Assignment 02

AERO 455 - CFD for Aerospace Applications

Instructor: Dr. Ziad Boutanios
Concordia University - MIAE

Given: 27th February 2022
Due: 5pm EST on 12th March 2022
No extensions

1 Finite Difference Schemes (45 points)

In lecture 05, slides 10 to 28, you have seen how to derive a finite difference schemes for the first and second derivatives for arbitrary orders of accuracy and different stencils. The procedure was also generalized.

1.1 Second-order first derivative schemes

1.1.1 The forward three-point scheme

(10 points)
Following the same procedure given in the lecture derive a *second-order forward* finite difference scheme for the first derivative using a three-point stencil. You will need to set up Taylor expansions for the solution variable q at points x_{i+1} and x_{i+2}.

1.1.2 The backward three-point scheme

(10 points)
Repeat the same procedure and derive a *second-order backward* finite difference scheme for the first derivative using a three-point stencil. You will need to set up Taylor expansions for the solution variable q at points x_{i-1} and x_{i-2}.

1.2 First-order second derivative schemes

1.2.1 The forward three-point scheme

(10 points)
Following the same procedure derive a *first-order forward* finite difference scheme for the second derivative using a three-point stencil. You will need to set up Taylor expansions for the solution variable q at points x_{i+1} and x_{i+2}.

1.2.2 The backward three-point scheme

(10 points)
Repeat the same procedure and derive a *first-order backward* finite difference scheme for the second derivative using a three-point stencil. You will need to set up Taylor expansions for the solution variable q at points x_{i-1} and x_{i-2}.

1.3 Scheme validity

(5 points)
How do you know whether your schemes are correct? Is there a quick check you can perform to find out? If so, show how for all four schemes derived.

2 Advanced Concepts (55 points)

All questions below relate to lecture 07.

2.1 Accuracy vs. Stability

Answer the following questions.

1. What is the typical trade-off between accuracy and stability for finite difference schemes? (2 points)

2. What is the Godunov theorem and which scheme introduced in the Godunov finite-volume method does it embody? (5 points)

3. What is the Iserles barrier theorem and which natural conclusion can be drawn from it for upwind schemes? (5 points)

4. What is the total variation of a variable q? Provide mathematical expressions of total variation of a continuous variable $q(x, t)$ and its discrete version q_i^t. (5 points)

5. What is a total variation diminishing scheme? Give an example of a scheme that is total variation diminishing, and an example of a scheme that is not. (5 points)

6. What is the MUSCL scheme, what is the motivation behind it and what is the order of accuracy of its original version as introduced by van Leer? (5 points)

2.2 Error analysis

Answer the following questions.

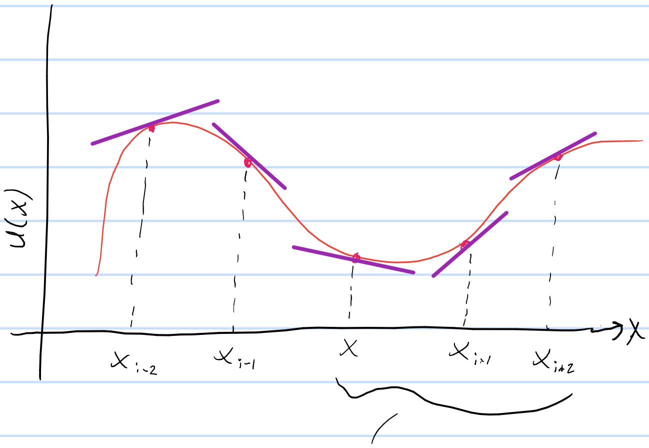
1. What is well-posedness of an initial value problem? Provide a mathematical expression of it. (3 points)
2. What is consistency of a finite difference scheme? Provide a mathematical expression of it. (3 points)
3. What does the convergence property of a finite difference scheme tell us? (2 points)
4. What are the sources of numerical error? (2 points)
5. What is the roundoff error? (2 points)

2.3 Stability analysis and time stepping

Answer the following questions.

