Computational Fluid Dynamics: Lecture 4 (ME EN 6720)

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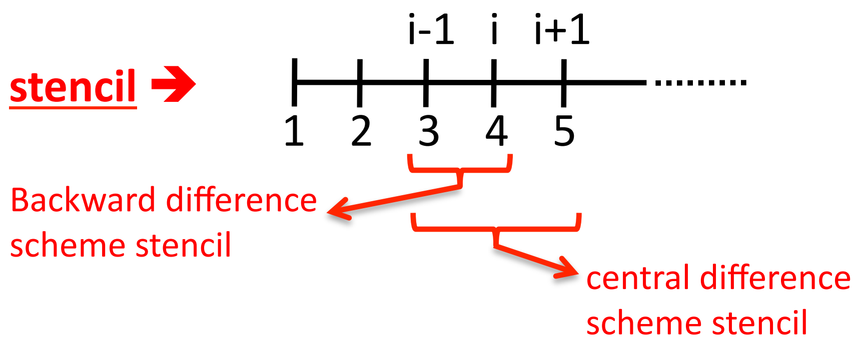
Finite difference approximations from polynomials

Other ways to develop finite difference approximations (besides Taylor Series)

- **curve fitting** through points:

  -We can fit a polynomial of degree n-1 (where n is our stencil size)



- Example: fitting a 1st order polynomial (stencil with n=2)

  -The equation for a line in point-slope form is:

$$(y - y_1) = m(x - x_1) \quad \text{where } m = \frac{y_1 - y_2}{x_1 - x_2}$$

  -For our two points we have:

$$\left.\begin{aligned}(x_1, y_1) &= (x_i, u_i)\\(x_2, y_2) &= (x_{i-1}, u_{i-1})\end{aligned}\right\} \quad \text{where } m = \frac{u_i - u_{i-1}}{x_i - x_{i-1}}$$

Finite difference approximations from polynomials

-Inserting these into our equation of a line:

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

-We want $\frac{\partial u}{\partial x}$ (or in this case $\frac{\partial y}{\partial x}$) ➔ taking 1st derivative of the above equation

$$\frac{\partial y}{\partial x} = \frac{u_i - u_{i-1}}{x_i - x_{i-1}}, \quad x_i - x_{i-1} = \Delta x_i, \quad \Rightarrow \boxed{\frac{\partial u}{\partial x} = \frac{u_i - u_{i-1}}{\Delta x_i}}$$

Our backwards difference scheme

-We could also do this with a stencil of 3 (i-1, i, i+1) and fit a 2nd order polynomial (parabola) to the points

-This is a little more difficult algebraically (3 coefficients, 3 points, 3 equations) and for our 1st derivative we can obtain

$$\frac{\partial u}{\partial x} = \frac{u_{i+1}(\Delta x_i)^2 - u_{i-1}(\Delta x_{i+1})^2 + u_i\left[(\Delta x_{i+1})^2 - (\Delta x_i)^2\right]}{\Delta x_{i+1}\Delta x_i(\Delta x_{i+1} + \Delta x_i)}$$

-Note, we haven't assumed uniform grid spacing ($\Delta x_i = \Delta x_{i-1} = \Delta x_{i+1}$) if we do ➔

$$\boxed{\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x}}$$

Our central difference scheme

Finite difference approximations from linear combinations

Finite difference schemes as linear combinations

•Another (very similar) way to look at this is as follows (ex 1st derivative):

$$\frac{\partial u}{\partial x} = \alpha u_i + \beta u_{i-1} + \gamma u_{i+1} \quad \text{(assume 1st derivative is a linear combination of 3 points)}$$

-we can examine the Taylor series approximation for each term:

$$u_{i+1} = u_i + \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!} + O(\Delta x^4)$$
$$u_i = u_i$$
$$u_{i-1} = u_i - \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!} - \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!} + O(\Delta x^4)$$

-substituting these into *

$$\frac{\partial u}{\partial x} = \alpha u_i + \beta\left[u_i - \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!} - \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!} + O(\Delta x^4)\right] +$$
$$\gamma\left[u_i + \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!} + O(\Delta x^4)\right]$$

-we can sub α, β, γ into our original linear combination to obtain our 2nd order centered difference for the 2nd derivative

