HW1 ME 573 Computational fluid dynamics summer 2015

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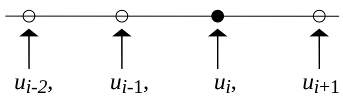
Contents

0.1 Problem 1

1. Use a Taylor table to derive a third order accurate scheme for a 1st derivative. Use 4 grid points: two points to the left, one at the point of interest, and one to the right:



Be sure to verify that it is third order accurate (e.g. not 2nd or 4th).

Let

$$\frac{du}{dx} \approx \left.\frac{\delta u}{\delta x}\right|_i = au_{i-2} + bu_{i-1} + cu_i + du_{i+1} \tag{1}$$

We now set up the Taylor table as explained in the lecture notes using h in place of dx for the spatial grid spacing in order to simplify the notation. Since we want to find 4 unknowns (a, b, c, d), then we need at least 4 columns. But we generate 5 in order to check for the order of the error using the last column. Therefore, the Taylor table with 5 columns is

	u_i	$\left.\frac{\partial u}{\partial x}\right\|_i$	$\left.\frac{\partial^2 u}{\partial x^2}\right\|_i$	$\left.\frac{\partial^3 u}{\partial x^3}\right\|_i$	$\left.\frac{\partial^4 u}{\partial x^4}\right\|_i$
u_{i-2}	1	$-2h$	$(-2h)^2 \frac{1}{2!}$	$(-2h)^3 \frac{1}{3!}$	$(-2h)^4 \frac{1}{4!}$
u_{i-1}	1	$-h$	$(-h)^2 \frac{1}{2!}$	$(-h)^3 \frac{1}{3!}$	$(-h)^4 \frac{1}{4!}$
u_i	1	0	0	0	0
u_{i+1}	1	h	$h^2 \frac{1}{2!}$	$h^3 \frac{1}{3!}$	$h^4 \frac{1}{4!}$

We now add the coefficients a, b, c, and d to obtain

	u_i	$\left.\frac{\partial u}{\partial x}\right\|_i$	$\left.\frac{\partial^2 u}{\partial x^2}\right\|_i$	$\left.\frac{\partial^3 u}{\partial x^3}\right\|_i$	$\left.\frac{\partial^4 u}{\partial x^4}\right\|_i$
au_{i-2}	a	$a(-2h)$	$a(-2h)^2 \frac{1}{2!}$	$a(-2h)^3 \frac{1}{3!}$	$a(-2h)^4 \frac{1}{4!}$
bu_{i-1}	b	$b(-h)$	$b(-h)^2 \frac{1}{2!}$	$b(-h)^3 \frac{1}{3!}$	$b(-h)^4 \frac{1}{4!}$
cu_i	c	0	0	0	0
du_{i+1}	d	$d(h)$	$d(h)^2 \frac{1}{2!}$	$d(h)^3 \frac{1}{3!}$	$d(h)^4 \frac{1}{4!}$

Expanding and summing each column gives

	u_i	$\left.\frac{\partial u}{\partial x}\right\|_i$	$\left.\frac{\partial^2 u}{\partial x^2}\right\|_i$	$\left.\frac{\partial^3 u}{\partial x^3}\right\|_i$	$\left.\frac{\partial^4 u}{\partial x^4}\right\|_i$
au_{i-2}	a	$a(-2h)$	$a(-2h)^2 \frac{1}{2!}$	$a(-2h)^3 \frac{1}{3!}$	$a(-2h)^4 \frac{1}{4!}$
bu_{i-1}	b	$b(-h)$	$b(-h)^2 \frac{1}{2!}$	$b(-h)^3 \frac{1}{3!}$	$b(-h)^4 \frac{1}{4!}$
cu_i	c	0	0	0	0
du_{i+1}	d	$d(h)$	$d(h)^2 \frac{1}{2!}$	$d(h)^3 \frac{1}{3!}$	$d(h)^4 \frac{1}{4!}$
Σ	$a+b+c+d$	$(-2a-b+d)h$	$\left(2a+\frac{b}{2}+\frac{d}{2}\right)h^2$	$\left(-\frac{8}{6}a-\frac{b}{6}+\frac{d}{6}\right)h^3$	$\left(\frac{16}{24}a+\frac{b}{24}+\frac{d}{24}\right)h^4$
	0	1	0	0	check if zero

