Sharif University of Technology
School of Mechanical Engineering
Center of Excellence in Energy Conversion

Computational Fluid Dynamics

Analysis of Methods

M.T. Manzari

Model Equations

- **To understand the performance of the numerical methods when applied to flow problems, we first examine them on simple model equations that represent various features of the Navier-Stokes equations.**
- **These are:**
  - **First order linear wave equation:** $\boxed{\dfrac{\partial u}{\partial t} + a\dfrac{\partial u}{\partial x} = 0 \quad (a > 0)}$
  - **Transient Diffusion:** $\boxed{\dfrac{\partial u}{\partial t} - \alpha\dfrac{\partial^2 u}{\partial x^2} = 0 \quad (\alpha > 0)}$
  - **Laplace Equation:** $\boxed{\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = 0}$
  - **Burger's Inviscid Equation:** $\boxed{\dfrac{\partial u}{\partial t} + u\dfrac{\partial u}{\partial x} = 0}$
  - **Burger's Viscous Equation:** $\boxed{\dfrac{\partial u}{\partial t} + u\dfrac{\partial u}{\partial x} = \mu\dfrac{\partial^2 u}{\partial x^2}}$

Solution in Wave Space

- Let us consider the linear convection equation with a periodic boundary condition (bi-convection problem) and $u(x,0) = u_0(x)$ as initial condition:

$$\boxed{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0}$$

- In this case, the waveform travels through one boundary and re-appears at the other boundary, eventually returning to its initial position. This process continues forever without any change in the shape of the solution.
- Preserving the shape of the initial condition $u_0(x)$ can be a difficult challenge for a numerical problem.
- Another type of boundary condition for the linear convection equation is defined by prescribing the value of $u(x)$ on one boundary. This corresponds to a wave entering the domain through this <u>inflow</u> boundary. No boundary condition is given at the opposite side, the <u>outflow</u> boundary.

Solution in Wave Space…

- **Now, let us consider an initial condition (** $0 \le x \le 2\pi$ **)**

$$\boxed{u(x,0) = f(0)\, e^{i\kappa x}}$$

- **Where** $f(0)$ **is a <u>complex constant</u> and** κ **is the wave-number.**

  In order to satisfy the periodic boundary condition, κ **must be <u>integer</u>. The solution for our bi-convection problem is:**

$$\boxed{u(x,t) = f(t)\, e^{i\kappa x}}$$

- **Substituting this solution into the equation gives:**

$$\boxed{\frac{df}{dt} = -ia\kappa f \quad \rightarrow \quad f(t) = f(0)\, e^{-ia\kappa t}}$$

- **Therefore,**

$$\boxed{u(x,t) = f(0)\, e^{i\kappa(x-at)} = f(0)\, e^{i(\kappa x - \omega t)}}$$

- **Where the <u>frequency</u>** ω **is defined as**

$$\boxed{\omega = \kappa a} \qquad \textbf{(dispersion relation)}$$

Solution in Wave Space…

- The dispersion relation $\omega = \kappa a$ is a characteristic of wave propagation in a <u>non-dispersive</u> medium. This means that the phase speed is the same for all wave-numbers.
- **We will see that most numerical methods introduce some dispersion, that is, waves with different wave-numbers travel at different speeds.**
- **An arbitrary initial waveform can be described by its M modes as ($\kappa_1 \le \kappa_2 \le \cdots \le \kappa_M$)**

$$\boxed{u(x,0) = \sum_{m=1}^{M} f_m(0) \exp(i\kappa_m x)}$$

- **Then, the solution becomes:**

$$\boxed{u(x,t) = \sum_{m=1}^{M} f_m(0) \exp\left[i\kappa_m \left(x - at\right)\right]}$$

- **Dispersion and dissipation resulting from a numerical approximation will cause the shape of the solution to change from that of the original waveform.**

Solution in Wave Space…

- **Now, let us consider the diffusion:**

$$\boxed{\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} \qquad 0 \le x \le \pi \qquad BC:\; u(0) = u_a \quad , \quad u(\pi) = u_b}$$

- **The steady-state solution of this is** $h(x) = u_a + \frac{x}{\pi}(u_b - u_a)$

- **Let the initial condition be (** κ must be integer to satisfy BC**)**

$$\boxed{u(x,0) = \sum_{m=1}^{M} f_m(0)\, Sin(\kappa_m x) + h(x)}$$

- **Substituting this into the equation, we find that**

$$\boxed{\frac{df_m}{dt} = -\kappa_m \nu\, f_m \quad \rightarrow \quad f_m(t) = f_m(0)\exp(-\kappa_m^2 \nu\, t)}$$

