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Optimal Numerical Schemes for Time Accurate Compressible Large Eddy Simulations:

Comparison of Artificial Dissipation and Filtering Schemes

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Research Supported by AFOSR (Drs. Fahroo and Li, PMs)

67th American Physical Society (APS) Meeting
Division of Fluid Dynamics

San Francisco, CA

November 23-25, 2014



UCLA

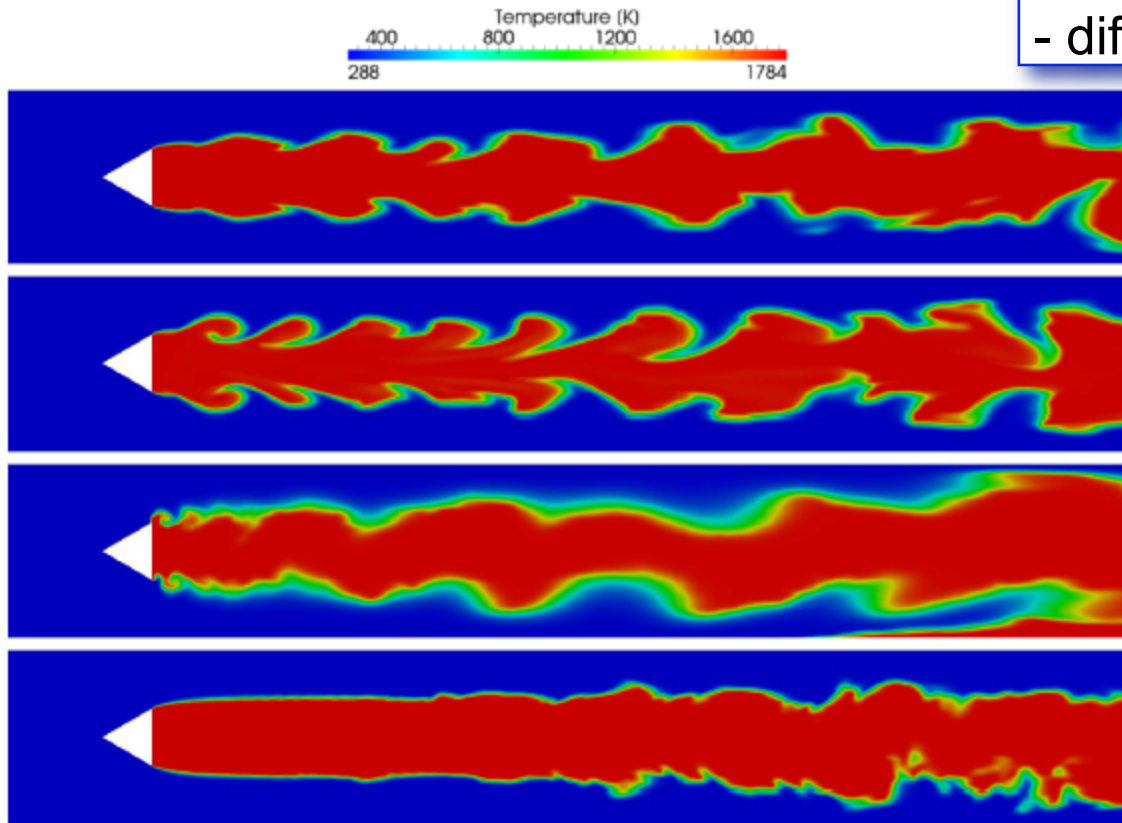
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RESEARCH
LABORATORY**



Challenges: Reactive LES

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 schemes for Reacting LES

Objectives

GOAL:

damp high frequency errors while preserving low wave content (ie: low-pass response)

- 1) compare damping character of Artificial Dissipation and Filtering
- 2) formulate filter as an equivalent Artificial Dissipation scheme
 - consequence of filter damping for stiff problems
- 3) insight on achieving “ideal” low-pass response for general problems

- von Neumann Analysis
- Crank-Nicolson w/ 6th order central differencing

von Neumann Analysis

1D Euler System (quasi-linear form):

$$\frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = 0$$

$$Q_i = \sum_k \hat{Q}(k) e^{ikx}$$

$$Q_{i+i} = \sum_k \hat{Q}(k) e^{ik(x+\Delta x)} = \sum_k \hat{Q}(k) e^{ik\Delta x} e^{ikx} \quad k\Delta x = \theta$$

with $\theta \in [-\pi, \pi]$

$$Q^{n+1} = G(\theta) Q^n$$

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

Growth Factor

$$|g_i|_2$$

Phase Error

$$\frac{\phi}{\phi_{exact}} = \frac{-\tan^{-1} \{ \text{Im}(g_i) / \text{Re}(g_i) \}}{CFL_i \times \theta}$$