Since first derivative approximation is sought, we want the $\frac{\partial u}{\partial x}$ column to sum to one, and the other columns to sum to zero. This gives four equations to solve for a, b, c and d

$$
\begin{aligned}
a+b+c+d &= 0\\
(-2a-b+d)\,h &= 1\\
\left(2a+\frac{b}{2}+\frac{d}{2}\right)h^2 &= 0\\
\left(-\frac{8}{6}a-\frac{b}{6}+\frac{d}{6}\right)h^3 &= 0
\end{aligned}
$$

Since $h \neq 0$ these reduce to

$$
\begin{aligned}
a+b+c+d &= 0\\
-2a-b+d &= \frac{1}{h}\\
2a+\frac{b}{2}+\frac{d}{2} &= 0\\
-\frac{8}{6}a-\frac{b}{6}+\frac{d}{6} &= 0
\end{aligned}
$$

Solving gives $a=\frac{1}{6h}, b=-\frac{1}{h}, c=\frac{1}{2h}, d=\frac{1}{3h}$. Therefore (1) becomes

$$
\begin{aligned}
\left.\frac{du}{dx}\right|_{x_i} \approx \left.\frac{\delta u}{\delta x}\right|_i &= a u_{i-2} + b u_{i-1} + c u_i + d u_{i+1}\\
&= \frac{\frac{1}{6}u_{i-2} - u_{i-1} + \frac{1}{2}u_i + \frac{1}{3}u_{i+1}}{h}\\
&= \frac{u_{i-2} - 6u_{i-1} + 3u_i + 2u_{i+1}}{6h}
\end{aligned}
$$

To determine the truncation error the last column in the Taylor table above is checked if it sums to non-zero. If the sum turns out to be zero, the next column after that must then be checked.

$$
\begin{aligned}
\left(\frac{16}{24}a+\frac{b}{24}+\frac{d}{24}\right)h^4 &= \left(\frac{16}{24}\frac{1}{6h}-\frac{1}{24h}+\frac{1}{3\,(24)\,h}\right)h^4\\
&= \left(\frac{16}{24}\frac{1}{6}-\frac{1}{24}+\frac{1}{3\,(24)}\right)h^3\\
&= \frac{1}{12}h^3
\end{aligned}
$$

Since the sum is not zero, there is no need to check any more columns and the truncation error is verified to be third order $O\left(h^3\right)$.

0.2 Problem 2

2. Use the spectral analysis method to find the effective wave number for this method. Plot the real and imaginary components of $k_{\text{effective}}$. Compare with the exact wave number and comment on any differences.

Using result from problem 1

$$
\left.\frac{\delta u}{\delta x}\right|_i = \frac{u_{i-2} - 6u_{i-1} + 3u_i + 2u_{i+1}}{6h} \tag{1}
$$

Using

$$u(x) = \sum_k \hat{u}_k e^{jkx}$$

Where $\hat{u}_k$ are the Fourier coefficients, which are functions of k, and are complex numbers in general . Looking at one mode only (one specific k), then we let k run over its range, where k is called the wave number which is related to the wave length λ by

$$k = \frac{2\pi}{\lambda}$$

j above is $\sqrt{-1}$(We could also have used $\hat{\imath}$ for $\sqrt{-1}$ but it looked very close to the index i and can be confusing). Hence[1]

$$u(x) = \hat{u}_k e^{jkx}$$

Equation (1) now can be written as

$$\begin{aligned}\frac{\partial u}{\partial x} &= \frac{\partial}{\partial x}\hat{u}_k e^{jkx}\\ &= (jk)\,\hat{u}_k e^{jkx}\\ &= (jk)\,u(x) \qquad (2)\end{aligned}$$

