Computational Fluid Dynamics: Lecture 3 (ME EN 6720)

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Conservation Equations

<u>summing up our equations:</u>

- conservation of mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0$$

- conservation of momentum

$$\rho \frac{\partial\left(u_i\right)}{\partial t} + \rho u_j \frac{\partial\left(u_i\right)}{\partial x_j} = \frac{\partial\left(\tau_{ij}\right)}{\partial x_j} - \frac{\partial\left(P\right)}{\partial x_i} + \rho g_i \qquad \left\{ \begin{aligned} \tau_{ij} &= 2\mu D_{ij} - \tfrac{2}{3}\mu\delta_{ij}\frac{\partial u_k}{\partial x_k} \\ D_{ij} &= \tfrac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \end{aligned} \right.$$

- conservation of energy

$$-\frac{\partial}{\partial x_j}\left[\rho u_j\left(e + \tfrac{1}{2}u_i u_i\right)\right] - \frac{\partial q_i}{\partial x_i} - \frac{\partial\left(P u_i\right)}{\partial x_j} + \frac{\partial\left(\tau_{ij} u_i\right)}{\partial x_j} = \frac{\partial}{\partial t}\left[\rho\left(e + \tfrac{1}{2}u_i u_i\right)\right]$$

- conservation of scalar concentration

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x_i}\left(\phi u_i\right) = r_g - r_d$$

Conservation of Momentum

- An equivalent index-notation form of the momentum equation is:

$$\frac{\partial\left(\rho u_i\right)}{\partial t}+\frac{\partial\left(\rho u_i u_j\right)}{\partial x_j}=\frac{\partial\left(\tau_{ij}\right)}{\partial x_j}-\frac{\partial\left(P\right)}{\partial x_i}+\rho g_i$$

- Forms of the Momentum Equation
  - **Differential** vs. **Integral**
  - **Eulerian** vs. **Lagrangian**
  - **Conservative** vs. **Non conservative**

- For the integral equations, **conservative** means all terms are written in the form of a divergence (e.g.,)
- For Finite Volume formulations, using a conservative form instead of the non conservative form guarantees the velocity field will be divergent free (a requirement for realizeability) $\nabla \cdot \vec{V}$

Systems of Equations

- **<u>Last Notes on Equations</u>:**

- In Lecture 2, we mentioned a plus of the conservative form (flux form) of the equations.
- All equations (mass, momentum, energy, scalar) have a divergence term for the integral form (e.g.,$\nabla \cdot \vec{V}$) or flux term for the differential form of the equations
- in 1-D

  - ρu flux of mass
  - $\rho u u$ flux of momentum
  - $\rho\left(e+\dfrac{u^2}{2}\right)u$ flux of total energy (E)

- We can summarize the equations for these fluxes into one compact form:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}=\mathbf{G}$$

$$\underbrace{\mathbf{U}=\begin{bmatrix}\rho\\ \rho u\\ \rho E\end{bmatrix}}_{\text{Solution Vector}} \qquad \underbrace{\mathbf{F}=\begin{bmatrix}\rho u\\ \left(\rho u^2+P-\tau_{xx}\right)\\ \left(Eu+Pu-k\dfrac{\partial T}{\partial x}-u\tau_{xx}\right)\end{bmatrix}}_{\text{Flux Vector}} \qquad \underbrace{\mathbf{G}=\begin{bmatrix}0\\ \rho f_x\\ \left(\rho\left(uf_x\right)+\rho\dot{q}\right)\end{bmatrix}}_{\text{Source Term Vector}}$$

- Note, the form described above could be termed the "strong" conservative form since all of the terms appear inside the spatial derivatives.
- Practically, this indicates that all of our equations are a form of the same PDE.

Process of CFD

As discussed in previous lectures our general process in CFD is:

Determine physics ➔ determine appropriate PDE ➔ **Discretize**

Discretization techniques:

finite differences

- use differential form of the equations
- construct approximate difference operators

e.g. $$\frac{\partial \phi}{\partial x} \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

finite volumes

- use integral form of the equations
- approximate fluxes at "volume" interfaces and gradients discretely

variational method

- leave differential operators unchanged
- approximate the solution space:

$$\phi(x) = \sum_{i=1}^{N} \underbrace{a_i}_{\text{expansion coefficients}} \underbrace{\Psi_i}_{\text{trial functions}}(x)$$

- 2 types of trial functions

-local ➔ finite elements

-Global ➔ spectral methods

Finite difference approximations

<u>Finite Difference Approximations</u> (Ferziger chapter 3)

