HW1 ME 573 Computational fluid dynamics summer 2015

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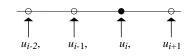
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0.1 Problem 1

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

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

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	$\frac{\partial u}{\partial x}\Big _{i}$	$\frac{\partial^2 u}{\partial x^2}\Big _i$	$\frac{\partial^3 u}{\partial x^3}\Big _i$	$\frac{\partial^4 u}{\partial x^4}\Big _i$
<i>u</i> _{<i>i</i>-2}	1	-2h	$(-2h)^2 \frac{1}{2!}$	$(-2h)^3 \frac{1}{3!}$	$(-2h)^4 \frac{1}{4!}$
<i>u</i> _{<i>i</i>-1}	1	-h	$(-h)^2 \frac{1}{2!}$	$(-h)^3 \frac{1}{3!}$	$(-h)^4 \frac{1}{4!}$
<i>u</i> _i	1	0	0	0	0
<i>u</i> _{<i>i</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

	<i>u</i> _i	$\frac{\partial u}{\partial x}\Big _i$	$\frac{\partial^2 u}{\partial x^2}\Big _i$	$\frac{\partial^3 u}{\partial x^3}\Big _i$	$\frac{\partial^4 u}{\partial x^4}\Big _i$
au _{i-2}	а	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)	$b(-h)^2 \frac{1}{2!}$	$b(-h)^3 \frac{1}{3!}$	$b(-h)^4 \frac{1}{4!}$
си _i	С	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	$\frac{\partial u}{\partial x}\Big _i$	$\frac{\partial^2 u}{\partial x^2}\Big _i$	$\frac{\partial^3 u}{\partial x^3}\Big _i$	$\frac{\partial^4 u}{\partial x^4}\Big _i$
au _{i-2}	а	a (-2h)	$a(-2h)^2 \frac{1}{2!}$	$a(-2h)^3\frac{1}{3!}$	$a(-2h)^4 \frac{1}{4!}$
bu _{i-1}	Ь	b (-h)	$b(-h)^2 \frac{1}{2!}$	$b(-h)^3\frac{1}{3!}$	$b(-h)^4 \frac{1}{4!}$
си _i	С	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	$\left(-2a-b+d\right)h$	$\left(2a + \frac{b}{2} + \frac{d}{2}\right)h^2$	$\left(-\frac{8}{6}a - \frac{b}{6} + \frac{d}{6}\right)h^3$	$\left(\frac{16}{24}a + \frac{b}{24} + \frac{d}{24}\right)h^4$
	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*

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

Since $h \neq 0$ these reduce to

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

Solving gives $a = \frac{1}{6h}, b = -\frac{1}{h}, c = \frac{1}{2h}, d = \frac{1}{3h}$. Therefore (1) becomes $\frac{du}{dx}\Big|_{x_i} \approx \frac{\delta u}{\delta x}\Big|_i = au_{i-2} + bu_{i-1} + cu_i + du_{i+1}$ $= \frac{\frac{1}{6}u_{i-2} - u_{i-1} + \frac{1}{2}u_i + \frac{1}{3}u_{i+1}}{du_i + 1}$

$$=\frac{u_{i-2}-6u_{i-1}+3u_i+2u_{i+1}}{6h}$$

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.

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

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 $O(h^3)$.

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

$$u\left(x\right) = \sum_{k} \hat{u}_{k} e^{jkx}$$

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{i} for $\sqrt{-1}$ but it looked very close to the index *i* and can be confusing). Hence¹

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

Equation (1) now can be written as

$$\frac{\partial u}{\partial x} = \frac{\partial}{\partial x} \hat{u}_k e^{jkx}
= (jk) \hat{u}_k e^{jkx}
= (jk) u(x)$$
(2)

For finite difference the above can be written as

¹We 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.

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

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

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

$$(jk)_{eff} = \frac{e^{-2jkh} - 6e^{-jkh} + 3 + 2e^{jkh}}{6h}$$

$$= \frac{(\cos 2kh - j\sin 2kh) - 6(\cos kh - j\sin kh) + 3 + 2(\cos kh + j\sin kh)}{6h}$$

$$= \frac{j}{6h}(-\sin 2kh + 6\sin kh + 2\sin kh) + \frac{1}{6h}(\cos 2kh - 6\cos kh + 3 + 2\cos kh)$$

Therefore

$$(jk)_{eff} = \overline{j\left(\frac{8\sin kh - \sin 2kh}{6h}\right)} + \frac{1}{6h}\left(\cos 2kh - 4\cos kh + 3\right)$$

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

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

2*x*

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

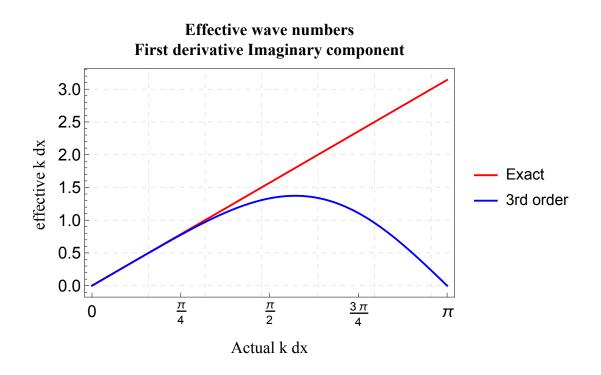
$$k_{eff_{\rm complex}}(x) = \frac{8\sin x - \sin x}{6}$$