For finite difference the above can be written as

$$\left.\frac{\delta u}{\delta x}\right|_i = (jk)_{eff}\, u_i$$

And the goal is to determine $(jk)_{eff}$ using (1) above and compare it to the actual (jk) from (2). From (1) we obtain for the RHS

$$\begin{aligned}(jk)_{eff}\, u_i &= \frac{\hat{u}_k e^{jk(x_i-2h)} - 6\hat{u}_k e^{jk(x_i-h)} + 3\hat{u}_k e^{jkx_i} + 2\hat{u}_k e^{jk(x_i+h)}}{6h}\\ (jk)_{eff}\, u_i &= \left(\frac{e^{-2jkh} - 6e^{-jkh} + 3 + 2e^{jkh}}{6h}\right)\hat{u}_k e^{jkx_i}\\ (jk)_{eff}\, u_i &= \overbrace{\frac{e^{-2jkh} - 6e^{-jkh} + 3 + 2e^{jkh}}{6h}}^{\text{effective wave number}} u_i\end{aligned}$$

Therefore the effective wave number$(jk)_{eff}$ is

$$\begin{aligned}(jk)_{eff} &= \frac{e^{-2jkh} - 6e^{-jkh} + 3 + 2e^{jkh}}{6h}\\ &= \frac{(\cos 2kh - j\sin 2kh) - 6(\cos kh - j\sin kh) + 3 + 2(\cos kh + j\sin kh)}{6h}\\ &= \frac{j}{6h}(-\sin 2kh + 6\sin kh + 2\sin kh) + \frac{1}{6h}(\cos 2kh - 6\cos kh + 3 + 2\cos kh)\end{aligned}$$

[1]We could also write $u(x) = \hat{u}_k e^{jkx}$ instead of $u(x) = \hat{u}_k e^{-jkx}$. Both are valid expressions, but the first one is more common.

Therefore

$$(jk)_{eff} = j\overbrace{\left(\frac{8\sin kh - \sin 2kh}{6h}\right)}^{\text{complex part}} + \overbrace{\frac{1}{6h}\left(\cos 2kh - 4\cos kh + 3\right)}^{\text{real part}}$$

We see that $(jk)_{eff}$ has both a complex part and a real part. But the exact wave number (jk) is only complex. This is the first major difference we see. Now we will plot the real and the imaginary parts of $(jk)_{eff}$. The complex part is

$$(jk)_{eff_{\text{complex}}} = \frac{8\sin kh - \sin 2kh}{6}$$

And the second is the real part

$$(jk)_{eff_{\text{real}}} = \frac{\cos 2kh - 4\cos kh + 3}{6}$$

We now use x for kh as the argument to simplify the notation and plot it

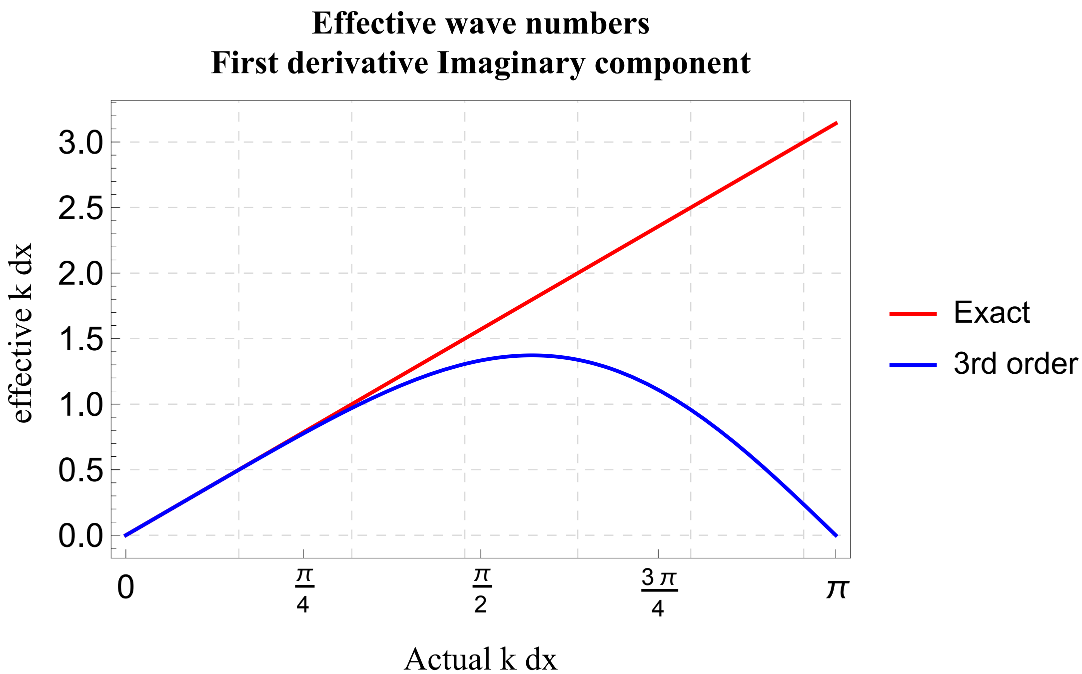
$$k_{eff_{\text{complex}}}(x) = \frac{8\sin x - \sin 2x}{6}$$

