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Investigation of Optimal Numerical Methods for High Reynolds Number Unsteady Simulations

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8th SoCal Symposium on Flow Physics

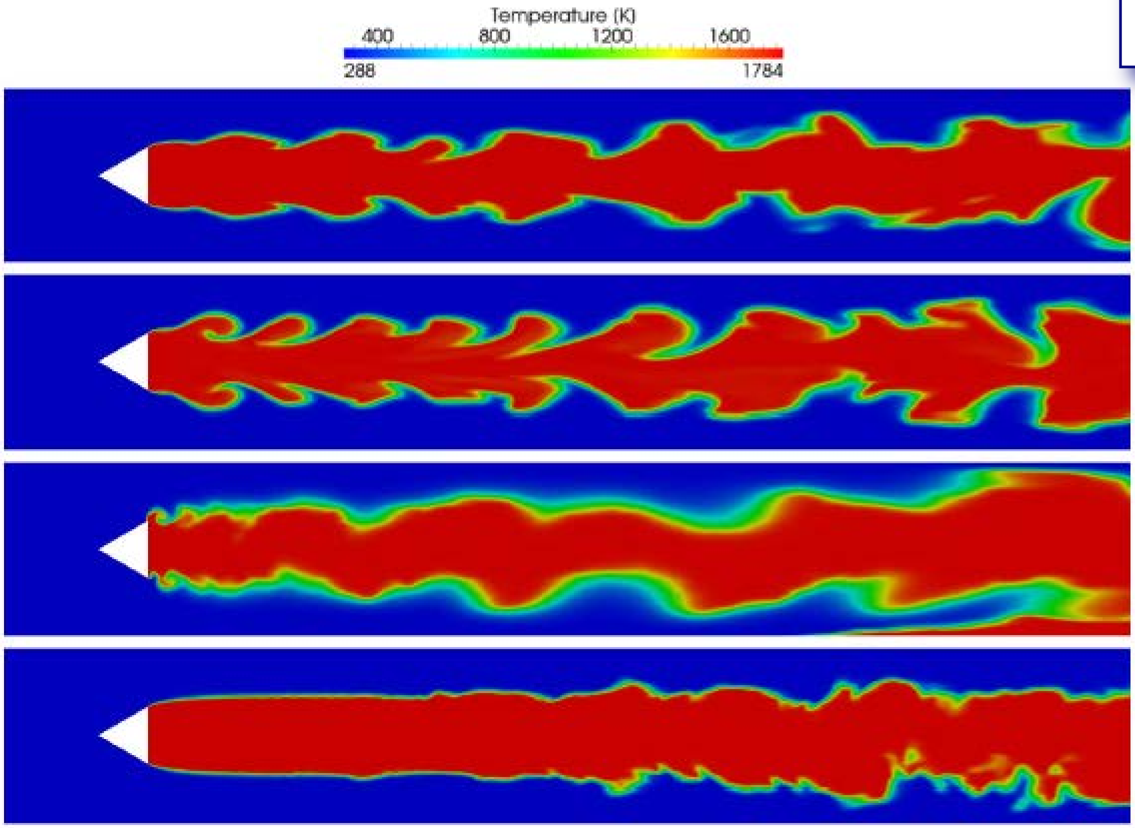
April 12, 2014

UCLA
ENERGY &
PROPULSION
RESEARCH
LABORATORY

Motivation: Large-Eddy Simulation (LES) Challenges

Instantaneous Temperature

Algorithm Comparisons
- identical subgrid modeling
- differences reside in numerics



CHARLES (Stanford)

LESLIE3D (Georgia Tech)

OpenFOAM (OpenCFD)

Fluent (Ansys)

Ref: 2013 - Cocks, Sankaran, Soteriou, “Is LES of reacting flow predictive? Part 1: Impact of Numerics”

Need to determine BEST discretization scheme for Reacting LES

Approach

- Investigate dissipation and dispersion characteristics of schemes
    - tied to solution accuracy
    - use Von Neumann Stability Analysis

- Schemes to investigate:
    - Standard Collocated Grid
    - Standard Staggered Grid
    - Kinetic Energy Preserving
        - Collocated & Staggered

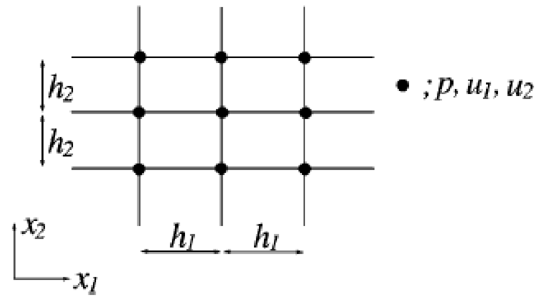


FIG. 1. Regular grid system.

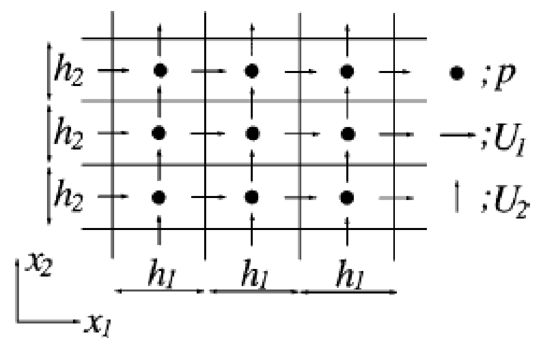


FIG. 2. Staggered grid system.