Artificial Dissipation

$$\frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x} = \sum_m (-1)^{m-1} (\Delta x)^{2m-1} \epsilon_{2m} |\lambda_{u+c}| \frac{\partial^{2m} Q}{\partial x^{2m}}$$

governing equations augmented with dissipation terms

$$\epsilon_2 = 1/2$$

$$\epsilon_4 = 1/12$$

$$\epsilon_6 = 1/60$$

upwind biased stencils

$$\begin{aligned} m = 1: & \quad \frac{Q_{i+1} - Q_{i-1}}{2\Delta x} - \frac{1}{2} \left(\frac{Q_{i+1} - 2Q_i + Q_{i-1}}{\Delta x} \right) = \frac{Q_i - Q_{i-1}}{\Delta x} \\ m = 2: & \quad \frac{-Q_{i+2} + 8Q_{i+1} - 8Q_{i-1} + Q_{i-2}}{12\Delta x} + \frac{1}{12} \left(\frac{Q_{i+2} - 4Q_{i+1} + 6Q_i - 4Q_{i-1} + Q_{i-2}}{\Delta x} \right) = \frac{4Q_{i+1} + 6Q_i - 12Q_{i-1} + 2Q_{i-2}}{12\Delta x} \\ \text{etc...} & \end{aligned}$$

Filtering (Explicit)

$$Q_i = \left[1 + \sum_m S_{2m} (\Delta x)^{2m} \frac{\partial^{2m}}{\partial x^{2m}} \right] Q_i^*$$

smoothing of solution as post-process of integration step

represent total amplification of filter scheme as:

$$G(\theta) = R(\theta) G^*(\theta)$$

with
$$\begin{cases} |R(\theta)|_2 \leq 1 \\ R(\theta = \pm\pi) = 0 \end{cases}$$

NOTE: filter is purely dissipative and does not alter original scheme's phase behavior

Filtering (Implicit)

$$\left[1 + \sum_m S'_{2m} (\Delta x)^{2m} \frac{\partial^{2m}}{\partial x^{2m}} \right] Q_i = \left[1 + \sum_m S_{2m} (\Delta x)^{2m} \frac{\partial^{2m}}{\partial x^{2m}} \right] Q_i^*$$