And the real part is

$$k_{eff_{\text{real}}}(x) = \frac{\cos 2x - 4\cos x + 3}{6}$$

The plots of the imaginary part is given below

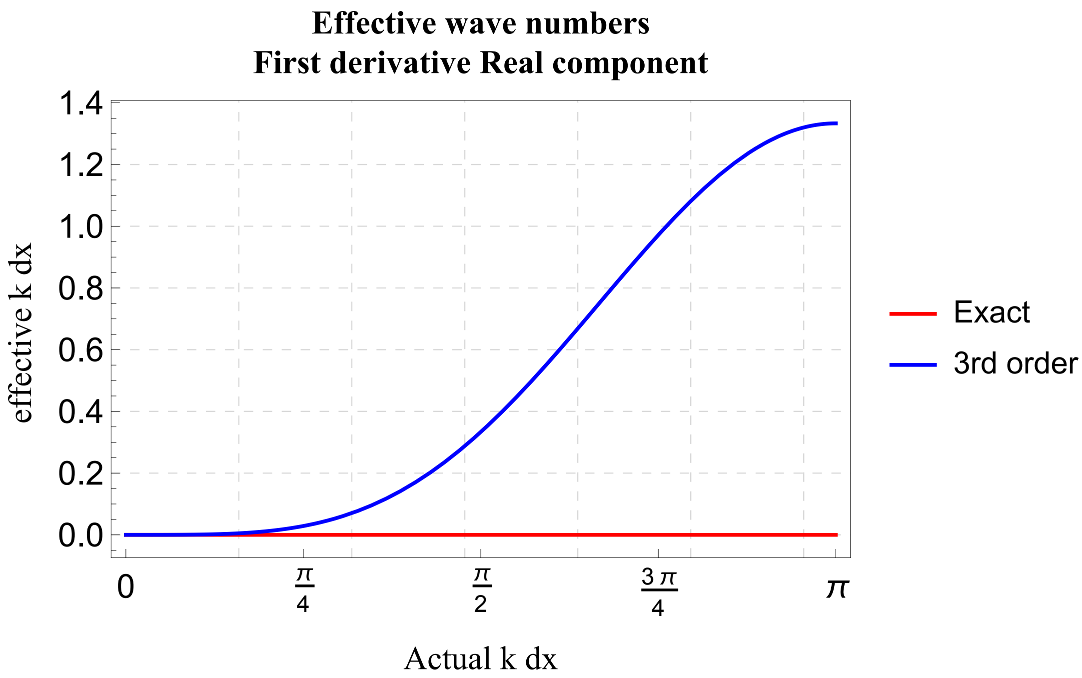
```
f[x_] := (8 Sin[x] - Sin[2 x])/6
Plot[{x, f[x]}, {x, 0, Pi}, Frame -> True,
FrameTicks -> {{Automatic, None}, {Range[0, Pi, Pi/4], None}},
FrameLabel -> {{Text@Style["effective k dx"],
None}, {Text@Style["Actual k dx"],
Text@Style[
Column[{"Effective wave numbers",
"First derivative Imaginary component"}, Alignment -> Center],
Bold]}}, BaseStyle -> 14,
PlotLegends -> {"Exact", "3rd order"}, GridLines -> Automatic,
GridLinesStyle -> Directive[LightGray, Dashed],
PlotStyle -> {Red, Blue}]
```