1. Is the Neumann stability analysis linear or non-linear? (2 points)
2. What is a transient explicit scheme? (2 points)
3. What is a transient implicit scheme? (2 points)
4. What is the physical meaning of the Courant number? Give a couple of examples using linear advection and linear diffusion. (10 points)

1.1.1) We are using a 3-Point Stencil. We want to use 2^{nd} order forward finite difference.



We will need to use all these points for a 3-Point stencil forward finite difference scheme

We need to find the Taylor Series expansions for each point

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} + \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(\Delta x^4) \quad (1)$$
$$u_{i+2} = u_i + 2\Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{(2\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} + \frac{(2\Delta x)^3}{3!}\Big|_{x_i} + O(\Delta x^4) \quad (2)$$

Solving (1) & (2) for $\frac{\partial u}{\partial x}$

$$\frac{\partial u}{\partial x}\Big|_{x_i} = \left(\frac{u_{i+1}-u_i}{\Delta x}\right) - \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(\Delta x^3) \quad (3)$$

$$\frac{\partial u}{\partial x}\Big|_{x_i} = \left(\frac{u_{i+2}-u_i}{2\Delta x}\right) - \frac{2\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{(2\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3} + O(\Delta x^3) \quad (4)$$

Now we need to combine them to make them 2^{nd} order. We want the following.

$\frac{\partial u}{\partial x}\Big|_{x_i} = a(3) + b(4)$ Note we want LHS to remain constant. As such we know
$a + b = 1$

We also want to cancel out the $O(\Delta x)$ term leaving just $O(\Delta x^2)$ term
$\frac{a}{2} + b = 0$

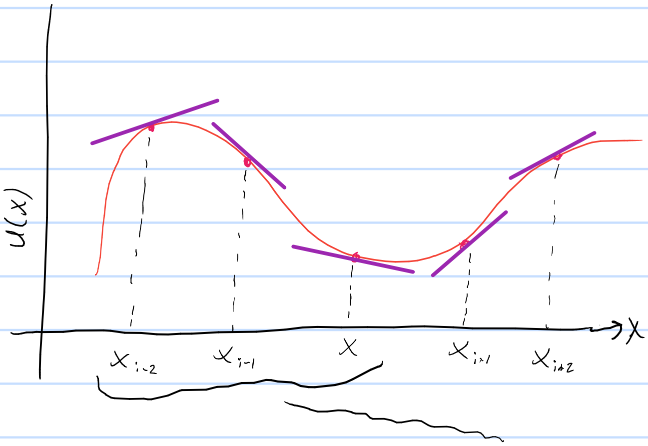
We can solve this system of equations

$$\left[\begin{array}{cc|c} 1 & 1 & 1 \\ \frac{1}{2} & 1 & 0 \end{array}\right] \xrightarrow{-\frac{1}{2}R_2 + R_1 \to R_1} \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{array}\right] \xrightarrow{2R_2 \to R_2} \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 0 & 1 & -1 \end{array}\right] \xrightarrow{-R_2 + R_1 \to R_1} \left[\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & -1 \end{array}\right] \qquad \begin{array}{l} a = 2 \\ b = -1 \end{array}$$

$$\frac{\partial u}{\partial x}\Big|_{x_i} = 2\left(\frac{u_{i+1}-u_i}{\Delta x}\right) - \cancel{2\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i}} - \frac{2\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} - \left(\frac{u_{i+2}-u_i}{2\Delta x}\right) + \cancel{\frac{2\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i}} + \cancel{\frac{(2\Delta x)^2}{3!}}\frac{\partial^3 u}{\partial x^3}$$

$$\frac{\partial u}{\partial x}\Big|_{x_i} = \frac{4u_{i+1}-4u_i}{2\Delta x} - \frac{(u_{i+2}-u_i)}{2\Delta x} = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + O(\Delta x^2)$$

1.1.2) We are using a 3-Point Stencil. We want to use 2^{nd} order backward finite difference.



We will need to use all these points for a 3-Point stencil forward finite difference scheme

We need to find the Taylor Series expansions for each point

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(x^4) \quad (5)$$
$$u_{i-2} = u_i - 2\Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{(2\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{(2\Delta x)^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(x^4) \quad 6$$

Solving 5 & 6 for $\frac{\partial u}{\partial x}\Big|_{x_i}$

$$\frac{\partial u}{\partial x} = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3} + O(x^3) \quad (7)$$
$$\frac{\partial u}{\partial x} = \frac{u_i - u_{i-2}}{2\Delta x} + \frac{2\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{(2\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3} + O(\Delta x^3) \quad (8)$$

Now we need to combine them to make them 2^{nd} order. We want the following.