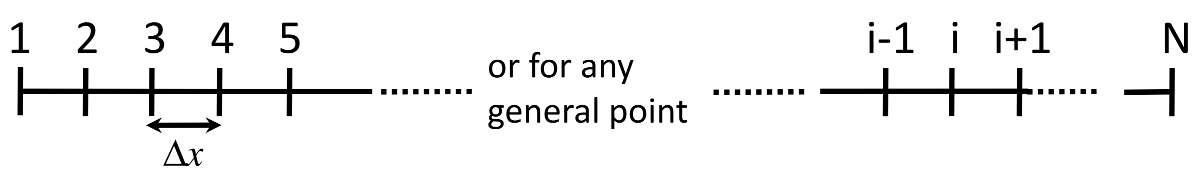
- goal: build a <u>discrete analog</u> to the continuous problem

<u>Discretization</u> ➔ <u>Finite Difference Equation</u> (FDE)

Represent variables at points

- Algebraic representation of PDE
- Solve using Linear algebra

- space (1-D):

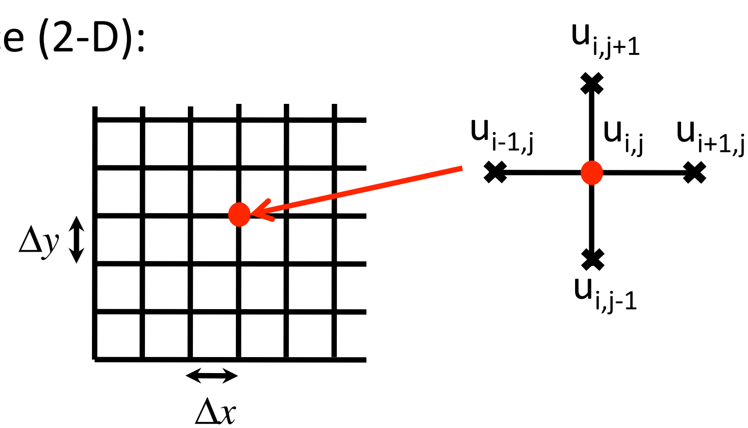


where $\Delta x = \dfrac{1}{N-1}$

and $x_i = (i-1)\Delta x$

for i=1,2,...,N

- space (2-D):



<u>definitions:</u>

$u_{i,j} = u(x_o, y_o)$

$u_{i+1,j} = u(x_o + \Delta x, y_o)$

$u_{i,j-1} = u(x_o, y_o - \Delta y)$

and so forth...

Finite difference approximations

• Recall the definition of a derivative:

for a function $u(x,y)$ at a point $(x_o,y_o) \Rightarrow \dfrac{\partial u}{\partial x} = \lim\limits_{\Delta x \to 0} \dfrac{u(x_o+\Delta x, y_o) - u(x_o,y_o)}{\Delta x}$

-for a continuous *u* (continuum assumption for fluids), the above will be "reasonable" for a "sufficiently" small Δ*x*

• we can develop a more formal definition using a Taylor series expansion of *u*

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j}\Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^3}{3!} + \cdots + \underbrace{\text{H.O.T}}_{\text{Higher-Order Terms}}$$

This is mathematically exact if [one or both]:

1) Δ*x*→0
2) The number of terms is infinite and the series converges

• from the Taylor series we can quickly come up with an approximation for $\left(\dfrac{\partial u}{\partial x}\right)_{i,j}$ by solving for it:

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} - \underbrace{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\frac{\Delta x}{2!} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\frac{(\Delta x)^2}{3!} + \cdots + \text{H.O.T}}_{\mathbf{O}(\Delta x)}$$

[note: **O**(Δ*x*) means "on the order of" Δ*x* which is the order of error of the approximation

Finite difference approximations

Finite Difference Approximations for 1st derivatives

- using the above index notation and a Taylor series approximation

$$* \quad u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{3!} + \mathrm{H.O.T}$$

we can get:

$$\boxed{\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + \mathbf{O}(\Delta x)}$$

Forward difference approximation

(because we expanded "forward" in space)

- we can do the same thing backwards:

$$** \quad u_{i-1,j} = u_{i,j} - \left(\frac{\partial u}{\partial x}\right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2!} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{3!} + \mathrm{H.O.T}$$

➔

$$\boxed{\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + \mathbf{O}(\Delta x)}$$