smoothing of solution as post-process of integration step

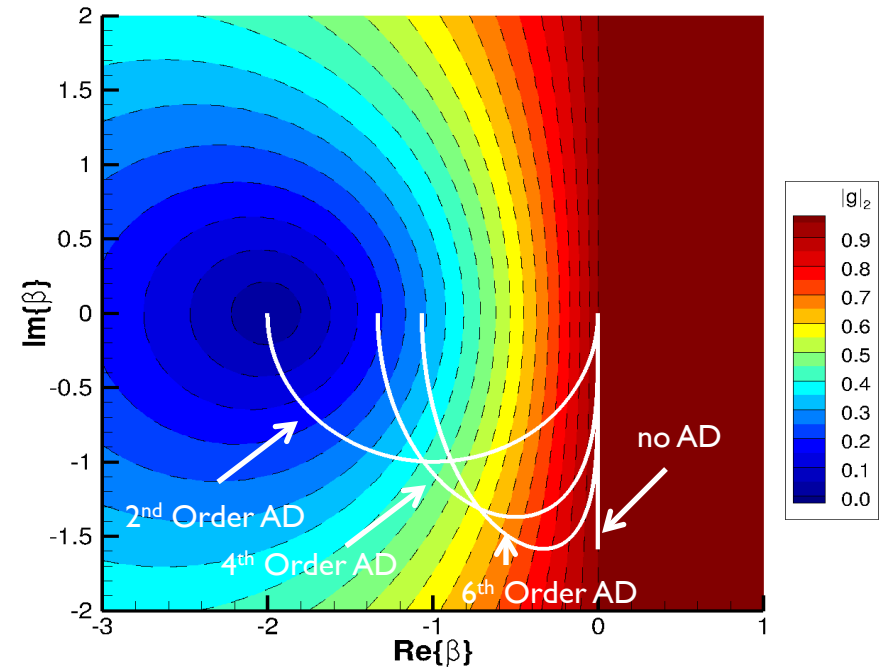
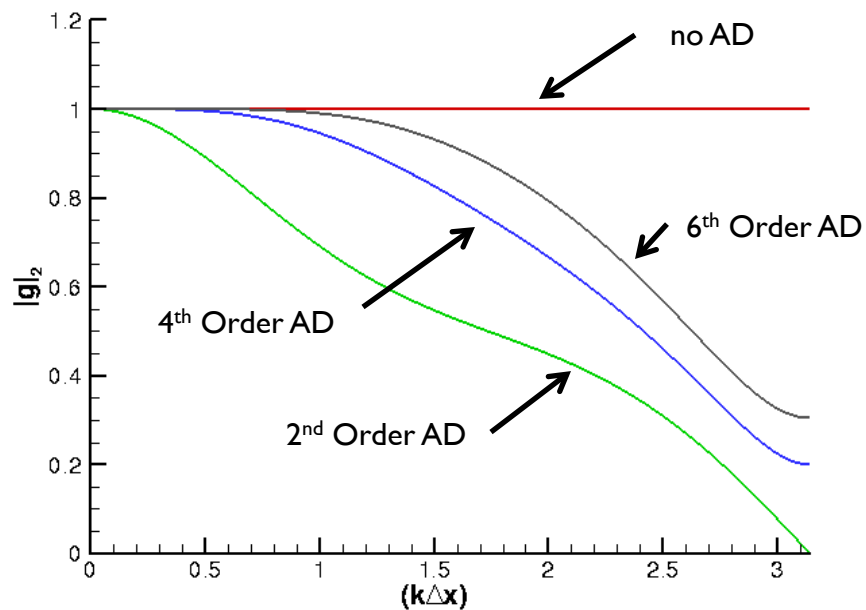
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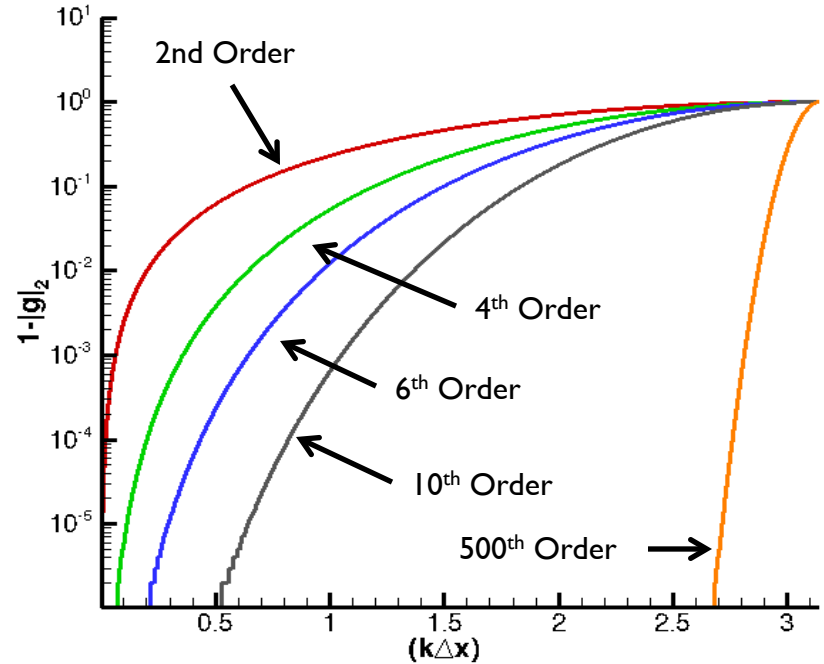
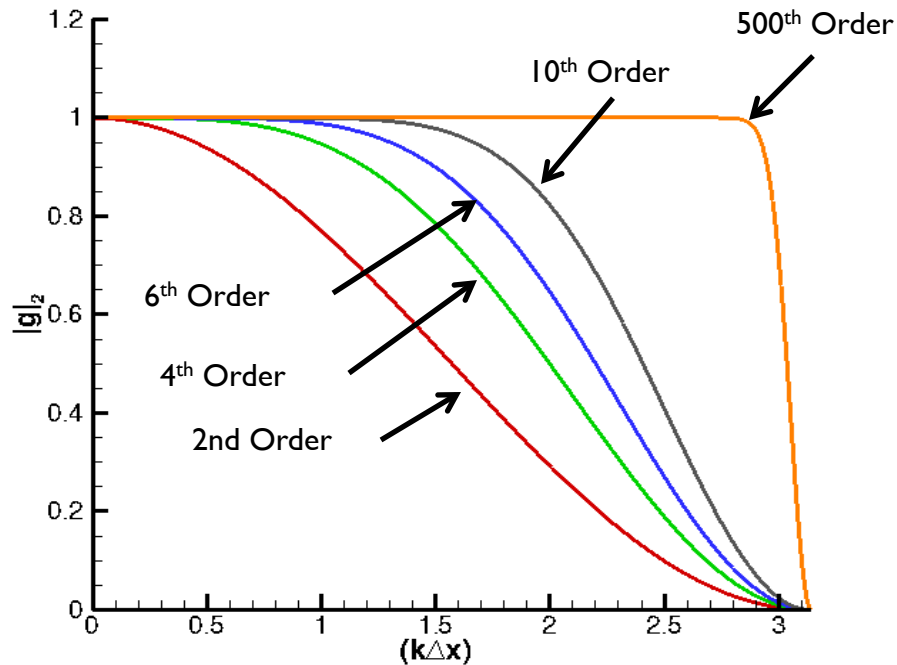
NOTE: filter is purely dissipative and does not alter original scheme's phase behavior

