Progress in Accuracy & Stability Improvement of Nonlinear Filter Methods for Long Time Integration of Compressible Flows

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Outline

- Objective
- Technical Challenge
- Approach

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- Results
- Current & Future Plan

Objectives

Construction of High Order Shock-Capturing Methods to Improve Predictability & Reliability of Turbulent Simulations

Challenges in Numerical Method Development

(Multiscale DNS & LES, and Aeroacoustic Turbulence Applications)

- **Accurate schemes developed for short time integration might suffer from nonlinear instability for longer time integration**

- **Numerical stability & accuracy requirements are an intricate balancing act**
  - > More stable schemes usually contain more numerical dissipation than their higher accuracy schemes counterparts
  - > Turbulence cannot tolerate numerical dissipation
  - > Proper amount of numerical dissipation is required for stability in the vicinity of discontinuities
  - > Reacting/combustion flows containing stiff source terms:
    - Numerical dissipation & under-resolved grid may lead to incorrect shock speed
    - Need well-balanced schemes to preserved certain physical steady states exactly

- **DNS & LES of turbulent flows containing both shock-free turbulence, and strong shocks & high gradient/shocklets during the entire computational time evolution cannot be solved accurately with standard numerical method construction**

- **Forced compressible turbulence can initially start with shock-free turbulence and might develop into flows with moderate to strong shock waves at a later time evolution (Kotov et al. JCP, 2016)**

→ **Stable & Accurate Temporal & Spatial Low Dissipative & Dispersive methods applicable to long time integration are required**

(Yee & Sjogreen, 2007-2017, Sjogreen & Yee, 2016-2017, Wang et al., 2009-2015, Kotov et al., 2011-2016)

Numerical Examples

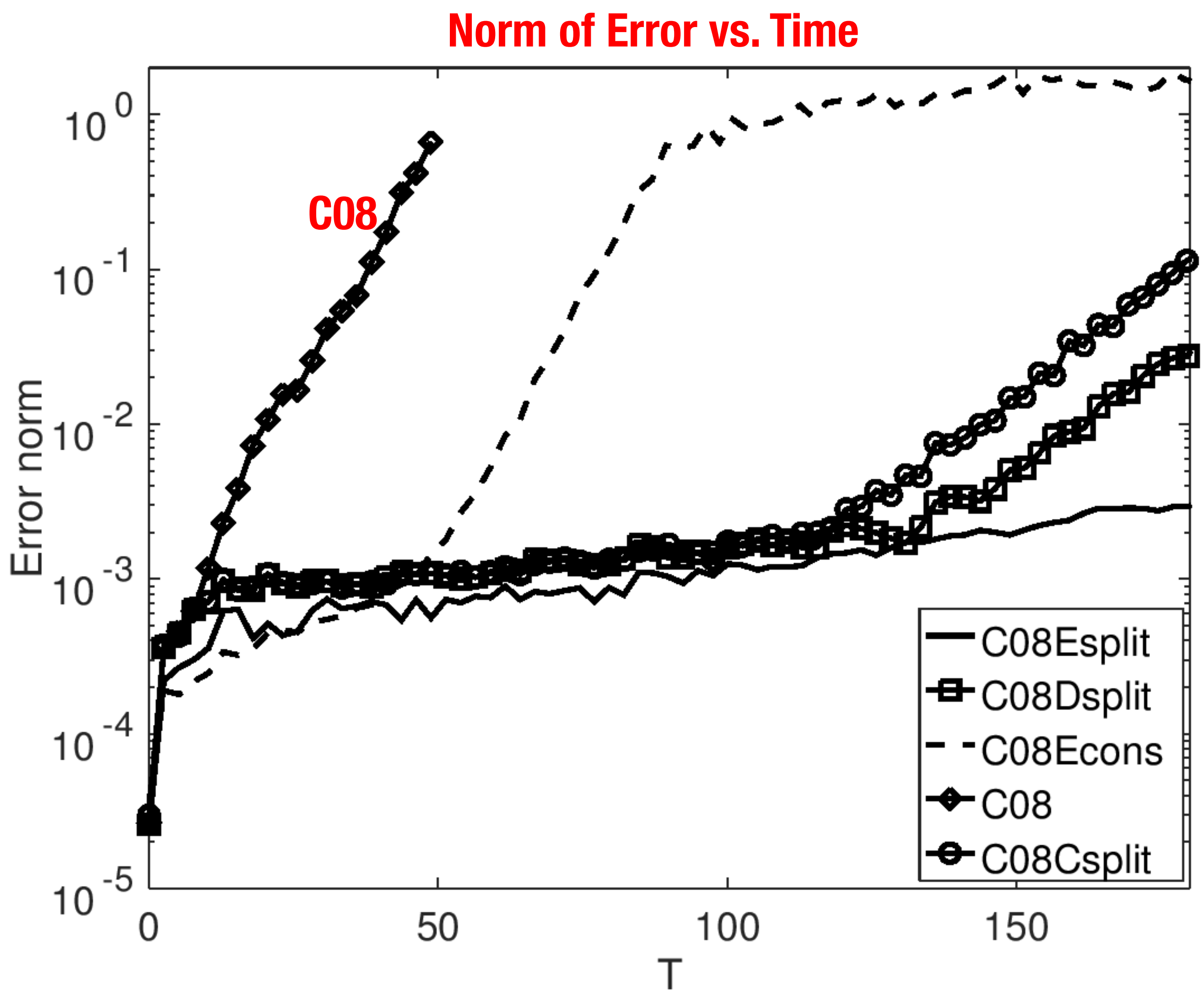
DNS Computations of Smooth Flows & Turbulence with Discontinuities