Von Neumann Analysis

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = 0 \quad \text{1D Euler Eqns} \quad \rightarrow \quad \frac{\partial Q}{\partial t} + A\frac{\partial Q}{\partial x} = 0 \quad \text{with}\, A = \partial E / \partial Q$$

Eigenvalues of the amplification matrix specify growth factor and phase errors.

$$Q^{n+1} = GQ^n$$

Staggered Grid Scheme/ Quasi-Linear Form

$$\Gamma_{ce}\left(\frac{\partial Q_{pT}}{\partial t} + \frac{\partial Q_u}{\partial t}\right)_i + \Gamma_m\left(\frac{\partial Q_{pT}}{\partial t} + \frac{\partial Q_u}{\partial t}\right)_{i+1/2} + A_{ce}\left(\frac{\partial Q_{pT}}{\partial x} + \frac{\partial Q_u}{\partial x}\right)_i + A_m\left(\frac{\partial Q_{pT}}{\partial x} + \frac{\partial Q_u}{\partial x}\right)_{i+1/2} = 0$$

$$Q_{pT} = \begin{pmatrix} p \\ 0 \\ T \end{pmatrix}$$

Continuity/Energy

Momentum

$$Q_u = \begin{pmatrix} 0 \\ u \\ 0 \end{pmatrix}$$

Growth Factor

$$||g_i||$$

Phase Error

$$\frac{\phi}{\phi_{exact}} = \frac{-\tan^{-1}\{Imag(g_i)/Re(g_i)\}}{CFL \times \beta}$$

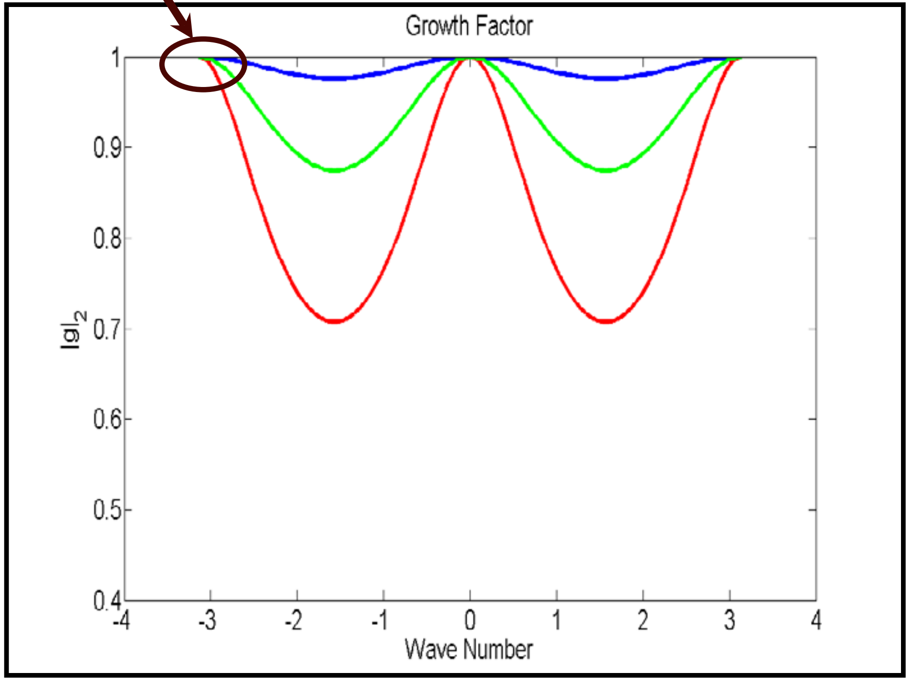
Stability Analysis

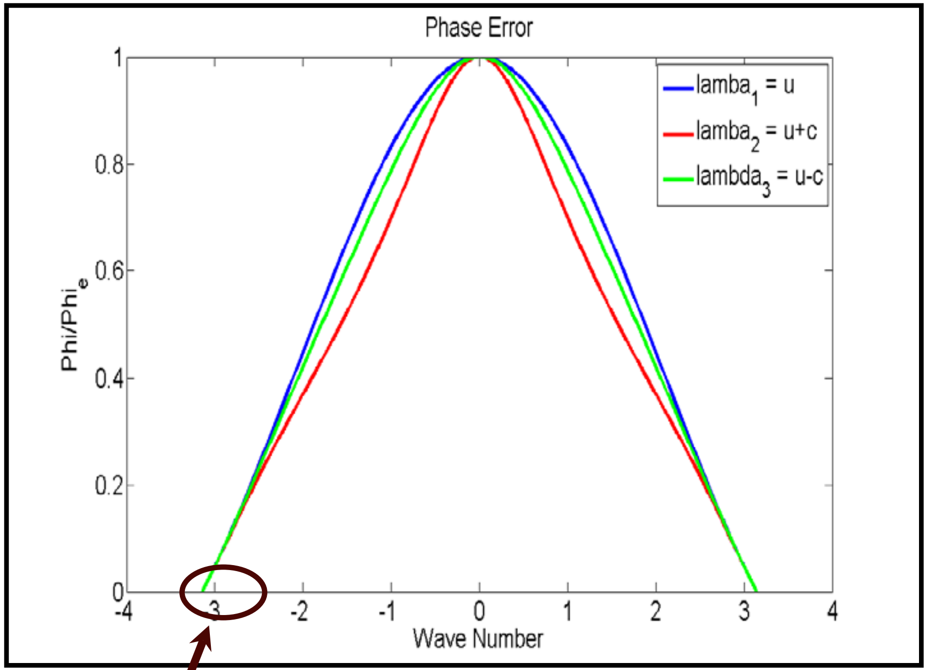
Euler Implicit Scheme (Collocated Grid)