Backwards difference approximation

Finite difference approximations

- if we subtract ** from * and rearrange we can get:

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

<u>centered</u> **difference approximation**

<u>Finite difference approximations for 2nd derivatives</u>

- if we add * and ** and rearrange we can get:

$$\boxed{\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} \underbrace{- \left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j} \frac{(\Delta x)^2}{12} + \text{H.O.T}}_{\mathbf{O}\left(\Delta x^2\right)}}$$

- This is a 2nd order-centered difference scheme for the 2nd derivative. It is one of the most popular schemes for 2nd derivatives in FD

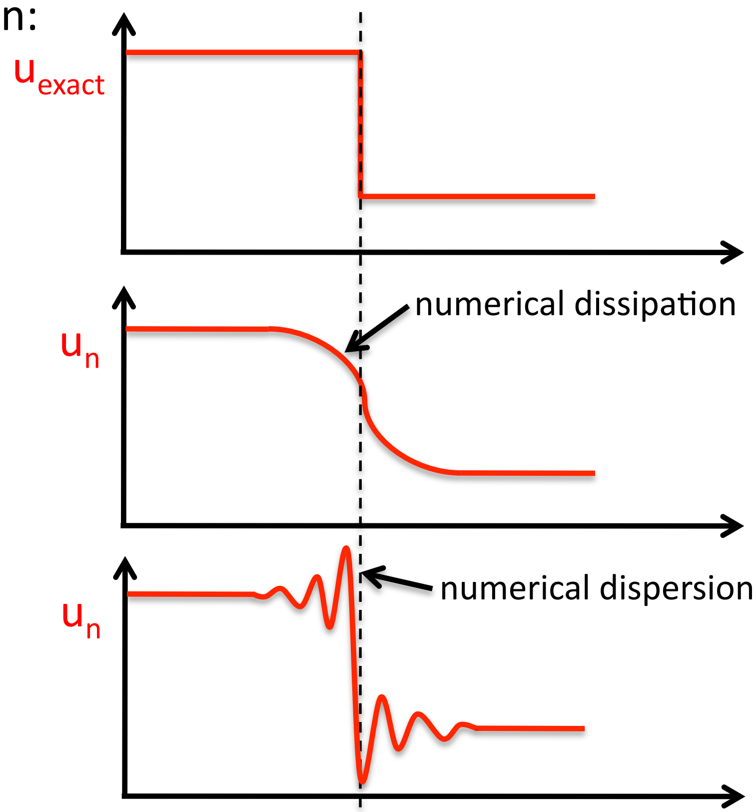
Truncation Error

Effect of Truncation Error (TE) on Solutions

• Two types of errors result from truncation of Taylor series for FD schemes such as those discussed above (and for other types of techniques we haven't talked about).

- **Numerical dissipation** and **Numerical dispersion**

• given a solution:



Why do we get one or the other?

Choice of FD scheme
• CDS → dispersion
• FDS → dissipation

Numerical dissipation is a direct result of **even** derivatives in the leading term of the TE

Numerical dispersion is a direct result of **odd** derivatives in the leading term of the TE

Accuracy of F.D. schemes

A few notes about the accuracy of numerical schemes

- a definition: If the T.E. of a scheme behaves like ~(Δx)^q then the scheme is called q-order

- **How can we compute the error?** (two measures for now)

a) Error Norms:

continuous: $\varepsilon_P = \left[\int_0^1 \left| u_e - u_n \right|^P \right]^{\frac{1}{P}}$

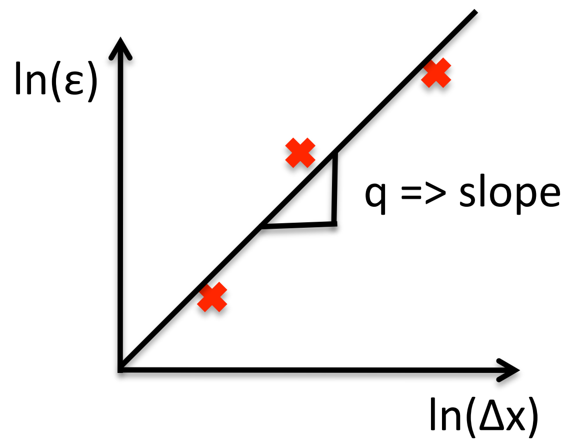
discrete: $\varepsilon_P = \left[\frac{1}{N} \sum_{i=1}^{N} \left| u_{e,i} - u_{n,i} \right|^P \right]^{\frac{1}{P}}$

u_e is the exact solution

u_n is the numerical solution

b) Relative error: $\varepsilon_r = \left| \frac{u_e - u_n}{u_e} \right|$

How can we use the error to verify the order of a scheme?