- Accurate schemes developed for short time integration might suffer from nonlinear instability for longer time integration
- Standard shock-capturing methods are too diffusive for long time integration

2D Isentropic Vortex Convection

Translation of initial data exactly if no numerical dissipation added

8^{th} order central (C08) vs. 4 different 8^{th}-order skew-symmetric splittings



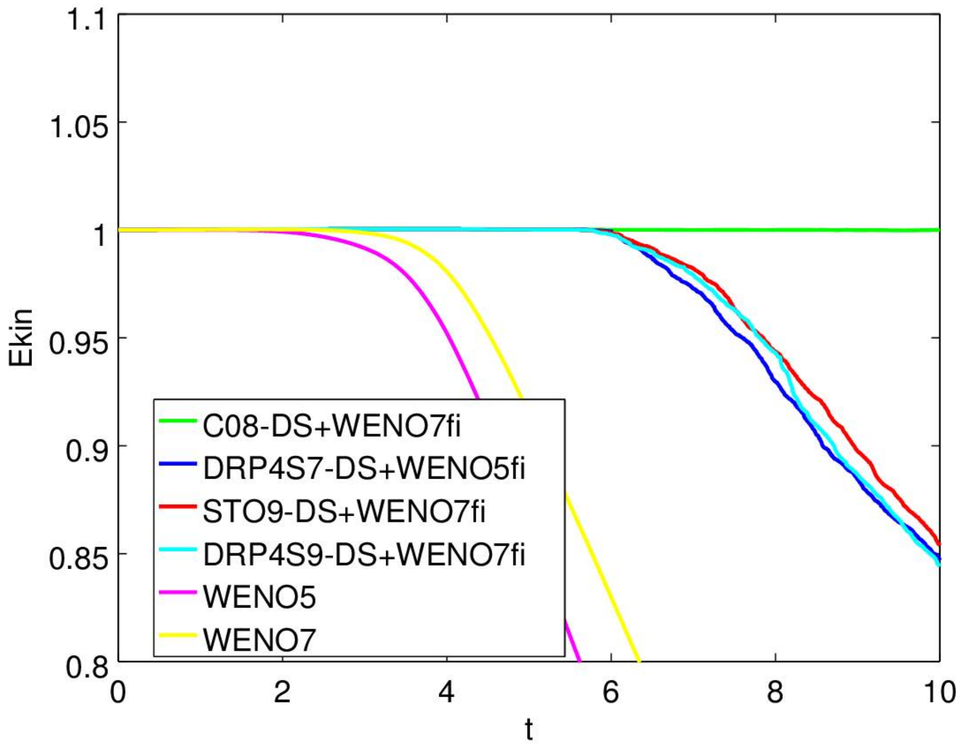
Improve numerical stability
for longer time integrations
by skew-symmetric splittings
(different accuracy)

