

Based on “Computational Methods For Fluid Dynamics” by Ferziger & Peric (2002)

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i \approx \frac{\left(\frac{\partial \phi}{\partial x}\right)_{i+1/2} - \left(\frac{\partial \phi}{\partial x}\right)_{i-1/2}}{0.5(x_{i+1} - x_{i-1})} \approx \frac{\frac{\phi_{i+1} + \phi_i}{\Delta x_i} - \frac{\phi_i + \phi_{i-1}}{\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} = \left[\frac{\phi_{i+1}\Delta x_{i-1} + \phi_{i-1}\Delta x_i}{\Delta x_i + \Delta x_{i-1}} - \phi_i \right] \times \frac{2}{\Delta x_i \Delta x_{i-1}}$$

Let's find out what is the leading truncation error term.

Firstly, assume Δx_i is the grid size from 'i' to 'i+1', however, both sides of node point 'i+0.5 Δx_i ' should have the same grid size:

$$\begin{aligned} \phi_{i+\Delta x_i} &= \phi_{i+0.5\Delta x_i} + (0.5\Delta x_i) \left(\frac{\partial \phi}{\partial x}\right)_{i+0.5\Delta x_i} + \frac{(0.5\Delta x_i)^2}{2} \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i+0.5\Delta x_i} + \frac{(0.5\Delta x_i)^3}{6} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i} + \frac{(0.5\Delta x_i)^4}{24} \left(\frac{\partial^4 \phi}{\partial x^4}\right)_{i+0.5\Delta x_i} + O(\Delta x_i^5) \\ \phi_i &= \phi_{i+0.5\Delta x_i} - (0.5\Delta x_i) \left(\frac{\partial \phi}{\partial x}\right)_{i+0.5\Delta x_i} + \frac{(0.5\Delta x_i)^2}{2} \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i+0.5\Delta x_i} - \frac{(0.5\Delta x_i)^3}{6} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i} + \frac{(0.5\Delta x_i)^4}{24} \left(\frac{\partial^4 \phi}{\partial x^4}\right)_{i+0.5\Delta x_i} + O(\Delta x_i^5) \end{aligned}$$

The upper one minus the lower one,

$$\phi_{i+\Delta x_i} - \phi_i = (\Delta x_i) \left(\frac{\partial \phi}{\partial x}\right)_{i+0.5\Delta x_i} + \frac{(0.5\Delta x_i)^3}{3} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i} + O(\Delta x_i^4)$$

Therefore, the 1st order derivative with derived with leading truncation error is:

$$\left(\frac{\partial \phi}{\partial x}\right)_{i+0.5\Delta x_i} = \frac{\phi_{i+\Delta x_i} - \phi_i}{\Delta x_i} - \frac{(\Delta x_i)^2}{24} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i}$$

Similarly,

$$\left(\frac{\partial \phi}{\partial x}\right)_{i-0.5\Delta x_{i-1}} = \frac{\phi_i - \phi_{i-\Delta x_{i-1}}}{\Delta x_{i-1}} - \frac{(\Delta x_{i-1})^2}{24} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i-0.5\Delta x_{i-1}}$$

Now, let's consider

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i = \left(\frac{\partial}{\partial x} \frac{\partial \phi}{\partial x}\right)_i = \left(\frac{\partial}{\partial x} \Phi\right)_i \quad \text{where } \Phi = \frac{\partial \phi}{\partial x}$$

More attention should be paid here since the grid size is different for two sides of node point 'i': left is Δx_{i-1} and right is Δx_i .

$$\Phi_{i+0.5\Delta x_i} = \Phi_i + (0.5\Delta x_i) \left(\frac{\partial \Phi}{\partial x}\right)_i + \frac{(0.5\Delta x_i)^2}{2} \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_i + \frac{(0.5\Delta x_i)^3}{6} \left(\frac{\partial^3 \Phi}{\partial x^3}\right)_i + \frac{(0.5\Delta x_i)^4}{24} \left(\frac{\partial^4 \Phi}{\partial x^4}\right)_i + O(\Delta x_i^5)$$

$$\Phi_{i-0.5\Delta x_{i-1}} = \Phi_i - (0.5\Delta x_{i-1}) \left(\frac{\partial \Phi}{\partial x}\right)_i + \frac{(0.5\Delta x_{i-1})^2}{2} \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_i - \frac{(0.5\Delta x_{i-1})^3}{6} \left(\frac{\partial^3 \Phi}{\partial x^3}\right)_i + \frac{(0.5\Delta x_{i-1})^4}{24} \left(\frac{\partial^4 \Phi}{\partial x^4}\right)_i + O(\Delta x_{i-1}^5)$$

