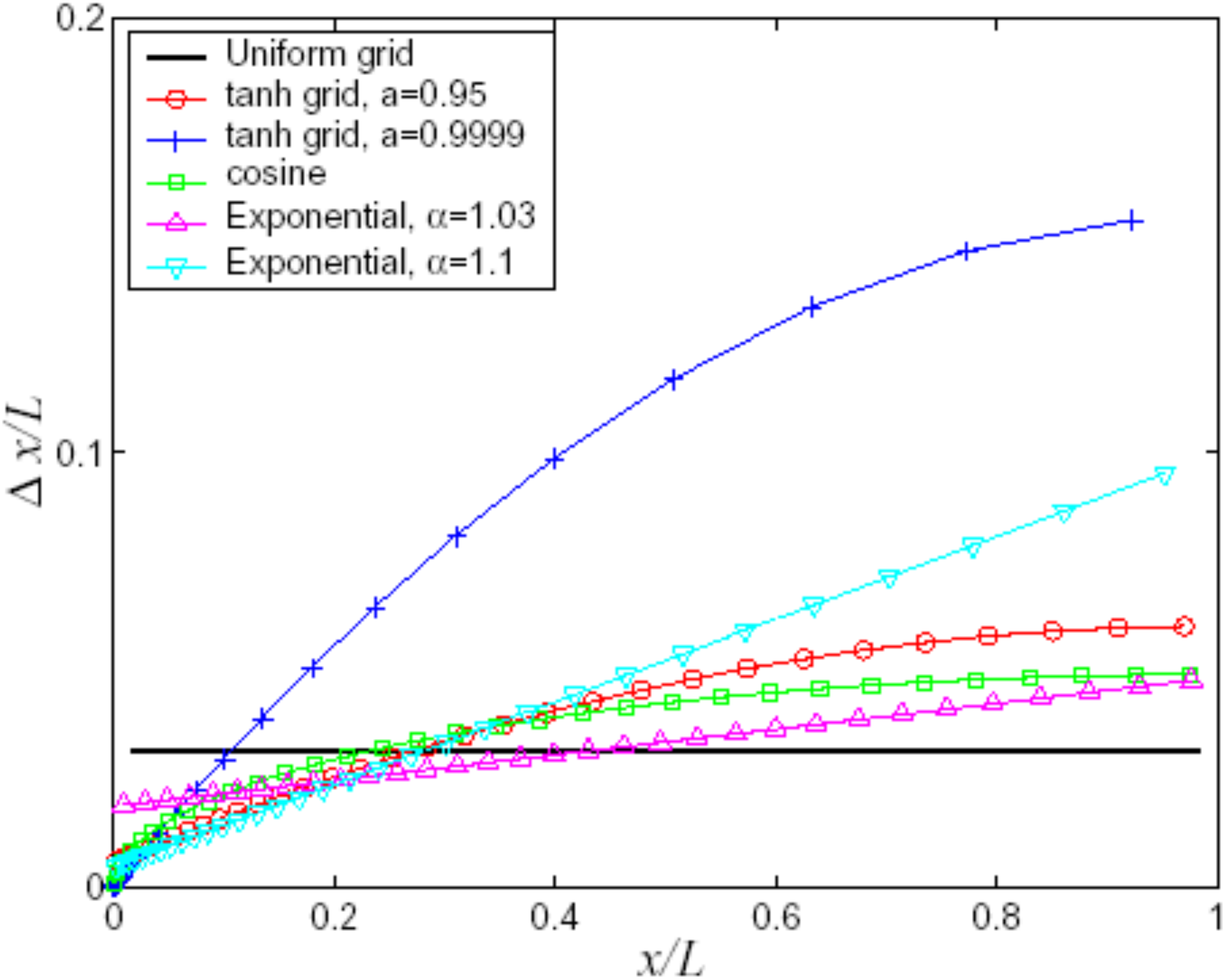
- Cosine

$$x_j = L\left(-1 + \cos\theta_j\right); \qquad \theta_j = \frac{j-1}{N}\frac{\pi}{2};$$