Discussion: We see from the above that the imaginary part of the effective wave number is accurate and close to the exact value for small wave numbers. After about $kh \approx \frac{\pi}{3}$, then it is no longer accurate. Smaller k implies larger wave length λ which in turn puts a limits of the grid size h.

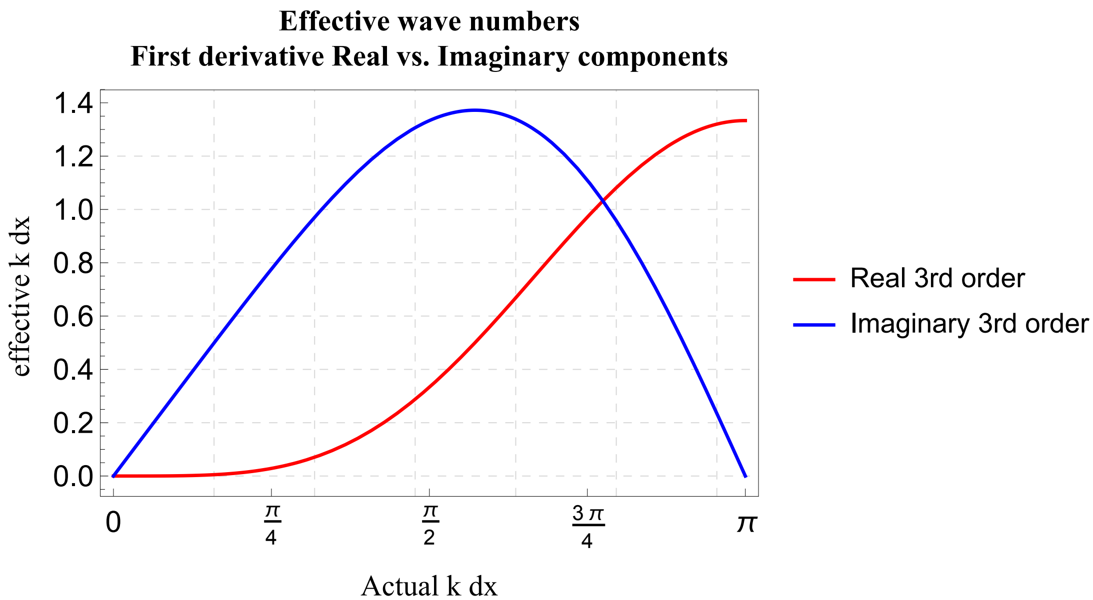
The real part plot is below

```
f[x_] := (Cos[2 x] - 4 Cos[x] + 3)/6
Plot[{0, f[x]}, {x, 0, Pi}, Frame -> True,
FrameTicks -> {{Automatic, None}, {Range[0, Pi, Pi/4], None}},
FrameLabel -> {{Text@Style["effective k dx"],
None}, {Text@Style["Actual k dx"],
Text@Style[
Column[{"Effective wave numbers",
"First derivative Real component"}, Alignment -> Center],
Bold]}}, BaseStyle -> 14, PlotLegends -> {"Exact", "3rd order"},
GridLines -> Automatic,
GridLinesStyle -> Directive[LightGray, Dashed],
PlotStyle -> {Red, Blue}]
```