Discretized equations

Example of a discretized equation

- 1-D heat equation: $$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

- two different FDE representations of this are:

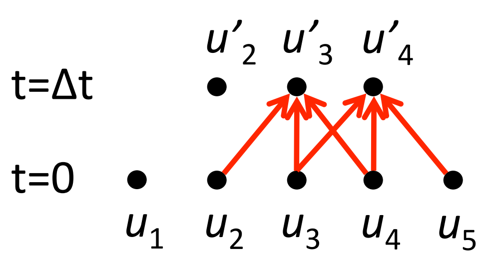
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{1}{(\Delta x)^2}\left[u_{i+1}^n - 2u_i^n + u_{i-1}^n\right] \qquad \text{(explicit)}$$

and

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{1}{(\Delta x)^2}\left[u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right] \qquad \text{(implicit)}$$

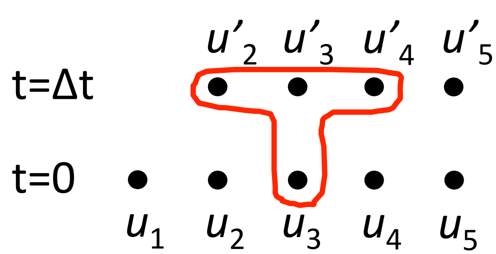
- graphically we can represent the points used by these two schemes as:

explicit



For example to get u'_3 and u'_4

implicit



For example to get u'_3

Truncation error in FDEs

- We can use our FDE equation above (explicit one) to look at the total TE of our solution
  - 1st we expand each *u* as a Taylor series about u^n_i:

$$u_i^{n+1} = u_i^n + \left(\frac{\partial u}{\partial t}\right)_i^n \Delta t + \left(\frac{\partial^2 u}{\partial t^2}\right)_i^n \frac{(\Delta t)^2}{2!} + \mathbf{O}\left(\Delta t^3\right)$$

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

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

  - substituting these into the FDE:

$$\frac{1}{\cancel{\Delta t}}\left[\cancel{u_i^n} + \left(\frac{\partial u}{\partial t}\right)_i^n \cancel{\Delta t} + \left(\frac{\partial^2 u}{\partial t^2}\right)_i^n \frac{(\Delta t)^{\cancel{2}}}{2!} + \mathbf{O}\left(\Delta t^{\cancelto{2}{3}}\right) - \cancel{u_i^n}\right] =$$

$$\frac{\alpha}{\cancel{\Delta x^2}}\left[\cancel{u_i^n} + \cancel{\left(\frac{\partial u}{\partial x}\right)_i^n \Delta x} + \left(\frac{\partial^2 u}{\partial x^2}\right)_i^n \frac{(\cancel{\Delta x})^2}{2!} + \cancel{\left(\frac{\partial^3 u}{\partial x^3}\right)_i^n \frac{(\Delta x)^3}{3!}} + \mathbf{O}\left(\Delta x^{\cancelto{2}{4}}\right) - \cancel{2u_i^n} + \cancel{u_i^n} - \cancel{\left(\frac{\partial u}{\partial x}\right)_i^n \Delta x} + \left(\frac{\partial^2 u}{\partial x^2}\right)_i^n \frac{(\cancel{\Delta x})^2}{2!} - \cancel{\left(\frac{\partial^3 u}{\partial x^3}\right)_i^n \frac{(\Delta x)^3}{3!}} + \mathbf{O}\left(\Delta x^{\cancelto{2}{4}}\right)\right]$$

  - cancelling terms (\\): $\left(\frac{\partial u}{\partial t}\right)_i^n + \left(\frac{\partial^2 u}{\partial t^2}\right)_i^n \frac{\Delta t}{2} + \mathbf{O}\left(\Delta t^2\right) = \alpha\left[\left(\frac{\partial^2 u}{\partial x^2}\right)_i^n + \mathbf{O}\left(\Delta x^2\right)\right]$
  - recovering the PDE: $\underbrace{\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}}_{\text{PDE}} + \underbrace{\mathbf{O}\left[\Delta t, \Delta x^2\right]}_{\text{TE}}$ ➔ **PDE + TE = FDE**

- this can be done for any FDE. Mixing schemes doesn't change the TE for individual terms