Therefore,

$$\Phi_{i+0.5\Delta x_i} - \Phi_{i-0.5\Delta x_{i-1}} = (0.5\Delta x_i + 0.5\Delta x_{i-1}) \left(\frac{\partial \Phi}{\partial x}\right)_i + \left[\frac{(0.5\Delta x_i)^2}{2} - \frac{(0.5\Delta x_{i-1})^2}{2} \right] \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_i + O(\Delta x_i^3)$$

Hence,

$$\left(\frac{\partial \Phi}{\partial x}\right)_i = \frac{\Phi_{i+0.5\Delta x_i} - \Phi_{i-0.5\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} - \left[\frac{(0.5\Delta x_i)^2}{2} - \frac{(0.5\Delta x_{i-1})^2}{2} \right] \left(\frac{\partial^2 \Phi}{\partial x^2}\right)_i + O(\Delta x_i^3)$$

Plug in $\Phi = \frac{\partial \phi}{\partial x}$, we get

$$\begin{aligned}
\left(\frac{\partial}{\partial x} \frac{\partial \phi}{\partial x}\right)_i &= \frac{\left(\frac{\partial \phi}{\partial x}\right)_{i+0.5\Delta x_i} - \left(\frac{\partial \phi}{\partial x}\right)_{i-0.5\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} - \left[\frac{(\Delta x_i)^2 - (\Delta x_{i-1})^2}{4(\Delta x_i + \Delta x_{i-1})}\right] \left(\frac{\partial^2}{\partial x^2} \frac{\partial \phi}{\partial x}\right)_i + O(\Delta x_i^3) \\
&\approx \frac{1}{0.5(\Delta x_i + \Delta x_{i-1})} \left[\frac{\phi_{i+\Delta x_i} - \phi_i}{\Delta x_i} - \frac{(\Delta x_i)^2}{24} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i} - \frac{\phi_i - \phi_{i-\Delta x_{i-1}}}{\Delta x_{i-1}} + \frac{(\Delta x_{i-1})^2}{24} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i-0.5\Delta x_{i-1}} \right] - \left[\frac{(\Delta x_i)^2 - (\Delta x_{i-1})^2}{4(\Delta x_i + \Delta x_{i-1})}\right] \left(\frac{\partial^2}{\partial x^2} \frac{\partial \phi}{\partial x}\right)_i
\end{aligned}$$

Finally,

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i = \frac{\frac{\phi_{i+\Delta x_i} - \phi_i}{\Delta x_i} - \frac{\phi_i - \phi_{i-\Delta x_{i-1}}}{\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} - \frac{1}{0.5(\Delta x_i + \Delta x_{i-1})} \left[\frac{(\Delta x_i)^2}{24} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i} - \frac{(\Delta x_{i-1})^2}{24} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i-0.5\Delta x_{i-1}} \right] - \frac{\Delta x_i - \Delta x_{i-1}}{4} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i$$

In “Computational Methods For Fluid Dynamics” by Ferziger & Peric (2002), it assumes that:

$$\left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i+0.5\Delta x_i} \approx \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{i-0.5\Delta x_{i-1}} \approx \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i$$

The finally formula becomes:

$$\begin{aligned}
\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i &= \frac{\frac{\phi_{i+\Delta x_i} - \phi_i}{\Delta x_i} - \frac{\phi_i - \phi_{i-\Delta x_{i-1}}}{\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} - \frac{1}{0.5(\Delta x_i + \Delta x_{i-1})} \left[\frac{(\Delta x_i)^2 - (\Delta x_{i-1})^2}{24} \right] \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i - \frac{\Delta x_i - \Delta x_{i-1}}{4} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i \\
&= \frac{\frac{\phi_{i+\Delta x_i} - \phi_i}{\Delta x_i} - \frac{\phi_i - \phi_{i-\Delta x_{i-1}}}{\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} - \frac{\Delta x_i - \Delta x_{i-1}}{12} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i - \frac{\Delta x_i - \Delta x_{i-1}}{4} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i \\
&= \frac{\frac{\phi_{i+\Delta x_i} - \phi_i}{\Delta x_i} - \frac{\phi_i - \phi_{i-\Delta x_{i-1}}}{\Delta x_{i-1}}}{0.5(\Delta x_i + \Delta x_{i-1})} - \frac{\Delta x_i - \Delta x_{i-1}}{3} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i
\end{aligned}$$

Which is exactly shown in the book:

$$\begin{aligned}
\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i &= \frac{\phi_{i+1}(x_i - x_{i-1}) + \phi_{i-1}(x_{i+1} - x_i) - \phi_i(x_{i+1} - x_{i-1})}{\frac{1}{2}(x_{i+1} - x_{i-1})(x_{i+1} - x_i)(x_i - x_{i-1})} - \\
&\quad \frac{(x_{i+1} - x_i) - (x_i - x_{i-1})}{3} \left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + H . \quad (3.31)
\end{aligned}$$