$$CFL = 1 = \frac{\lambda_2 \Delta t}{\Delta x}$$

$$Mach = 0.28$$

No damping of highest modes





No convection of highest modes

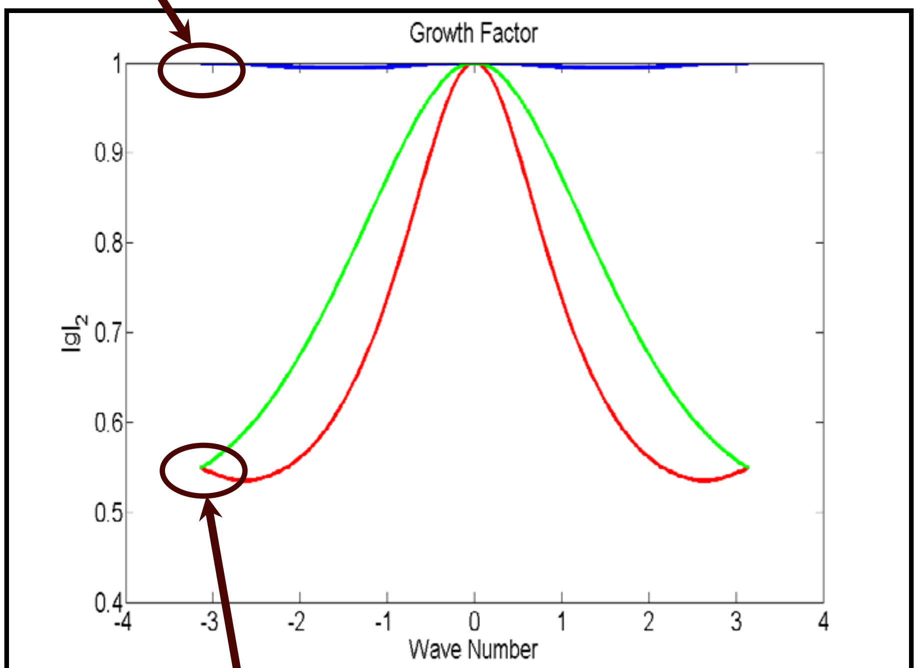
Stability Analysis

Euler Implicit Scheme (Staggered Grid)

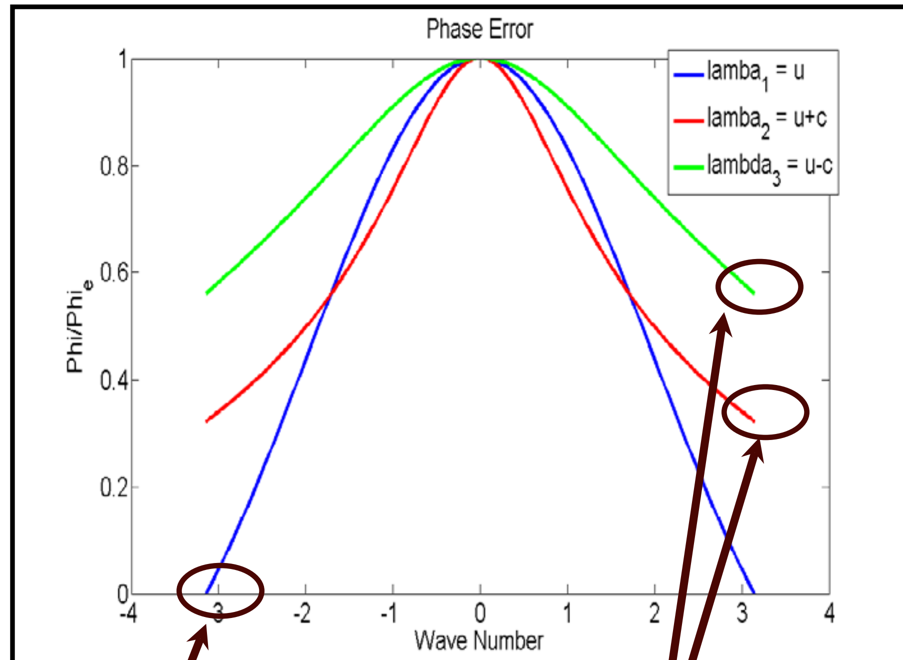
$$CFL = 1 = \frac{\lambda_2 \Delta t}{\Delta x}$$