Discussion: The exact value is zero for all wave numbers, since we know from the above, that the exact effective k has only complex part and no real part. but the effective k is only as accurate and close to zero for much smaller wave numbers. After about $kh \approx \frac{\pi}{4}$ it is no longer accurate. Having a real part in the effective wave number, implies the finite difference scheme will introduce damping effect in the result.

```
real[x_] := (Cos[2 x] - 4 Cos[x] + 3)/6
im[x_] := (8 Sin[x] - Sin[2 x])/6
Plot[{real[x], im[x]}, {x, 0, Pi}, Frame -> True,
FrameTicks -> {{Automatic, None}, {Range[0, Pi, Pi/4], None}},
FrameLabel -> {{Text@Style["effective k dx"],
None}, {Text@Style["Actual k dx"],
Text@Style[
Column[{"Effective wave numbers",
"First derivative Real vs. Imaginary components"},
Alignment -> Center], Bold]}}, BaseStyle -> 14,
PlotLegends -> {"Real 3rd order", "Imaginary 3rd order"},
GridLines -> Automatic,
GridLinesStyle -> Directive[LightGray, Dashed],
PlotStyle -> {Red, Blue}]
```



0.3 Problem 3

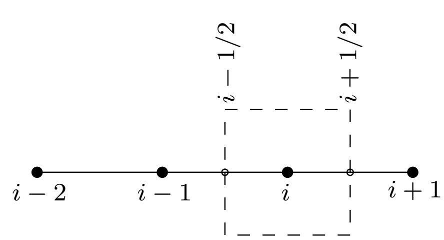
3. One way to generate finite difference expressions is to use points between grid points such as:

$$\frac{u_{i+1/2} - u_{i-1/2}}{dx}$$

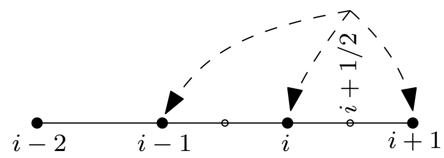
Then the (*i*+½) and (*i*-½) are defined by interpolation according to the method one wants to generate. (Note, this is common in finite volume methods). Use this approach and 3 point Lagrange interpolation (upwind) on a uniform grid to define the ½ cell points. Then analyze the method to determine its Taylor series accuracy. Discuss.

Hint: for this method you will end up using points at (*i*-2) (*i*-1) (*i*) and (*i*+1)

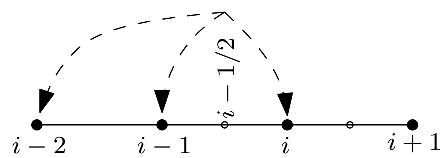
We need to derive approximation for $\left.\frac{du}{dx}\right|_{x_i} \approx \left.\frac{\delta u}{\delta x}\right|_i = \frac{u_{i+1/2}(x) - u_{i-1/2}(x)}{h}$ using 3 points Lagrangian interpolation. There are 4 points needed. The following diagram shows the cell structure used



When interpolating $u_{i+1/2}(x)$, the following 3 points are used



When interpolating for $u_{i-1/2}(x)$, the following 3 points are used



Therefore

$$\begin{aligned} u_{i+1/2}(x) &= u_{i-1}(\cdot) + u_i(\cdot) + u_{i+1}(\cdot) \\ &= u_{i-1}\frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + u_i\frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} + u_{i+1}\frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)} \end{aligned}$$

When x is midpoint between x_{i+1} and x_i, then the above reduces to (where $h = dx$) which is the grid size between each point:

$$\begin{aligned} u_{i+1/2}(x) &= u_{i-1}\frac{\left(\frac{h}{2}\right)\left(\frac{-h}{2}\right)}{(-h)(-2h)} + u_i\frac{\left(\frac{3}{2}h\right)\left(\frac{-h}{2}\right)}{(h)(-h)} + u_{i+1}\frac{\left(\frac{3}{2}h\right)\left(\frac{h}{2}\right)}{(2h)(h)} \\ &= -\frac{1}{8}u_{i-1} + \frac{3}{4}u_i + \frac{3}{8}u_{i+1} \end{aligned}$$