- Exponential

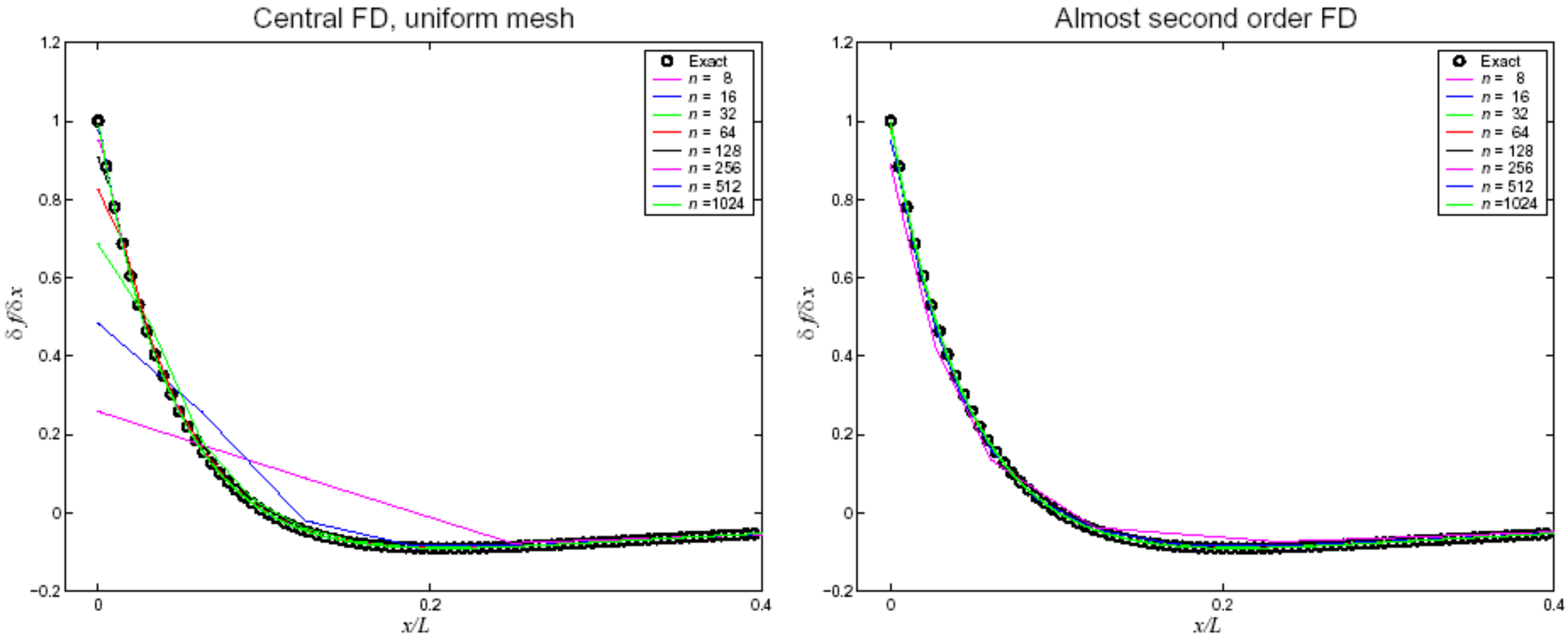
$$x_j = x_{j-1} + \Delta x_{j-1}; \qquad \Delta x_j = \Delta x_o \alpha^j;$$

Grid types



Uniform grid
tanh grid, a=0.95
tanh grid, a=0.9999
cosine
Exponential, α=1.03
Exponential, α=1.1
0.2
0.1
0
Δ x/L
0
0.2
0.4
0.6
0.8
1
x/L

Non-uniform grids



Non-uniform grids