Artificial Dissipation: Growth Factor



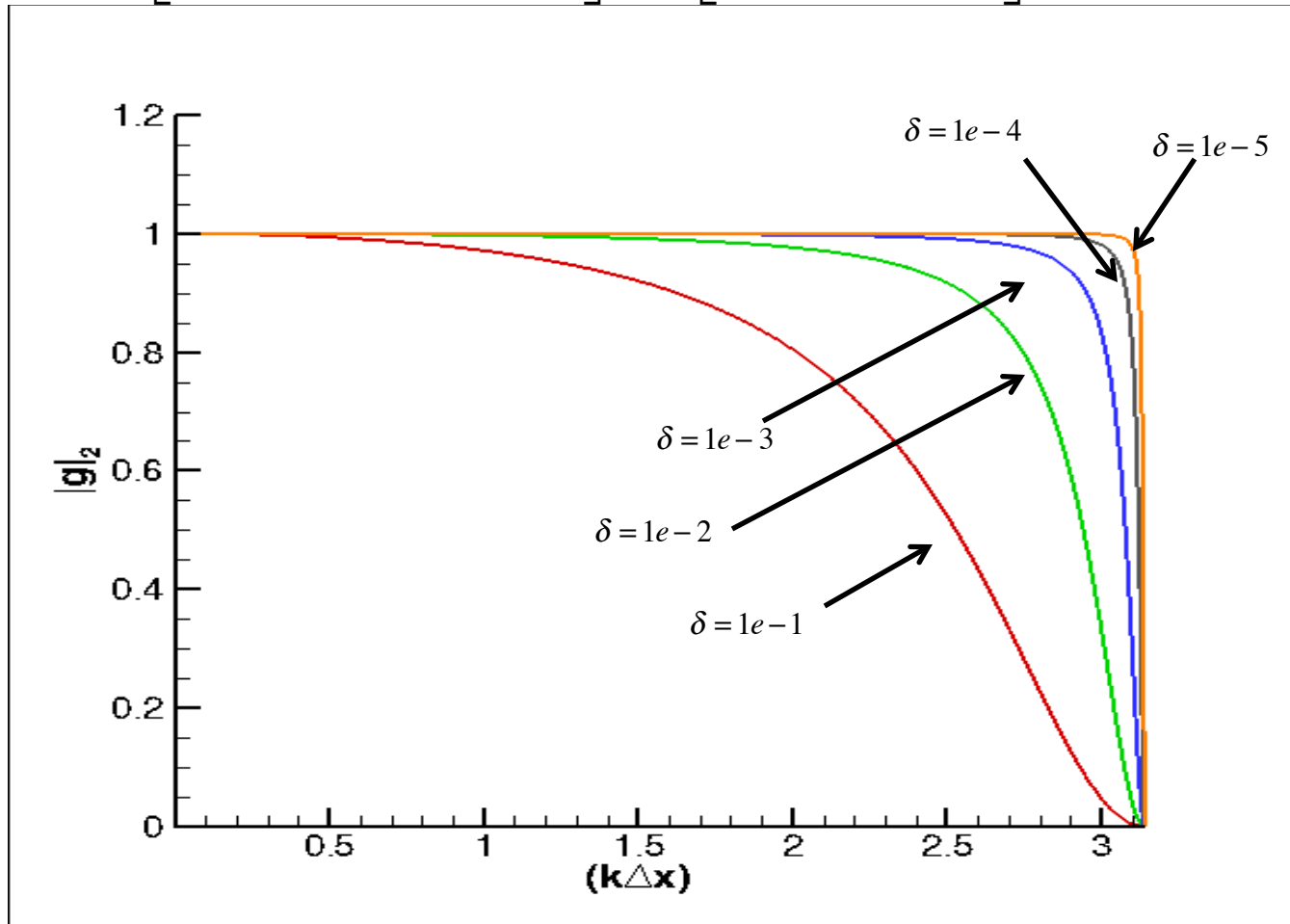
Explicit Filter: Growth Factor

Shapiro Filter (1975) $Q_i = \left[1 + S_m (\Delta x)^{2m} \frac{\partial^{2m}}{\partial x^{2m}} \right] Q_i^*$ with $S_m = \frac{(-1)^{m-1}}{2^{2m}}$