- **Therefore,**

$$\boxed{u(x,t) = \sum_{m=1}^{M} f_m(0)\exp(-\kappa_m^2 \nu\, t)\sin(\kappa_m x) + h(x)}$$

- **Note that <u>high wave-number</u> components (large κ_m) of the solution <u>decay more rapidly</u> than low wave-number components, consistent with the physics of diffusion.**

Fourier Error Analysis

- **This method can be used to evaluate the accuracy of a FDM formulation.**
- **An arbitrary periodic function can be decomposed into its Fourier components, which are in the form $\exp(i\kappa x)$, where κ is the wave number.**
- **It is of interest to examine how well a given FD operator approximates derivatives of $\exp(i\kappa x)$. The exact first derivative of $\exp(i\kappa x)$ is:**

$$\boxed{\frac{\partial e^{i\kappa x}}{\partial x} = i\kappa\, e^{i\kappa x}}$$

- **Applying a 2nd order centered difference operator to $u_j = \exp(i\kappa x_j)$ with $x_j = j\,\Delta x$, we get:**

$$\begin{aligned}
(\delta_x u)_j &= \frac{u_{j+1} - u_j}{2\Delta x} = \frac{\exp[i\kappa\,\Delta x\,(j+1)] - \exp[i\kappa\,\Delta x\,(j-1)]}{2\Delta x} \\
&= \frac{\exp(i\kappa\, x_j)}{2\Delta x}\{[\cos(\kappa\Delta x) + i\sin(\kappa\Delta x)] - [\cos(\kappa\Delta x) - i\sin(\kappa\Delta x)]\} \\
&= i\frac{\sin(\kappa\Delta x)}{\Delta x}\exp(i\kappa\, x_j) = i\kappa^* \exp(i\kappa\, x_j)
\end{aligned}$$

Fourier Error Analysis...

- **Note that the degree to which the modified wave number κ^* approximates the actual wave number is a measure of the <u>accuracy</u> of the approximation.**
- **Note also that**

$$\boxed{\kappa^* \equiv \frac{\sin \kappa \Delta x}{\Delta x} = \kappa - \frac{\kappa^3 \Delta x^2}{6} + \ldots = O(\Delta x^2)}$$

- **When applied to the linear convection equation, we have**

$$\boxed{\frac{df}{dt} = -ia\kappa^* f \quad \rightarrow \quad f(t) = f(0)e^{-ia\kappa^* t}}$$

- **And the solution becomes:**

$$\boxed{u_{numerical}(x,t) = f(0)\exp i\kappa(x - a^* t)}$$

- **Where a^* is the numerical (or modified) phase speed:**

$$\boxed{\frac{a^*}{a} = \frac{\kappa^*}{\kappa}}$$

- **Note that since $a^* / a \leq 1$, the numerical method introduces dispersion.**

Fourier Error Analysis…

- **In general, FD operators can be written as**

$$\boxed{\left(\delta_x\right)_j = \overbrace{\left(\delta_x^a\right)_j}^{anti-symmetric} + \overbrace{\left(\delta_x^s\right)_j}^{symmetric}}$$

- **For example, using nodes $j-3$ to $j+3$, then**

$$\left(\delta_x^a u\right)_j = \frac{1}{\Delta x}\left[a_1(u_{j+1} - u_{j-1}) + a_2(u_{j+2} - u_{j-2}) + a_3(u_{j+3} - u_{j-3})\right]$$

$$\left(\delta_x^S u\right)_j = \frac{1}{\Delta x}\left[d_0 + d_1(u_{j+1} + u_{j-1}) + d_2(u_{j+2} + u_{j-2}) + d_3(u_{j+3} + u_{j-3})\right]$$

- **The corresponding modified wave number is**

$$i\kappa^* = \frac{1}{\Delta x}\left[d_0 + 2(d_1 \cos\kappa\Delta x + d_2 \cos 2\kappa\Delta x + d_3 \cos 3\kappa\Delta x)\right.$$
$$\left. + 2i(a_1 \sin\kappa\Delta x + a_2 \sin 2\kappa\Delta x + a_3 sin 3\kappa\Delta x)\right]$$

- **When the FD operator is <u>anti-symmetric</u> (centered), the modified wave-number is <u>purely real</u>.**
- **When the FD operator is <u>symmetric</u>, the modified wave-number is <u>complex</u>, with the imaginary component being entirely error.**

Fourier Error Analysis…

- The real part of the modified wave-number determines the error in the phase speed ($a^* / a \neq 1$).
- The imaginary part of the modified wave-number leads to an error in the amplitude of the solution (Note: $df / dt = -ia\kappa^* f$).