Finite difference approximations from linear combinations

-grouping terms:

$$0 = u_i(\alpha+\beta+\gamma) + \left(\frac{\partial u}{\partial x}\right)_i(-1-\Delta x\beta+\Delta x\gamma) + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!}(\beta+\gamma) +$$

$$\left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!}(-\beta+\gamma) + O\left(\Delta x^4\right)$$

-now equating coefficients:

$\alpha+\beta+\gamma \quad = 0$ ⟵ should go away

what we want ⟶ $\Delta x(\gamma-\beta) \quad = 1$

$\beta+\gamma \quad = 0$ ⟵ should go away

Our leading order error term (truncation) is $= \frac{\Delta x^3}{3!}(-\beta+\gamma)$

-using our coefficients we get:

$$\alpha = 0, \quad \beta = {}^{1}\!/_{2\Delta x}, \quad \gamma = -{}^{1}\!/_{2\Delta x}$$

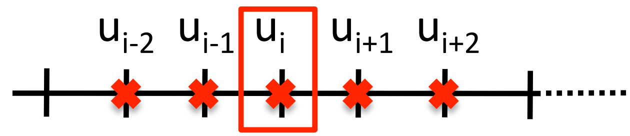
$$\Rightarrow \boxed{\frac{\partial u}{\partial x} = \frac{u_{i+1}-u_{i-1}}{2\Delta x}} \quad \text{our CDS}$$

Higher-order finite difference approximations

How can we get higher-order of accuracy from finite difference schemes?

• we can increase the accuracy of standard finite difference schemes **by expanding the stencil size**

5 point stencil ➔



• if we do a Taylor series expansion for each term, combine and cancel we can derive an estimate for the 1st derivative:

$$\left.\frac{\partial u}{\partial x}\right|_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{2\Delta x} + \mathbf{O}\left(\Delta x^4\right)$$

• and in a similar fashion we can develop an estimate for the 2nd derivative

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_i = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12\Delta x^2} + \mathbf{O}\left(\Delta x^4\right)$$

Higher-order finite difference approximations: Padé schemes

- Increasing our stencil width is not always desirable
- **One answer**: introduce $\frac{\partial u}{\partial x}$ estimates on the LHS when we do our linear combination:

$$\left.\frac{\partial u}{\partial x}\right|_{i} + \lambda \left.\frac{\partial u}{\partial x}\right|_{i-1} + \zeta \left.\frac{\partial u}{\partial x}\right|_{i+1} = \alpha u_i + \beta u_{i-1} + \gamma u_{i+1}$$

- our Taylor series for each term is:

$$u_{i+1} = u_i + \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!} + \left(\frac{\partial^4 u}{\partial x^4}\right)_i \frac{(\Delta x)^4}{4!} + \left(\frac{\partial^5 u}{\partial x^5}\right)_i \frac{(\Delta x)^5}{5!} + O\left(\Delta x^6\right)$$

$$u_i = u_i$$

$$u_{i-1} = u_i - \left(\frac{\partial u}{\partial x}\right)_i \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \frac{(\Delta x)^2}{2!} - \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^3}{3!} + \left(\frac{\partial^4 u}{\partial x^4}\right)_i \frac{(\Delta x)^4}{4!} - \left(\frac{\partial^5 u}{\partial x^5}\right)_i \frac{(\Delta x)^5}{5!} + O\left(\Delta x^6\right)$$

$$\left.\frac{\partial u}{\partial x}\right|_{i+1} = \left(\frac{\partial u}{\partial x}\right)_i + \left(\frac{\partial^2 u}{\partial x^2}\right)_i \Delta x + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^4 u}{\partial x^4}\right)_i \frac{(\Delta x)^3}{3!} + \left(\frac{\partial^5 u}{\partial x^5}\right)_i \frac{(\Delta x)^4}{4!} + O\left(\Delta x^5\right)$$

$$\left.\frac{\partial u}{\partial x}\right|_{i-1} = \left(\frac{\partial u}{\partial x}\right)_i - \left(\frac{\partial^2 u}{\partial x^2}\right)_i \Delta x + \left(\frac{\partial^3 u}{\partial x^3}\right)_i \frac{(\Delta x)^2}{2!} - \left(\frac{\partial^4 u}{\partial x^4}\right)_i \frac{(\Delta x)^3}{3!} + \left(\frac{\partial^5 u}{\partial x^5}\right)_i \frac{(\Delta x)^4}{4!} + O\left(\Delta x^5\right)$$