2nd Order Implicit Filter: Growth Factor

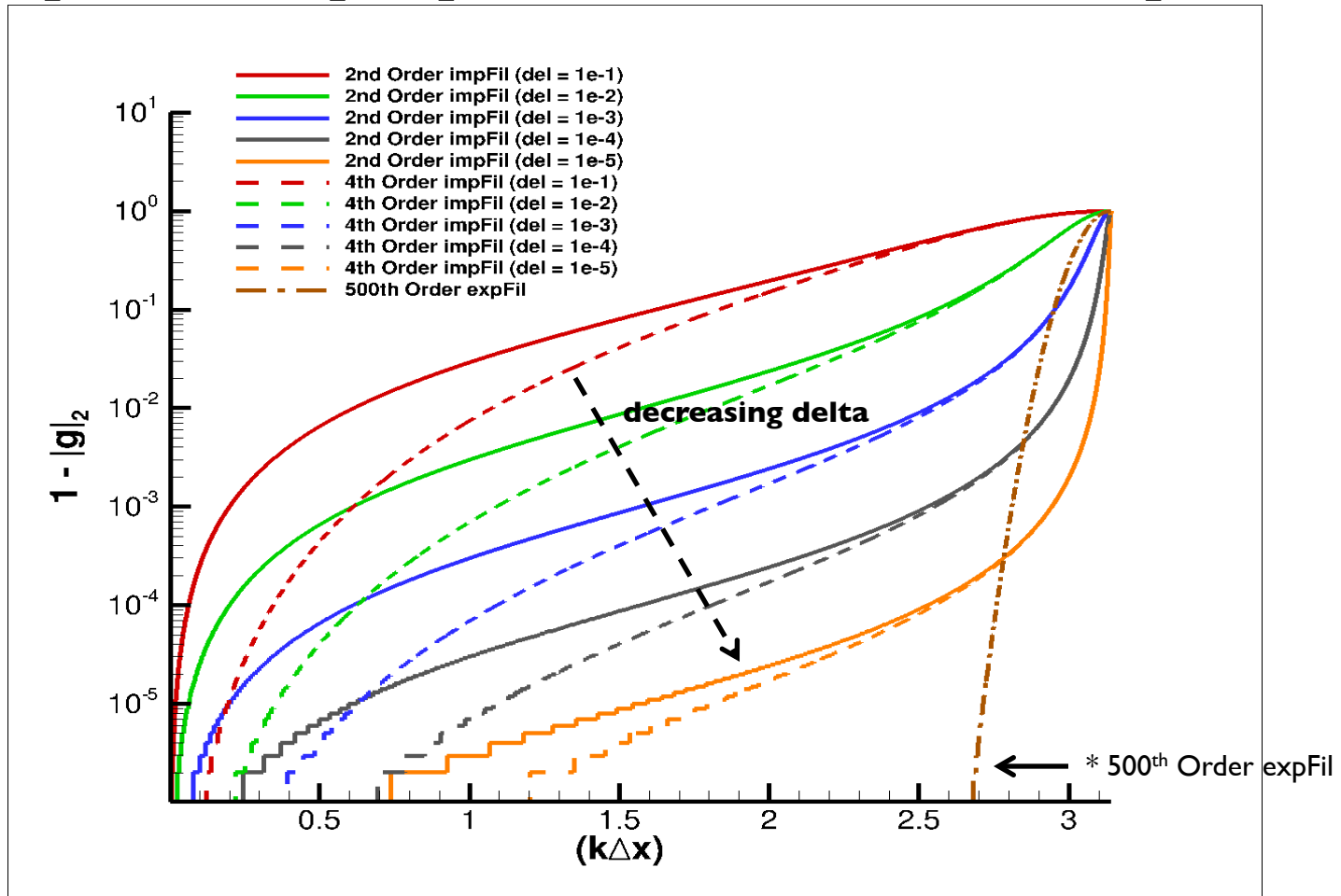
Long Filter (1971) $\left[1 + (1 - \delta)S(\Delta x)^2 \frac{\partial^2}{\partial x^2}\right] Q_i = \left[1 + S(\Delta x)^2 \frac{\partial^2}{\partial x^2}\right] Q_i^*$ with $\delta \in \langle 0, 1 \rangle$



2nd vs. 4th Order Implicit Filters: Growth Factor Error

4th order Lele
Filter (1992)

$$\left[1 + S(\Delta x)^2 \frac{\partial^2}{\partial x^2} \right] Q_i = \left[1 + S(\Delta x)^2 \frac{\partial^2}{\partial x^2} + \left(\frac{-\delta}{4 - 8\delta} \right) S(\Delta x)^4 \frac{\partial^4}{\partial x^4} \right] Q_i^* \quad \text{with } \delta \in \langle 0, 1 \rangle$$



Filtering as an Artificial Dissipation Scheme

$$Q_i^{n+1} = \left[1 + \frac{1}{4}(\Delta x)^2 \frac{\partial^2}{\partial x^2} \right] Q_i^*$$

$$= \left[1 + \frac{1}{4}(\Delta x)^2 \frac{\partial^2}{\partial x^2} \right] \left[Q_i^n - \Delta t(1-\theta) \frac{\partial E^n}{\partial x} + \Delta t\theta \frac{\partial E^*}{\partial x} \right] \text{ with } \theta \in [0,1]$$



$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} + (1-\theta) \frac{\partial E^n}{\partial x} + (\theta) \frac{\partial E^*}{\partial x} = \frac{1}{4} \frac{(\Delta x)^2}{\Delta t} \frac{\partial^2 Q^n}{\partial x^2} - (1-\theta) \frac{1}{4} (\Delta x)^2 \frac{\partial^3 E^n}{\partial x^3} - (\theta) \frac{1}{4} (\Delta x)^2 \frac{\partial^3 E^*}{\partial x^3}$$

dispersive terms:

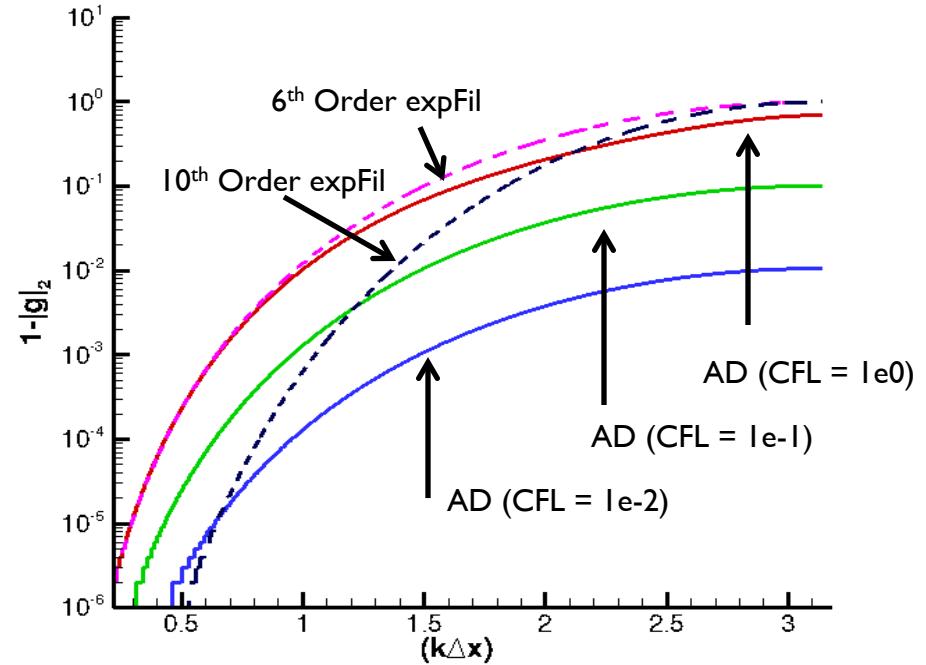
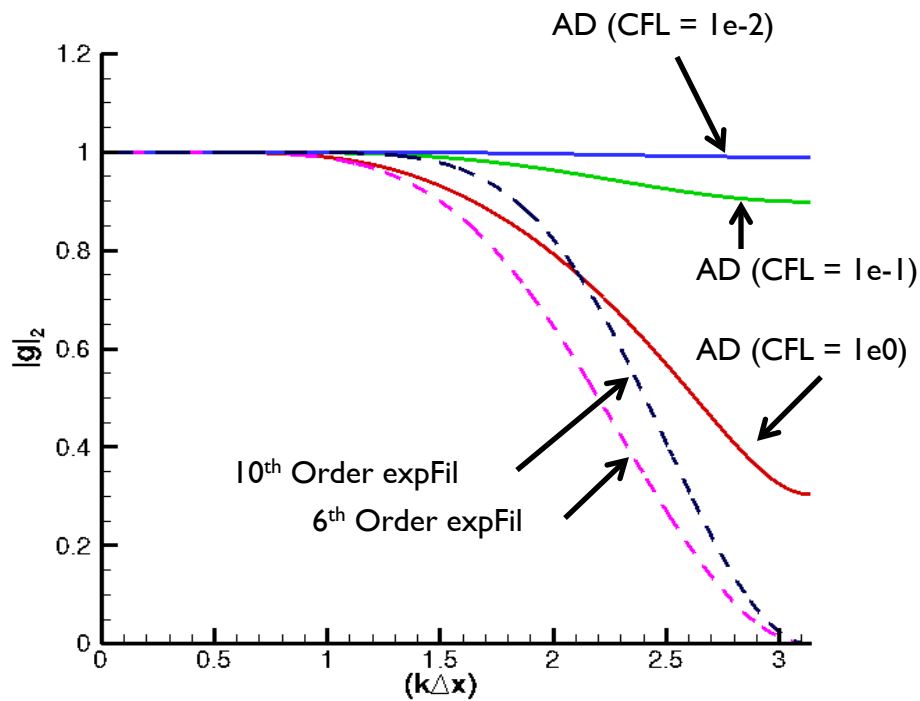
- restore phase of original scheme