$\frac{\partial u}{\partial x}\Big|_{x_i} = a(7) + b(8)$, Note we want LHS to remain constant. As such we know $a + b = 1$

We also want to cancel out the $O(\Delta x)$ term leaving just $O(\Delta x^2)$ term
$\frac{a}{2} + b = 0$

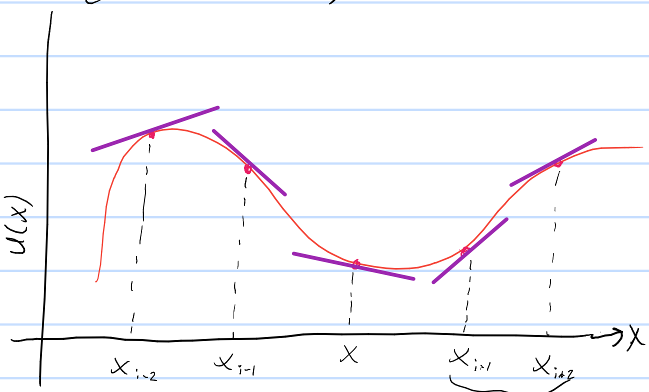
We can solve this system of equations

$$\left[\begin{array}{cc|c} 1 & 1 & 1 \\ \frac{1}{2} & 1 & 0 \end{array}\right] \xrightarrow{-\frac{1}{2}R_2 + R_1 \to R_1} \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{array}\right] \xrightarrow{2R_2 \to R_2} \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 0 & 1 & -1 \end{array}\right] \xrightarrow{-R_2 + R_1 \to R_1} \left[\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & -1 \end{array}\right] \quad \begin{array}{l} a = 2 \\ b = -1 \end{array}$$

$$\frac{\partial u}{\partial x} = 2\left(\frac{u_i - u_{i-1}}{\Delta x} + \cancel{\frac{2\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i}} - \cancel{\frac{2\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3}}\right) - \left(\frac{u_i - u_{i-2}}{2\Delta x} - \cancel{\frac{2\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i}} + \cancel{\frac{(2\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3}}\right)$$

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

1.2.1) find a 1^{st}-Order forward finite difference scheme for a second order derivative using a 3 point Stencil



Use these points

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} + \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(\Delta x^4) \quad (9)$$

$$u_{i+2} = u_i + 2\Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{(2\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} + \frac{(2\Delta x)^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(\Delta x^4) \quad (10)$$

Solving 9 & 10 for $\frac{\partial^2 u}{\partial x^2}$

$$-\frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} = u_i - u_{i+1} + \Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + O(\Delta x^3)$$

$$\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} = \frac{2(u_{i+1}-u_i)}{\Delta x^2} - \frac{2}{\Delta x}\frac{\partial u}{\partial x}\Big|_{x_i} - \frac{2\Delta x}{6}\partial^3 u/\partial x^3\Big|_{x_i} + O(\Delta x) \quad (11)$$

$$-2\Delta x^2\, \partial^2 u/\partial x^2\Big|_{x_i} = u_i - u_{i+2} + 2\Delta x\, \partial u/\partial x\Big|_{x_i} + O(\Delta x^3)$$