$$Mach = 0.28$$

No damping of PARTICLE WAVE's highest modes



Highest ACOUSTIC modes damped

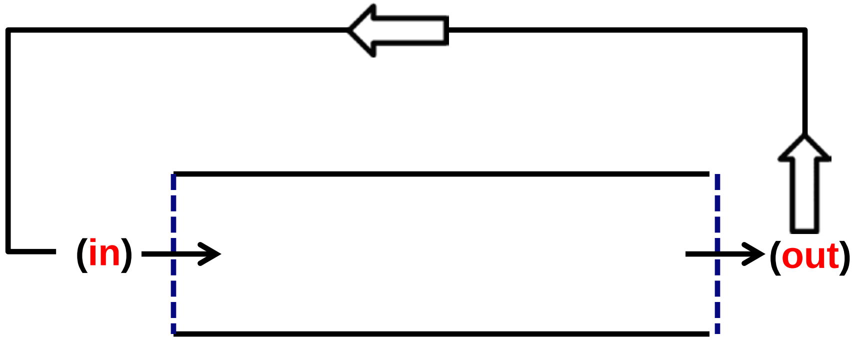


No convection of PARTICLE WAVE's highest modes

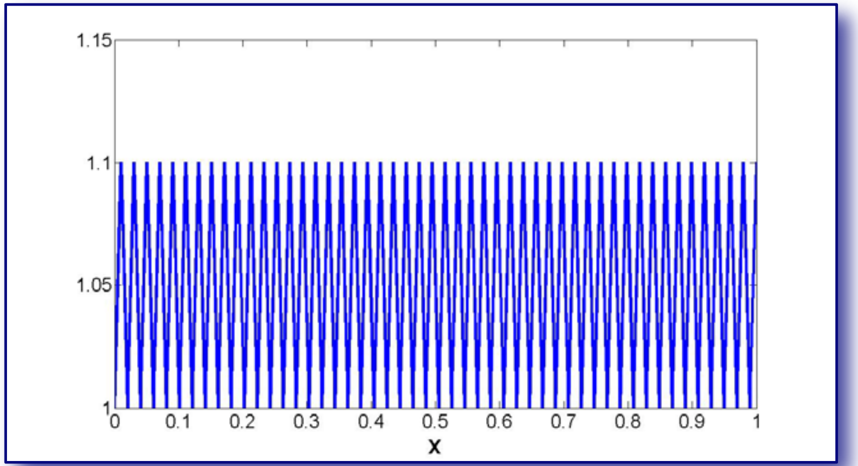
Slow convection of highest ACOUSTIC modes

Test Cases

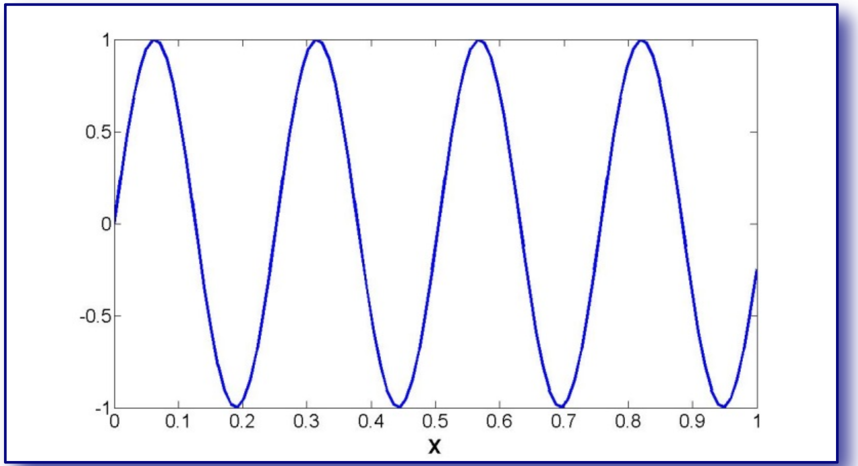
1D Duct
– Periodic BC's



Saw-tooth i.c.



Sinusoidal i.c.