dissipation term scales as $\varepsilon_2 \sim 1 / CFL_{u+c}$

- increased damping w/ decreasing time-step

Effect of CFL

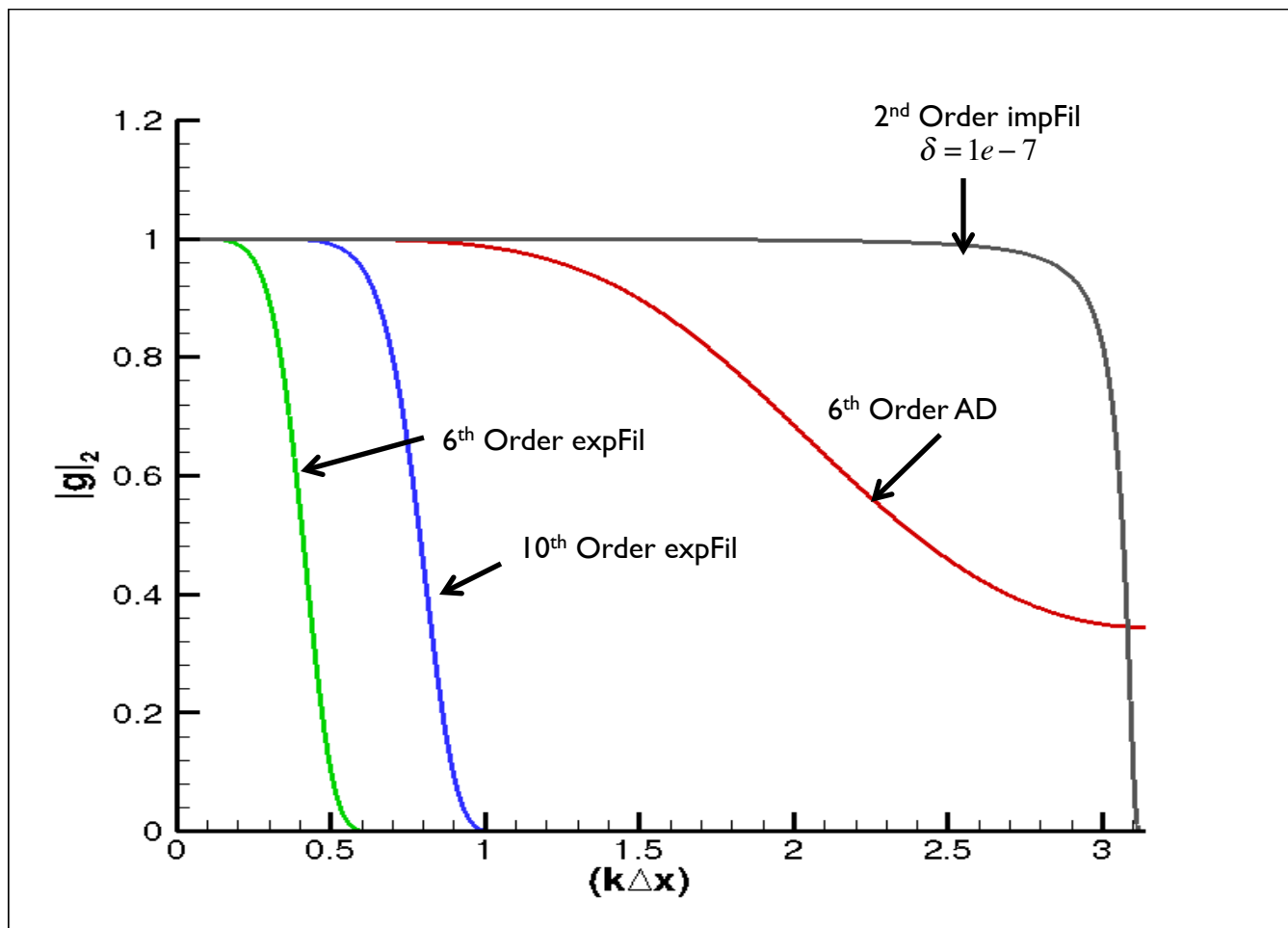
* AD shown is 6th order



Cumulative Low CFL Damping

$$CFL_{u+c} = 10^{-4}$$

$$Nsteps = 10^4$$



Summary

- Filtering is a form of artificial dissipation
 - damping behavior more predictable and tunable
- Explicit filters require very high order for low-pass response
 - overly dissipative for small time-steps
- Implicit filters can be efficiently designed for low-pass response
 - superior to artificial dissipation or explicit filters

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- Dr. Venke Sankaran (Edwards AFRL)
- Professor Ann Karagozian (UCLA)
- Professor Charles Merkle (Purdue)

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THANK YOU

Back-Up Slides

Staggered Grid Von Neumann Analysis

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = 0 \quad \text{1D Euler Eqns}$$

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

$$||g_i||$$

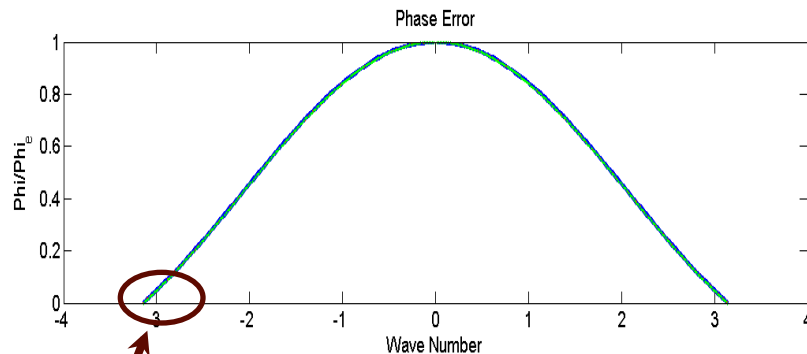
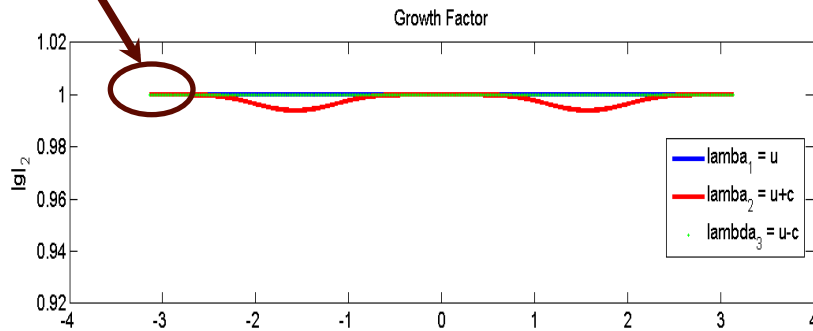
Phase Error