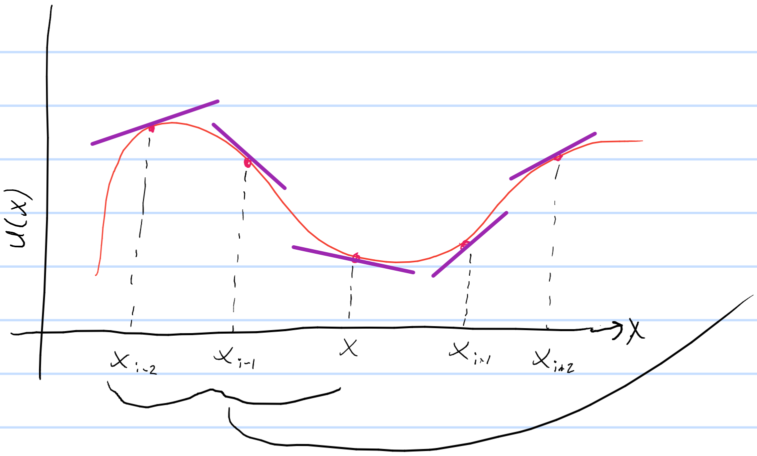
$$\partial^2 u/\partial x^2\Big|_{x_i} = \frac{(u_{i+2}-u_i)}{2\Delta x^2} - \frac{1}{\Delta x}\frac{\partial u}{\partial x}\Big|_{x_i} + O(\Delta x) \quad (12)$$

$\partial^2 u/\partial x^2|_{x_i} = a(11) + b(12)$ We want to keep the LHS, so $a+b=1$. Also we want to remove other derivatives so $\frac{a}{2}+b=0$. This is the same as 1.1, so $b=2$, $a=-1$

$$\frac{\partial^2 u}{\partial x^2} = -\frac{2(u_{i+1}-u_i)}{\Delta x^2} + \cancel{\frac{2}{\Delta x}\frac{\partial u}{\partial x}\Big|_{x_i}} + \frac{\cancel{2}(u_{i+2}-u_i)}{\cancel{2}\Delta x^2} - \cancel{\frac{2}{\Delta x}\frac{\partial u}{\partial x}\Big|_{x_i}}$$

$$\partial^2 u/\partial x^2 = \frac{-2u_{i+1} + 2u_i + u_{i+2} - u_i}{\Delta x^2} = \underline{\frac{u_i - 2u_{i+2} + u_{i+2}}{\Delta x^2}} + O(\Delta x)$$

1.2.1) find a 1st-Order forward finite difference scheme for a second order derivative using a 3 point Stencil



use these points

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(x^4) \quad (13)$$
$$u_{i-2} = u_i - 2\Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + \frac{(2\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2}\Big|_{x_i} - \frac{(2\Delta x)^3}{3!}\frac{\partial^3 u}{\partial x^3}\Big|_{x_i} + O(x^4) \quad (14)$$

Solve 13 & 14 for $\partial^2 u / \partial x^2 |_{x_i}$

$$-\Delta x^2/2 \; \partial^2 u/\partial x^2 = u_i - u_{i-1} - \Delta x \, \partial u/\partial x|_{x_i} + O(x^3)$$
$$\partial^2 u/\partial x^2|_{x_i} = \frac{2(u_{i-1}-u_i)}{\Delta x^2} + \frac{2}{\Delta x}\,\partial u/\partial x|_{x_i} + O(\Delta x) \quad (15)$$

$$-2\Delta x^2 \, \partial^2 u/\partial x^2 = u_i - u_{i-2} - 2\Delta x \frac{\partial u}{\partial x}\Big|_{x_i} + O(\Delta x^3)$$
$$\partial^2 u/\partial x^2|_{x_i} = \frac{u_{i-2}-u_i}{2\Delta x^2} + \frac{1}{\Delta x}\frac{\partial u}{\partial x}\Big|_{x_i} + O(\Delta x)$$

We find the coefficients using the same method as previously

$$\partial^2 u/\partial x^2 = \frac{-2(u_{i-1}-u_i)}{\Delta x^2} - \cancel{\frac{2}{\Delta x}\frac{\partial u}{\partial x}} + \frac{\cancel{2}(u_{i-2}-u_i)}{\cancel{2}\Delta x^2} + \cancel{\frac{2}{\Delta x}\frac{\partial u}{\partial x}} + O(\Delta x)$$

$$\partial^2 u/\partial x^2 = \frac{2u_i - 2u_{i-1} + u_{i-2} - u_i}{\Delta x^2} + O(\Delta x) = \frac{u_i - 2u_{i-1} + u_{i-2}}{\Delta x^2} + O(\Delta x)$$

1.1.3) In order to validate the schemes you can look at the coefficients of the point coordinates. The sum of these must be 0. This is true for each derived scheme.