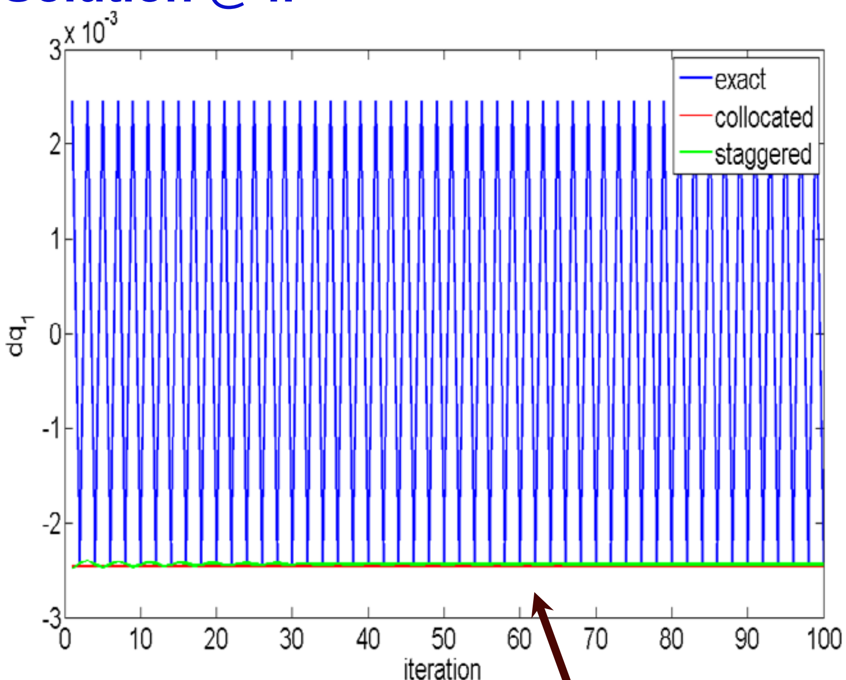


Particle Wave High Frequency Behavior

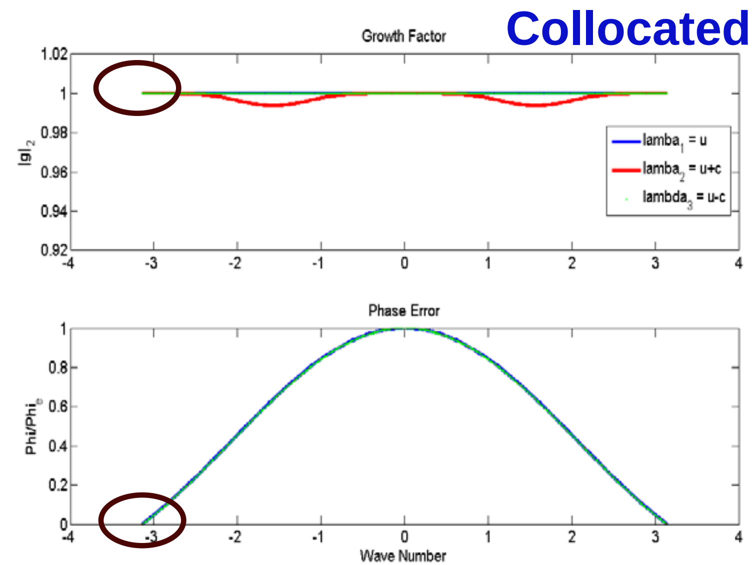
Runge Kutta Scheme

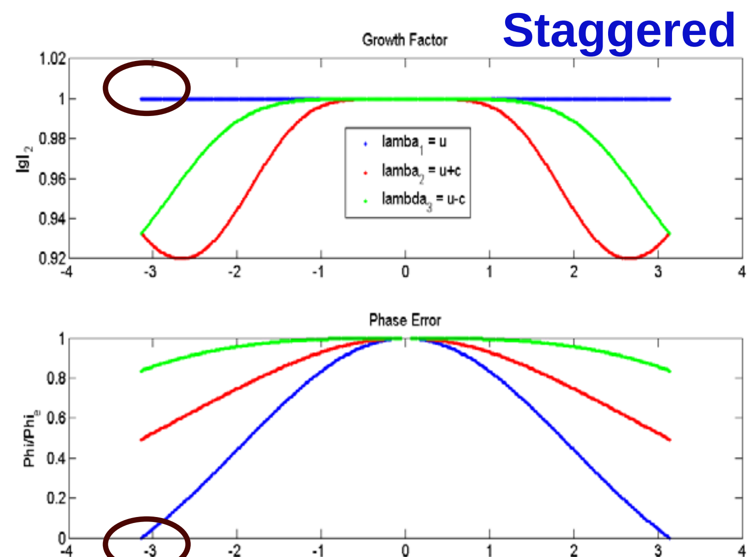
$$CFL = 1 = \frac{\lambda_2 \Delta t}{\Delta x}$$
$$Mach = 0.28$$
$$distrub = 0.01\%$$

Solution @ i:



Collocated AND Staggered:
- stationary & un-damped





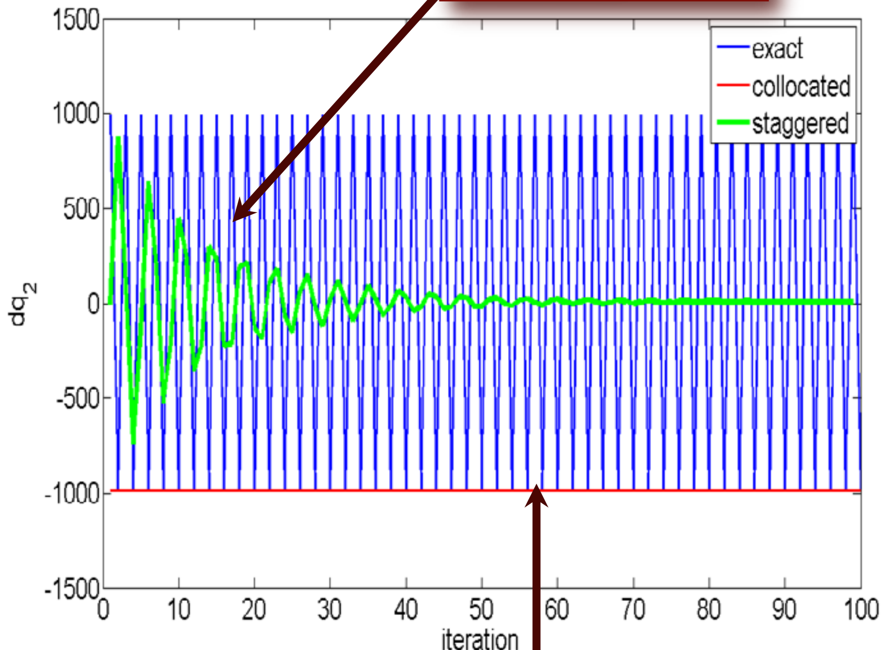
Acoustic Wave High Frequency Behavior

Runge Kutta Scheme

$$CFL = 1 = \frac{\lambda_2 \Delta t}{\Delta x}$$
$$Mach = 0.28$$
$$distrub = 0.01\%$$