And

$$\begin{aligned} u_{i-1/2}(x) &= u_{i-2}(\cdot) + u_{i-1}(\cdot) + u_i(\cdot) \\ &= u_{i-2}\frac{(x-x_{i-1})(x-x_i)}{(x_{i-2}-x_{i-1})(x_{i-2}-x_i)} + u_{i-1}\frac{(x-x_{i-2})(x-x_i)}{(x_{i-1}-x_{i-2})(x_{i-1}-x_i)} + u_i\frac{(x-x_{i-2})(x-x_{i-1})}{(x_{i+1}-x_{i-2})(x_i-x_{i-1})} \end{aligned}$$

When x is midpoint between x_i and x_{i-1}, then the above reduces to (where $h = dx$) which is the grid size between each point:

$$\begin{aligned} u_{i-1/2}(x) &= u_{i-2}\frac{\left(\frac{h}{2}\right)\left(-\frac{h}{2}\right)}{(-h)(-2h)} + u_{i-1}\frac{\left(\frac{3}{2}h\right)\left(\frac{-h}{2}\right)}{(h)(-h)} + u_i\frac{\left(\frac{3}{2}h\right)\left(\frac{h}{2}\right)}{(2h)(h)} \\ &= -\frac{1}{8}u_{i-2} + \frac{3}{4}u_{i-1} + \frac{3}{8}u_i \end{aligned}$$

Therefore

$$\begin{aligned} \left.\frac{\delta u}{\delta x}\right|_i &= \frac{u_{i+1/2}(x) - u_{i-1/2}(x)}{dx} \\ &= \frac{\left(-\frac{1}{8}u_{i-1} + \frac{3}{4}u_i + \frac{3}{8}u_{i+1}\right) - \left(-\frac{1}{8}u_{i-2} + \frac{3}{4}u_{i-1} + \frac{3}{8}u_i\right)}{h} \\ &= \frac{1}{8}\frac{3u_i - 7u_{i-1} + 3u_{i+1} + u_{i-2}}{h} \end{aligned}$$

To determine the Taylor series accuracy, we expand the RHS around x_i

$$\begin{aligned}
\Delta &= \frac{1}{8h}\left(3u_i - 7u_{i-1} + 3u_{i+1} + u_{i-2}\right) \\
&\approx \frac{1}{8h}\left[3u_i - 7\left(u_i - h\left.\frac{\delta u}{\delta x}\right|_i + O\left((-h)^2\right)\right) + 3\left(u_i + h\left.\frac{\delta u}{\delta x}\right|_i + O\left(h^2\right)\right) + \left(u_i - 2h\left.\frac{\delta u}{\delta x}\right|_i + O\left((-2h)^2\right)\right)\right] \\
&= \frac{1}{8h}\left[3u_i - 7u_i + 7h\left.\frac{\delta u}{\delta x}\right|_i + 7O\left(h^2\right) + 3u_i + 3h\left.\frac{\delta u}{\delta x}\right|_i + 3O\left(h^2\right) + u_i - 2h\left.\frac{\delta u}{\delta x}\right|_i + O\left(4h^2\right)\right] \\
&= \frac{1}{8h}\left[7h\left.\frac{\delta u}{\delta x}\right|_i + 7O\left(h^2\right) + 3h\left.\frac{\delta u}{\delta x}\right|_i + 3O\left(h^2\right) - 2h\left.\frac{\delta u}{\delta x}\right|_i + O\left(4h^2\right)\right] \\
&= \frac{1}{8h}\left(7h\left.\frac{\delta u}{\delta x}\right|_i + 3h\left.\frac{\delta u}{\delta x}\right|_i - 2h\left.\frac{\delta u}{\delta x}\right|_i + O\left(h^2\right)\right) \\
&= \frac{1}{8}\left(8\left.\frac{\delta u}{\delta x}\right|_i + O\left(h\right)\right) \\
&= \left.\frac{\delta u}{\delta x}\right|_i + O\left(h\right)
\end{aligned}$$

Therefore this is first order accurate.