- The number of points per wave-length (PPW) by which a given wave is resolved is given by $2\pi / \kappa\Delta x$.

- The resolving efficiency of a scheme can be expressed in terms of PPW required to produce errors below a specified level.
- For our 2nd order FD scheme, we need 80 PPW to produce an error in the phase speed of less than 0.1 percent.

Stability, Consistency and Convergence

- Let us start with the following definitions:

(Discretization error)= (Analytical solution)-(Ideal Numerical Solution)

(Truncation error)= (PD Equation)-(FD Equation)

(Discretization error)= (Truncation error)+(Errors due to BC)

(Round off error)= (Real Numerical solution)-(Ideal Numerical Solution)

- A numerical scheme is called STABLE if errors from any source (round off, truncation, mistakes) are not permitted to grow as the calculations proceeds.

Error	Stability
If the overall round off error grows	Strong instability
If the overall round off error does not grow	Strong stability
If a single general round off error grows	Weak Instability
If a single general round off error does not grow	Weak stability

- A method is CONVERGENT if the solution to the FD equation approaches the true solution to the PDE as the mesh is refined.

Fourier Stability Analysis…

- A difference method is called consistent if its truncation error approaches zero as its mesh size goes to zero.
- This is not true for all methods. For example, DuFort-Frankel method for solving the heat conduction equations is

$$\frac{1}{2\Delta t}\left(u_j^{n+1}-u_j^n\right)=\frac{\alpha}{\Delta x^2}\left(u_{j+1}^n-u_j^{n+1}-u_j^{n-1}+u_{j-1}^n\right)$$

- Whose truncation error is:

$$T.E.=\frac{\alpha}{12}\frac{\partial^4 u}{\partial x^4}\Delta x^2-\alpha\frac{\partial^2 u}{\partial t^2}\left(\frac{\Delta t}{\Delta x}\right)^2-\frac{1}{6}\frac{\partial^3 u}{\partial t^3}\Delta t^2+\ldots$$

- Now, note that if $\lim\limits_{\Delta t,\Delta x\to 0}\left(\Delta t/\Delta x\right)\neq 0$, then, DuFort-Frankel method in fact solves the following hyperbolic equation!

$$\frac{\partial u}{\partial t}+\alpha\left(\frac{\Delta t}{\Delta x}\right)^2\frac{\partial^2 u}{\partial t^2}=\alpha\frac{\partial^2 u}{\partial x^2}$$

Lax Equivalence Theorem

Given a properly posed initial value (linear) problem and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence.

Fourier or von Neumann Stability Analysis

- This method investigates the growth of the error of a difference equation. Let us show this by an example.
- Consider a simple explicit method for solving the heat conduction equation:

$$\boxed{\begin{array}{l} \dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \dfrac{\alpha}{\Delta x^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) \\ or \\ u_j^{n+1} = u_j^n + \dfrac{\alpha\,\Delta t}{\Delta x^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) \end{array}}$$

- Note that

$$\boxed{\overset{\text{Numerical solution}}{N} = \overset{\text{Exact solution}}{D} + \overset{\text{error}}{\varepsilon}}$$

- Substituting this in our FD equation, we get

$$\boxed{\dfrac{D_j^{n+1} + \varepsilon_j^{n+1} - D_j^n - \varepsilon_j^n}{\Delta t} = \dfrac{\alpha}{\Delta x^2}\left(D_{j+1}^n + \varepsilon_{j+1}^n - 2D_j^n - 2\varepsilon_j^n + D_{j-1}^n + \varepsilon_{j-1}^n\right)}$$

Fourier Stability Analysis…

- Since the exact solution satisfies the difference equation, then we have

$$\boxed{\frac{\varepsilon_j^{n+1}-\varepsilon_j^n}{\Delta t}=\frac{\alpha}{\Delta x^2}\left(\varepsilon_{j+1}^n-2\varepsilon_j^n+\varepsilon_{j-1}^n\right)}$$

- Now, express the error as

$$\boxed{\varepsilon(x,t)=\sum_m b_m(t)e^{i\kappa_m x} \quad with \quad \kappa_m=2\pi m/2L,\;\; m=0,1,\ldots,M=\frac{L}{\Delta x}}$$