Higher-order finite difference approximations: Padé schemes

- substituting these in and collecting terms:

$$\left.\frac{\partial u}{\partial x}\right|_i(1+\lambda+\zeta)+\Delta x\left.\frac{\partial^2 u}{\partial x^2}\right|_i(-\lambda+\zeta)+\frac{(\Delta x)^2}{2!}\left.\frac{\partial^3 u}{\partial x^3}\right|_i(\lambda+\zeta)+\frac{(\Delta x)^3}{3!}\left.\frac{\partial^4 u}{\partial x^4}\right|_i(-\lambda+\zeta)+\frac{(\Delta x)^4}{4!}\left.\frac{\partial^5 u}{\partial x^5}\right|_i(\lambda+\zeta)+O\left(\Delta x^5\right)=$$

$$u_i(\alpha+\beta+\gamma)+\Delta x\left.\frac{\partial u}{\partial x}\right|_i(-\beta+\gamma)+\frac{(\Delta x)^2}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_i(\beta+\gamma)+\frac{(\Delta x)^3}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_i(-\beta+\gamma)+$$

$$\frac{(\Delta x)^4}{4!}\left.\frac{\partial^4 u}{\partial x^4}\right|_i(\beta+\gamma)+\frac{(\Delta x)^5}{5!}\left.\frac{\partial^5 u}{\partial x^5}\right|_i(-\beta+\gamma)+O\left(\Delta x^6\right)$$

- if we now equate coefficients:

$$\begin{aligned}
0 &= \alpha+\beta+\gamma \\
1+\lambda+\zeta &= \Delta x(-\beta+\gamma) \\
\frac{(\Delta x)^2}{2!}(\lambda+\zeta) &= \frac{(\Delta x)^3}{3!}(-\beta+\gamma) \\
\Delta x(-\lambda+\zeta) &= \frac{(\Delta x)^2}{2}(\beta+\gamma) \\
\frac{(\Delta x)^3}{3!}(-\lambda+\zeta) &= \frac{(\Delta x)^4}{4!}(\beta+\gamma)
\end{aligned}$$

Our leading order error term (truncation) is $=\left[\frac{\Delta x^4}{4!}(\lambda+\zeta)-\frac{\Delta x^5}{5!}(-\beta+\gamma)\right]\left.\frac{\partial^5 u}{\partial x^5}\right|_i$

Higher-order finite difference approximations: Padé schemes

- solving for our coefficients:

$$\alpha = 0, \quad \beta = -\tfrac{3}{4\Delta x}, \quad \gamma = \tfrac{3}{4\Delta x}, \quad \lambda = -\tfrac{1}{4}, \quad \zeta = \tfrac{1}{4}$$

- so now our scheme is:

$$\boxed{\left.\frac{\partial u}{\partial x}\right|_{i-1} + 4\left.\frac{\partial u}{\partial x}\right|_{i} + \left.\frac{\partial u}{\partial x}\right|_{i+1} = \tfrac{3}{\Delta x}\left(u_{i+1} - u_{i-1}\right)} + O\left(\Delta x^4\right)$$

- this is usually referred to as a 4^{th}-order compact finite difference scheme or a 4^{th}-order Padé scheme

- another way to derive this is to find the highest order interpolant between three points ➔ Padé schemes are can be thought of as fitting splines

finite difference approximations for mixed derivatives

What about mixed partial derivatives?

- mixed derivatives can occur is we transform the equations of motion into different coordinate systems (e.g. spherical coordinates) or map between reference frames
- one option: $$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)$$
- we can use a central difference for $\frac{\partial u}{\partial x}$: $$\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathbf{O}\left(\Delta x^2\right)$$
- we now have $$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial y}\left(\frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathbf{O}\left(\Delta x^2\right)\right)$$
- if we also use central differences in y

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{1}{2\Delta y}\left(\frac{u_{i+1,j+1} - u_{i-1,j+1}}{2\Delta x} - \frac{u_{i+1,j-1} - u_{i-1,j-1}}{2\Delta x}\right) + \mathbf{O}\left(\Delta x^2\right) + \mathbf{O}\left(\Delta y^2\right)$$

- or $$\frac{\partial^2 u}{\partial x \partial y} = \frac{u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1}}{4\Delta x \Delta y} + \mathbf{O}\left[\Delta x^2, \Delta y^2\right]$$