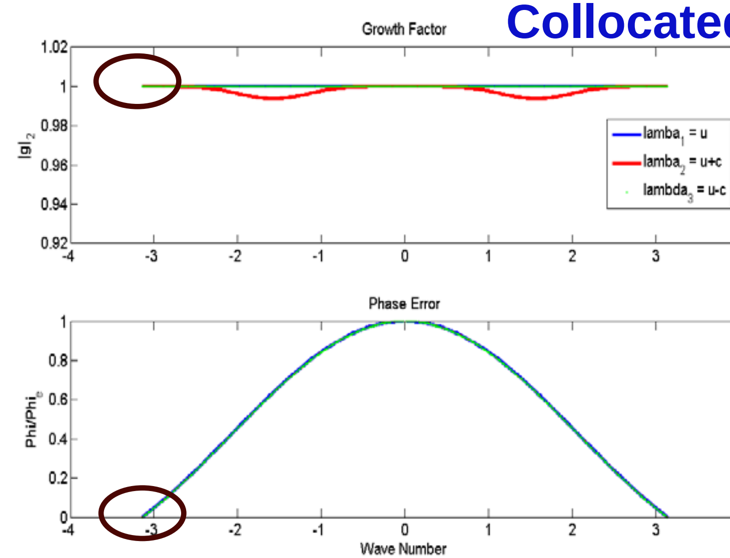
Staggered:
- DAMPED with mild phase error

Solution @ i:

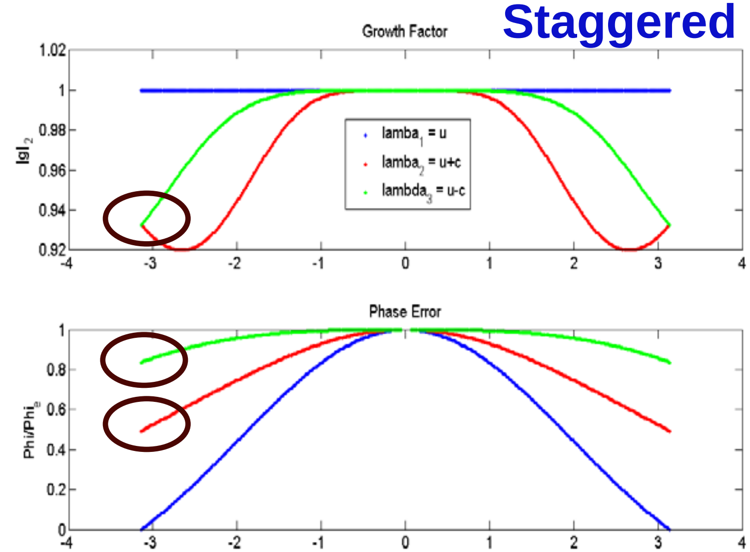


Collocated:
- stationary & un-damped

Collocated



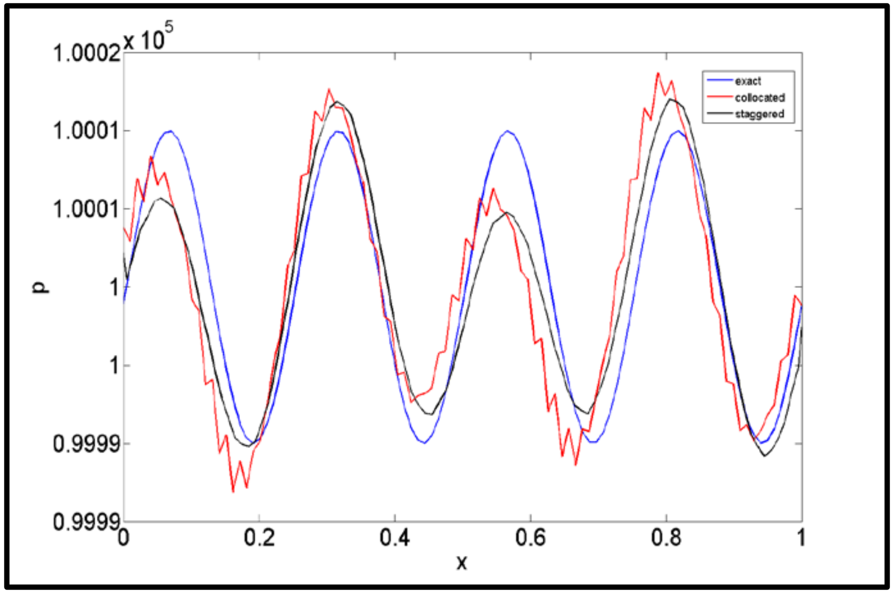
Staggered



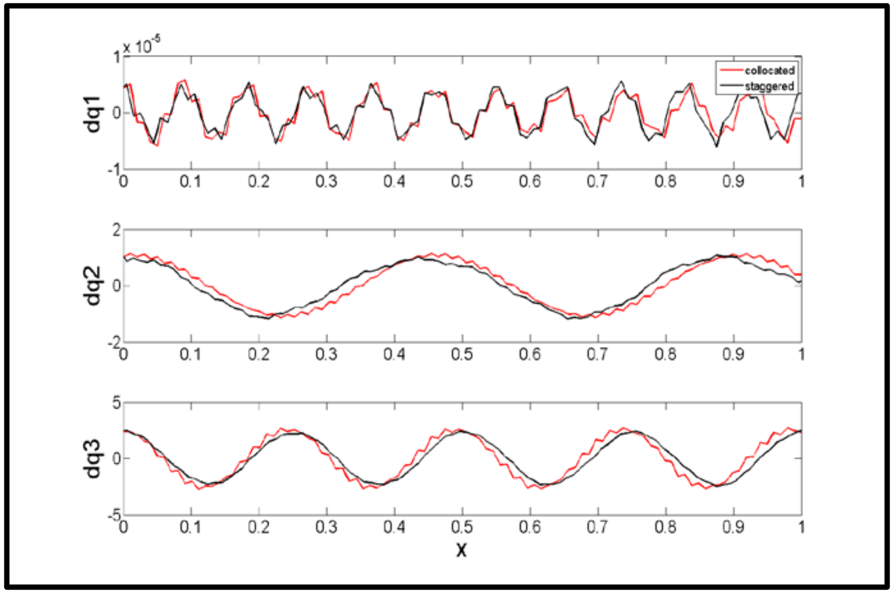
Effect of Boundary Conditions

$$CFL = 1 = \frac{\lambda_2 \Delta t}{\Delta x}$$
$$Mach = 0.28$$
$$distrub = 0.01\%$$

$$\Omega + [\Delta \hat{q}_{bc} - \Delta \hat{q}_{\text{int}}] = 0$$
$$\Omega_{inlet} = \begin{bmatrix} \rho u - \dot{m}_{in} \\ T - T_{in} \\ 0 \end{bmatrix}, \Omega_{outlet} = \begin{bmatrix} 0 \\ 0 \\ p - p_{out} \end{bmatrix}$$



Pressure at 10T$_3$



characteristic variables at 10T$_3$

- high frequency in Collocated pressure solution
- lack of acoustic damping

Kinetic Energy Preservation (KEP)

- "in computations of turbulent flow fields, dissipative errors show up at the level of kinetic energy" (Mahesh 2004)
- Robust at inviscid limit (Re → ∞)

Incompressible Flow:

$$u_i\left\{\frac{\partial u_i}{\partial t}+\frac{\partial u_i u_j}{\partial x_j}=\frac{1}{\rho}\left(-\frac{\partial P}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}\right)\right\}\xrightarrow{\frac{\partial u_j}{\partial x_j}=0}\frac{\partial}{\partial t}\left(\frac{1}{2}u_i^2\right)+\frac{\partial}{\partial x_j}\left(\frac{1}{2}u_i^2 u_j\right)=\frac{1}{\rho}\left(-\frac{\partial u_i P}{\partial x_i}+u_i\frac{\partial \tau_{ij}}{\partial x_j}\right)$$

- $K = \frac{1}{2} u_i^2$ bounded and constant at inviscid limit
- KEP schemes satisfy secondary equation discretely
- Richtmeyer & Morton (1967)
- Arakawa (1966)

Compressible Flow:

$$\frac{-u_i^2}{2}\left\{\frac{\partial}{\partial t}\rho+\frac{\partial}{\partial x_j}\rho u_j\right\}+u_i\left\{\frac{\partial}{\partial t}\rho u_i+\frac{\partial}{\partial x_j}\rho u_i u_j+\frac{\partial}{\partial x_i}P-\frac{\partial}{\partial x_j}\tau_{ij}\right\}=0$$

$$\longrightarrow \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i^2\right)+\frac{\partial}{\partial x_j}\left(\rho u_j\frac{u_i^2}{2}\right)=\frac{1}{\rho}\left(-u_i\frac{\partial P}{\partial x_i}+u_i\frac{\partial \tau_{ij}}{\partial x_j}\right)$$

- Discrete analogue seeks:
  - Accurate transport of KE → accurate physical transfer of energy: $E = KE + U_{int}$

KEP: Applied to 1D Euler

(Collocated Grid)

- compare Crank-Nicolson (CN) with Fully KEP scheme (F-KEP)

$$\frac{(\rho\phi_k)_i^{n+1} - (\rho\phi_k)_i^n}{\Delta t} + \frac{1}{V_i}\sum_f (\phi)_f^m (\rho \mathrm{u}_j)_f^{n+1/2} \cdot S_i + \frac{1}{V_i}\sum_f \left(\frac{\partial p\upsilon_{k,j}}{\partial x_j}\right)_f^{n+1/2} \cdot S_i = 0$$

Subbareddy/Candler(2009)
Merkle (2013)

$$\phi^m = \frac{1}{2}(\phi^{n+1} + \phi^n)$$

(CN)

$$\phi^m = \frac{(\sqrt{\rho}\phi)^{n+1} + (\sqrt{\rho}\phi)^n}{(\sqrt{\rho})^{n+1} + (\sqrt{\rho})^n}$$

(F-KEP)

$$\phi = \begin{bmatrix} 1 \\ u \\ e \\ Y_k \end{bmatrix}$$

- discrete secondary equation satisfied to machine zero if KEP

$$\frac{(\rho\phi_k^2)_i^{n+1} - (\rho\phi_k^2)_i^n}{2\Delta t} + \frac{1}{V_i}\sum_f (\rho \mathrm{u}_j{}^{n+1/2})_f \left(\frac{\phi_k^2}{2}\right)_f^m \cdot S_{f,i} + \phi_{k,i}^m \frac{1}{V_i}\sum_f (p\upsilon_{k,j})^{n+1/2} \cdot S_{f,i} = RESIDUAL$$