3D Taylor-Green Vortex (Compressible & Inviscid)

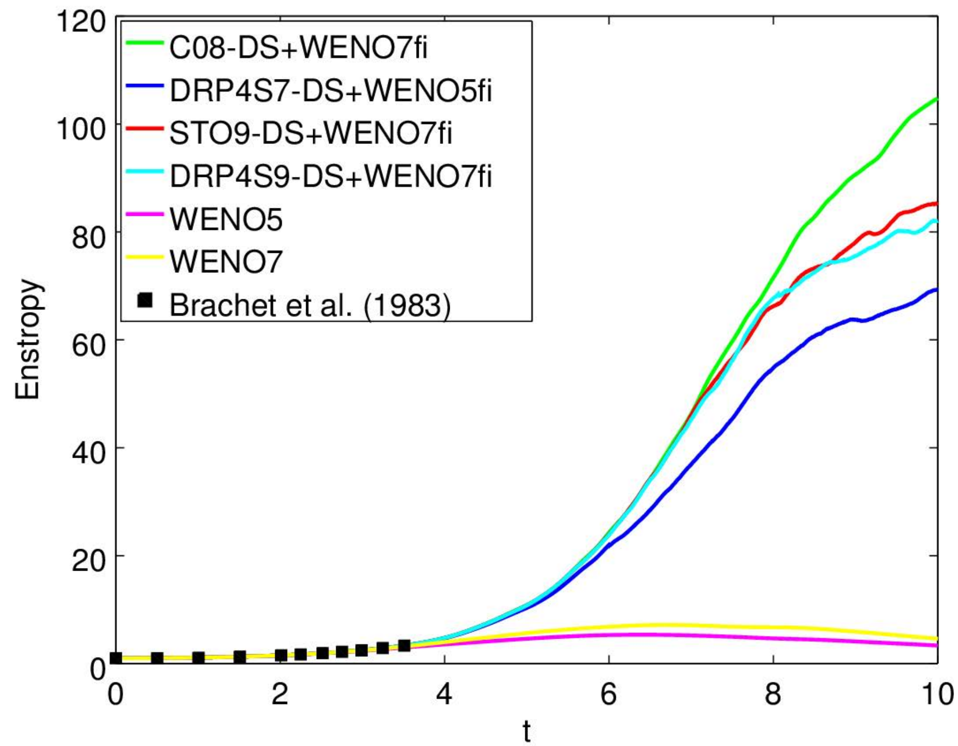
(Comparison of 4 Nonlinear Filter Methods, 64^3 grids)

Classical Central vs. DRP Central Base Schemes

Kinetic Energy



Enstrophy



C08-DS+WENO7fi: 8th-order central + Ducros et al. split +WENO7fi

DRP4S7-DS+WENO5fi: Tam & Webb 4th-order DRP, 7pt grid stencil + Ducros et al. split +WENO5fi