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

Runge Kutta 4: von Neumann

Collocated

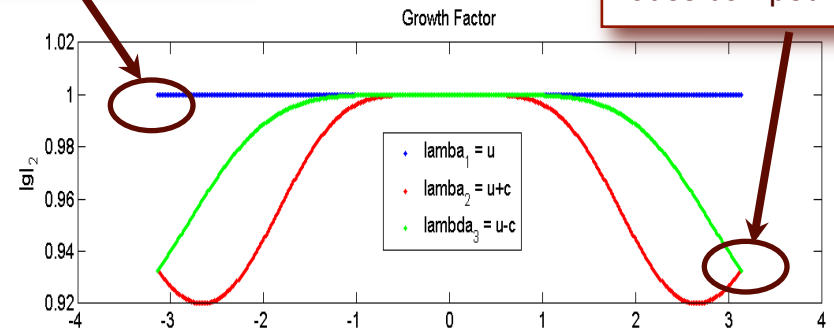
No damping of highest modes



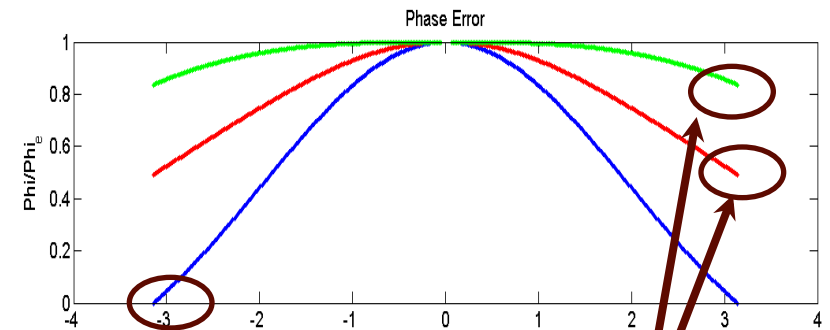
No convection of highest modes

Staggered

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

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 ($\text{Re} \rightarrow \infty$)

Incompressible Flow:

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

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

Compressible Flow:

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

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

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

KEP: Applied to 1D Euler

(Collocated Grid)

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

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

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

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

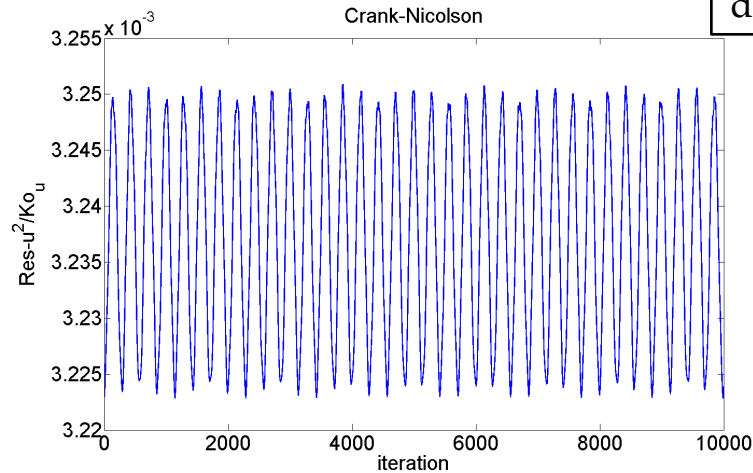
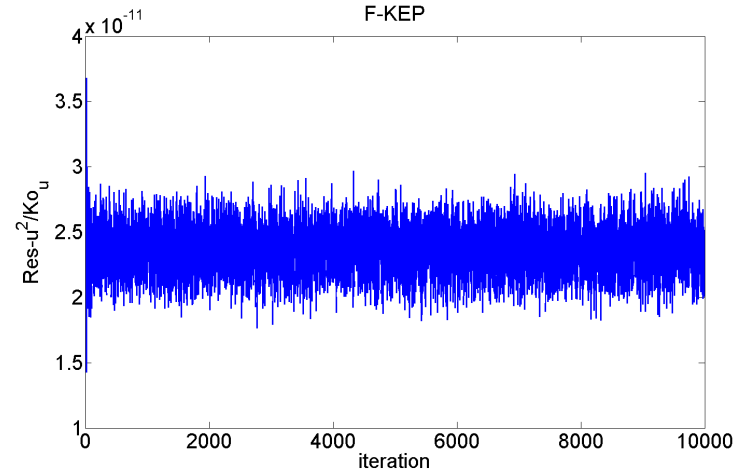
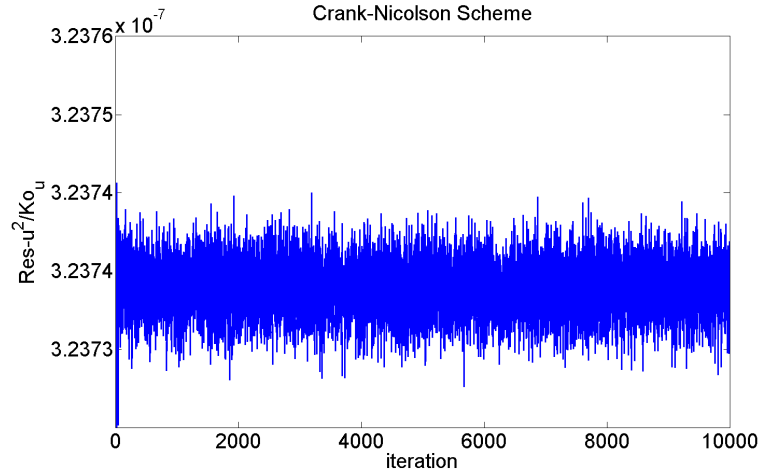
$$\text{with } \left(\frac{\phi_k^2}{2} \right)_f^m = \frac{1}{2} \left(\frac{\phi_k}{2} \right)_i^m \left(\frac{\phi_k}{2} \right)_{nbr}^m$$

Evaluating KEP: u^2

Mach = 0.859

disturb = 0.01%

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



disturb = 1%