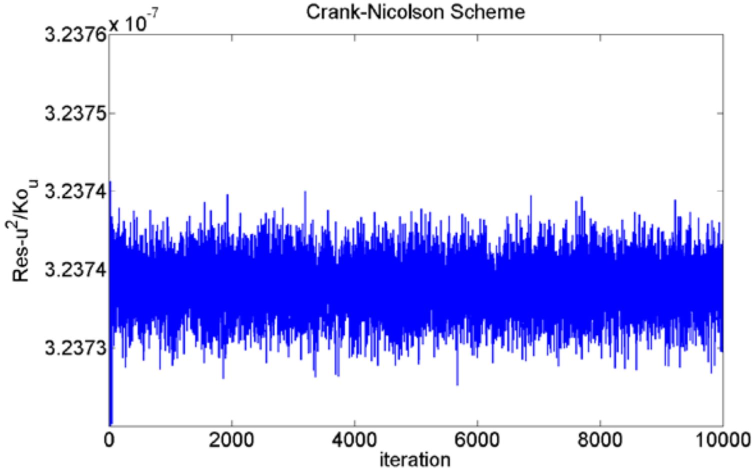
$$\text{with} \quad \left(\frac{\phi_k^2}{2}\right)_f^m = \frac{1}{2}\left(\frac{\phi_k}{2}\right)_i^m \left(\frac{\phi_k}{2}\right)_{nbr}^m$$

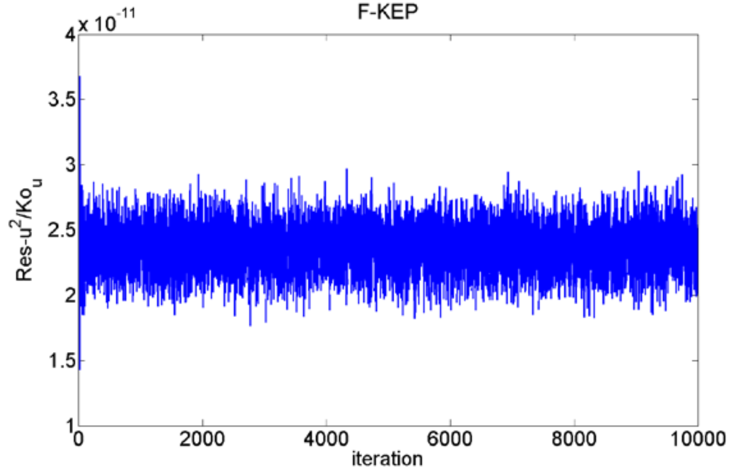
Evaluating KEP: u^2

Mach = 0.859

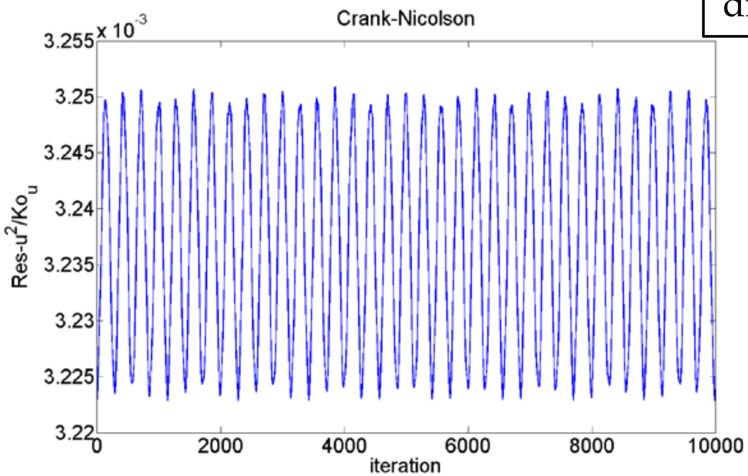
disturb = 0.01%

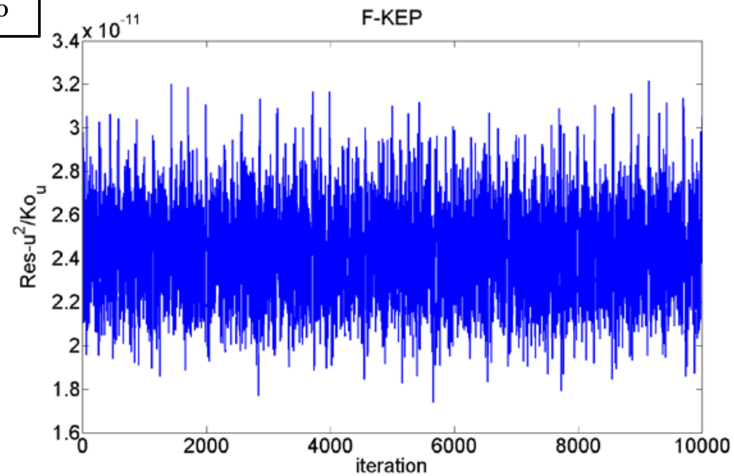
- F-KEP always secondary conservative
- CN KEP for low compressibility effects





disturb = 1%





Going Forward

- **Key Questions:**
  - What is the advantage of kinetic energy preservation for LES?
  - Does it help minimize or eliminate the need for artificial dissipation?
  - What about the relative importance of dispersion errors?

- **Implement Merkle's generalized KEP schemes**
  - Formulated for both staggered and collocated schemes
  - Major advantage is that it is KE preserving for the scalar transport as well
  - Can we minimize or eliminate the need for artificial dissipation for scalars?

- **Extend schemes to multi-dimensional code**
  - Apply to non-reacting and reacting LES computations

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