2.1.1) When using higher order schemes, the stability of the solution often suffers. This means the solution can oscillate, especially when discontinuities such as shock waves appear. However, the higher stability that comes with lower order schemes comes with a cost in accuracy.

2.1.2) Godunov's theorem states the following (taken from the class notes). "Linear numerical schemes for solving PDE's, having the property of not generating new extrema (monotone scheme), can be at most first-order accurate. This theorem applies to the monotone scheme.

2.1.3) Isersles barrier theorem states the following (taken from the class notes). "The maximum order of accuracy O(max) of a stable semi-discrete advection scheme with p upwind points and d downwind points is O(max)=min(p+d, 2p, 2d+2). This theorem helps realize that upwind biased schemes can often outperform pure upwind schemes in order to attain stble higher order accuracy since the upwinding can help stabilize the high-order part of the scheme, and in return the higher-order part can help reduce the upwinding diffusion.

2.1.4) The total varration of a variable helps measure the oscillations of a variable. It can be described continuously or discretely as follows

$$TV(q(x,t)) = \int_a^b \left| \frac{\partial q}{\partial x} \right| dx$$

$$TV(q_i^t) = \sum_{i=1}^{n} |q_{i+1}^t - q_i^t$$

2.1.5) for a scheme to be a total varration diminishing scheme it must satisfy

$$TV(q^{t+1}) \leq TV(q^t)$$

The first-order upwind differencing scheme is TVD while the second order central differencing scheme is not,

2.1.6) The MUSCL scheme is a finite volume method that can provide stable and accurate results, even for flows with discontinuities. This scheme is based on replacing the piecewise constant approximation of Godunovs method by reconstructed states derived from the solution at the previous time step. The van Leer version works with a order of accuracy of 2.

2.2.1) The stability of the initial value problem of a PDE is called well-posedness. An initial value problem is well-posed for a 1st order PDE if for any time $T \geq 0$ there is a constant C_T such that any solution $q(x,t)$ satisfies

$$\|q(x,t)\|^2 \leq C_T \|q(x,0)\|^2 \text{ for } 0 \leq t \leq T$$

2.2.2) Consistency describes how well a scheme describes a PDE it represents. A scheme is consistent with a PDE if the error between the scheme and PDE does not grow or is reduced as the time step & space intervals are refined. Mathematically this is described as.

$$Pq - P_{\Delta x}^{\Delta t} q \rightarrow O(\Delta x^r, \Delta t^s) \text{ as } \Delta x, \Delta t \rightarrow 0$$

2.2.3) Convergence tells us how constistent and stable the numerical solution of a PDE is. Basically, it tells us whether the solution will be stable, and if so how accurate the final solution will be once it stabilizes. The Lax-Friedrich theorem states that "A consistent finite difference scheme for a PDE for which the initial value problem is well-posed, will be convergent if and only if it is stable."

2.2.4) The sources of numerical error include the discretization error, and the round-off error. The discretization error is the error that stems from taking the numerical error to a problem, and is described by the order of accuracy of the scheme used. The round off error stems fom computers having to round off a number to a certain significant figure due to floating point approximation

2.2.5) The roundoff error occurs as the compter must round off numbers at a certain significant figure due to floating point approximation. For example, with a binary32 (single precision) number the machine error ranges from 2^-2 to 5.96e-8.

2.3.1) The Neumann stability analysis approach is a linear approach.

2.3.2) The transient explicit time stepping scheme describes a scheme where the solution values are only from the current and previous time levels in the scheme.

2.3.3) The transient implicit time stepping scheme describes a scheme where the solution values can include values from the next time level.

2.3.4) The physical meaning of the Courant number describes the ratio of the velocity that particles pass through a cell compared to the rate the information is able to pass through a cell. Basically, if the Courant number is above 1, a particle would be able to pass through a cell in the mesh faster than a timestep, and thus the solution will not be stable. Some examples include

$Cd = ud/ug < 0.5$ for linear diffusion flow. This indicate that the diffusive transport veloity cannot exceed half the speed at which information crosses an entire cell.

$Ca = \alpha/ug$ for linear advection. Again the physical transport velocity cannot exceed the grid numerical transport velocity. It is always true that the courant number must be less than one for all explicit schemes to be stable.