And the real part is

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

The plots of the imaginary part is given below

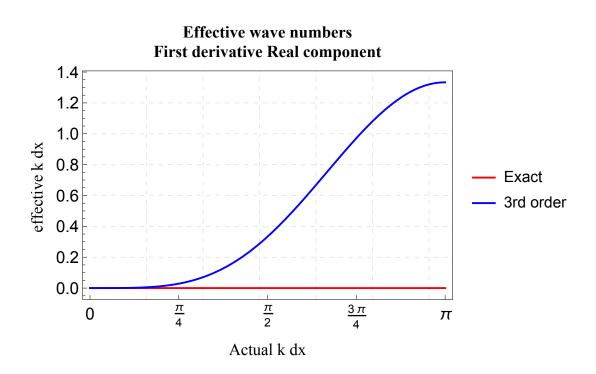
```
f[x_] := (8 Sin[x] - Sin[2 x])/6
Plot[{x, f[x]}, {x, 0, Pi}, Frame -> True,
FrameTicks -> {{Automatic, None}, {Range[0, Pi, Pi/4], None}},
FrameLabel -> {{Text@Style["effective k dx"],
None}, {Text@Style["Actual k dx"],
Text@Style[
Column[{"Effective wave numbers",
"First derivative Imaginary component"}, 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

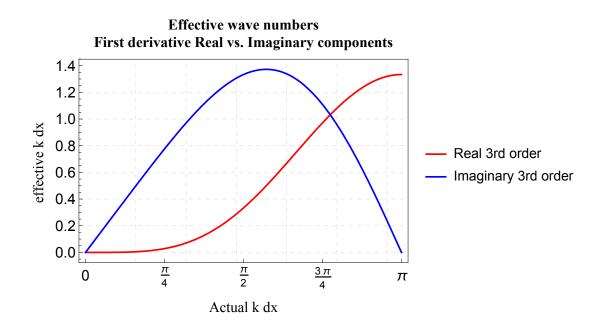
```
f[x_] := (Cos[2 x] - 4 Cos[x] + 3)/6
Plot[{0, f[x]}, {x, 0, Pi}, Frame -> True,
FrameTicks -> {{Automatic, None}, {Range[0, Pi, Pi/4], None}},
FrameLabel -> {{Text@Style["effective k dx"],
None}, {Text@Style["Actual k dx"],
Text@Style[
Column[{"Effective wave numbers",
    "First derivative Real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



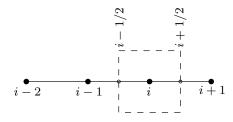
0.3 Problem 3

3. One way to generate finite difference expressions is to use points between grid points such as: $\frac{u_{i+1/2} - u_{i-1/2}}{dx}$

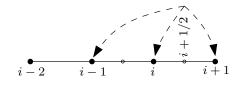
Then the $(i+\frac{1}{2})$ and $(i-\frac{1}{2})$ are defined by interpolation according to the method one wants to generate. (Note, this is common in finite volume methods). Use this approach and 3 point Lagrange interpolation (upwind) on a uniform grid to define the $\frac{1}{2}$ cell points. Then analyze 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)

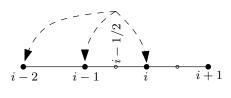
We need to derive approximation for $\frac{du}{dx}\Big|_{x_i} \approx \frac{\delta u}{\delta x}\Big|_i = \frac{u_{i+1/2}(x) - u_{i-1/2}(x)}{h}$ using 3 points Lagrangian interpolation. There are 4 points needed. The following diagram shows the cell structure used



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

$$u_{i+1/2}(x) = u_{i-1}(\cdot) + u_i(\cdot) + u_{i+1}(\cdot)$$

= $u_{i-1}\frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + u_i\frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} + u_{i+1}\frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$

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:

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

And

$$u_{i-1/2}(x) = u_{i-2}(\cdot) + u_{i-1}(\cdot) + u_i(\cdot)$$

= $u_{i-2} \frac{(x - x_{i-1})(x - x_i)}{(x_{i-2} - x_{i-1})(x_{i-2} - x_i)} + u_{i-1} \frac{(x - x_{i-2})(x - x_i)}{(x_{i-1} - x_{i-2})(x_{i-1} - x_i)} + u_i \frac{(x - x_{i-2})(x - x_{i-1})}{(x_{i+1} - x_{i-2})(x_i - x_{i-1})}$

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:

$$u_{i-1/2}(x) = u_{i-2} \frac{\binom{h}{2} \binom{-h}{2}}{(-h)(-2h)} + u_{i-1} \frac{\binom{3}{2}h}{(h)(-h)} + u_i \frac{\binom{3}{2}h}{(2h)(h)} + u_i \frac{\binom{3}{2}h}{(2h)(h)}$$
$$= -\frac{1}{8}u_{i-2} + \frac{3}{4}u_{i-1} + \frac{3}{8}u_i$$

Therefore

$$\frac{\delta u}{\delta x}\Big|_{i} = \frac{u_{i+1/2}(x) - u_{i-1/2}(x)}{dx}$$
$$= \frac{\left(-\frac{1}{8}u_{i-1} + \frac{3}{4}u_{i} + \frac{3}{8}u_{i+1}\right) - \left(-\frac{1}{8}u_{i-2} + \frac{3}{4}u_{i-1} + \frac{3}{8}u_{i}\right)}{h}$$
$$= \frac{1}{8}\frac{3u_{i} - 7u_{i-1} + 3u_{i+1} + u_{i-2}}{h}$$

To determine the Taylor series accuracy, we expand the RHS around \boldsymbol{x}_i

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

Therefore this is first order accurate.