- Or we can write (a is complex and κ_m is real)

$$\boxed{\varepsilon_m(x,t)=e^{at}e^{i\kappa_m x}}$$

- Substituting this form in our equation gives:

$$\boxed{e^{a(t+\Delta t)}e^{i\kappa_m x}-e^{at}e^{i\kappa_m x}=\frac{\overbrace{\alpha\Delta t}^{r}}{\Delta x^2}\left[e^{at}e^{i\kappa_m(x+\Delta x)}-2e^{at}e^{i\kappa_m x}+e^{at}e^{i\kappa_m(x-\Delta x)}\right]}$$

- The amplification factor G becomes: ($\beta=\kappa_m\Delta x$)

$$\boxed{G\equiv\frac{\varepsilon_j^{n+1}}{\varepsilon_j^n}=e^{a\Delta t}=1+2r(\cos\beta-1)=1-4r\sin^2(\beta/2)}$$

Fourier Stability Analysis…

- Thus, the error will not grow if

$$\boxed{|G| \equiv \left|\frac{\varepsilon_j^{n+1}}{\varepsilon_j^n}\right| = \left|1 - 4r\sin^2(\beta/2)\right| \le 1 \quad \rightarrow \quad r \le \frac{1}{2}}$$

- Since, G is <u>purely real</u> then the method has no phase angle.
- As another example, we can consider the Lax method for solving the first order wave equation:

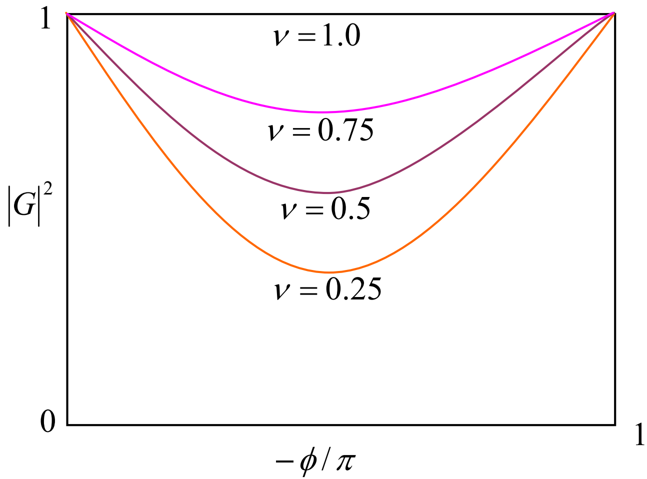
$$\boxed{\frac{1}{\Delta t}\left(u_j^{n+1} - \frac{u_{j+1}^n + u_{j-1}^n}{2}\right) + c\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) = 0}$$

- In this case: $(\nu = c\,\Delta t / \Delta x)$

$$\boxed{\begin{aligned} G &= \cos\beta - i\,\nu\sin\beta = |G|e^{i\phi} \\ &= \sqrt{\cos^2\beta + \nu^2\sin^2\beta}\ \exp\left[i\ \tan^{-1}(-\nu\tan\beta)\right] \end{aligned}}$$

- Here, ϕ is the phase angle.

Fourier Stability Analysis…



Fourier Stability Analysis…

- The Fourier method can be also applied to a system of equations. Consider:

$$\boxed{\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0}$$

- This can be linearized as

$$\boxed{\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{U}}{\partial x} = 0 \qquad \textit{with} \qquad \mathbf{A} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}}}$$

- Using the Lax method, we get

$$\boxed{\mathbf{U}_j^{n+1} = \frac{1}{2}\left(\mathbf{I} + \frac{\Delta t}{\Delta x}\mathbf{A}^n\right)\mathbf{U}_{j-1}^n + \frac{1}{2}\left(\mathbf{I} - \frac{\Delta t}{\Delta x}\mathbf{A}^n\right)\mathbf{U}_{j+1}^n}$$

- The amplification factor becomes

$$\boxed{\mathbf{G} = \mathbf{I}\cos\beta - i\tfrac{\Delta t}{\Delta x}\mathbf{A}\sin\beta}$$

- For a stable solution, the largest eigen-value of $\mathbf{G}$ must obey: ($\lambda_{\max}$ is the largest eigen-value of $\mathbf{A}$)

$$\boxed{\left|\rho_{\max}\right| \le 1 \qquad \rightarrow \qquad \left|\lambda_{\max}\frac{\Delta t}{\Delta x}\right| \le 1}$$