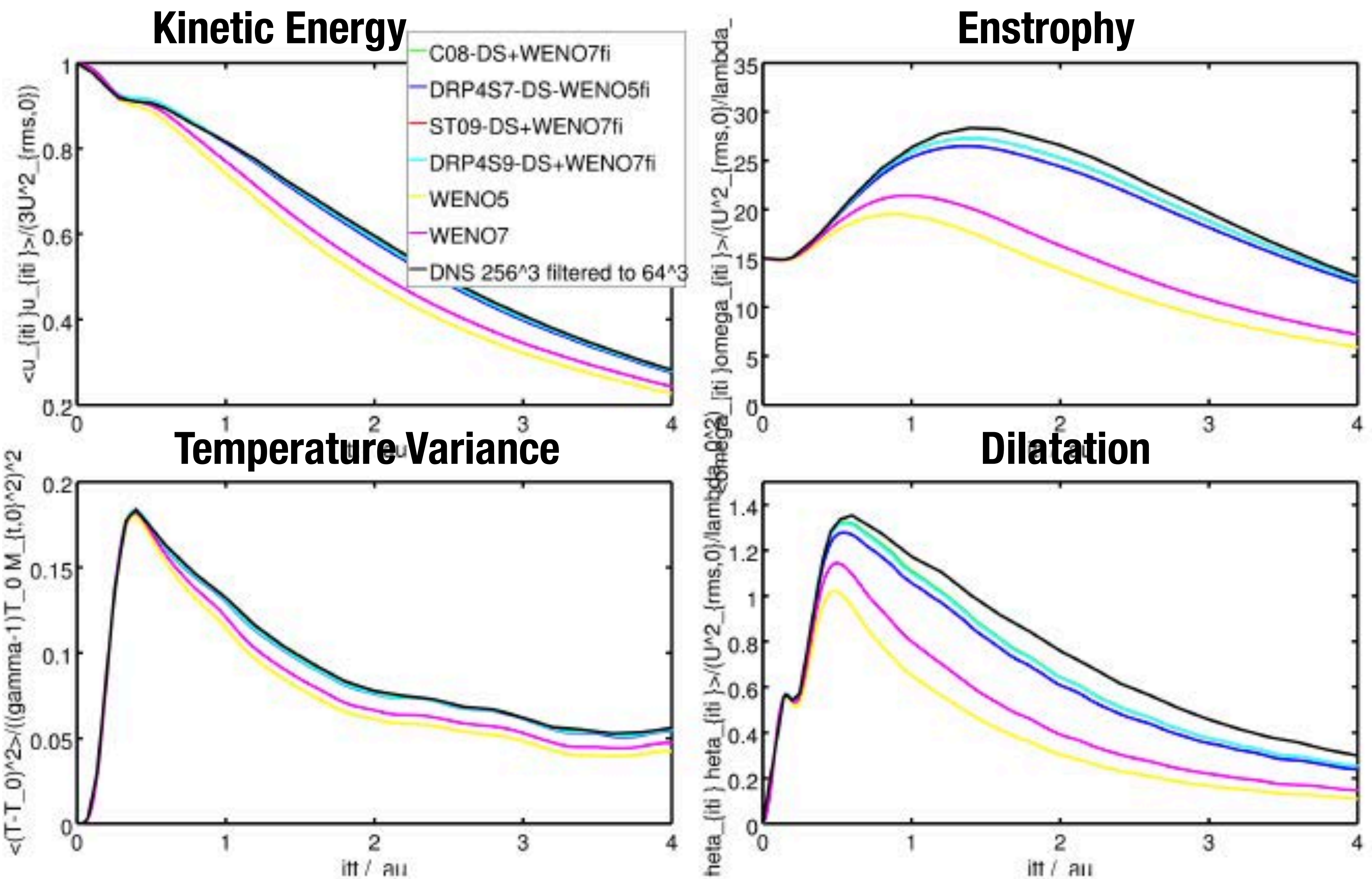
ST09-DS+WENO7fi: Bogey & Bailly 4th-order DRP, 9pt grid stencil + Ducros et al. split +WENO7fi

DRP4S9-DS+WENO7fi: Tam & Webb 4th-order DRP, 9pt grid stencil + Ducros et al. split +WENO7fi

3D Isotropic Turbulence with Shocklets

(Comparison of 4 Nonlinear Filter Methods, 64^3 grids)

Classical Central vs. DRP Central Base Schemes



Spurious Numerics Due to Source Terms

Source Terms: **Hyperbolic conservation laws with source terms – Balanced Law**

> *Most high order shock-capturing schemes are not well-balanced schemes*

> *High order WENO/Roe & their nonlinear filter counterparts are well-balanced for certain reacting flows – Wang et al. JCP papers (2010, 2011)*

Stiff Source Terms:

> *Numerical dissipation can result in wrong propagation speed of discontinuities for under-resolved grids if the source term is stiff (LeVeque & Yee, 1990)*

> *This numerical issue has attracted much attention in the literature – last 20 years (Improvement can be obtained for a single reaction case)*

> *A New Sub-Cell Resolution Method has been developed for stiff systems on coarse mesh (Wang et al., JCP, 2012)*

Nonlinear Source Terms:

> *Occurrence of spurious steady-state & discrete standing-wave numerical solutions -- due to fixed grid spacings & time steps (Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, 1990 – 2002)*

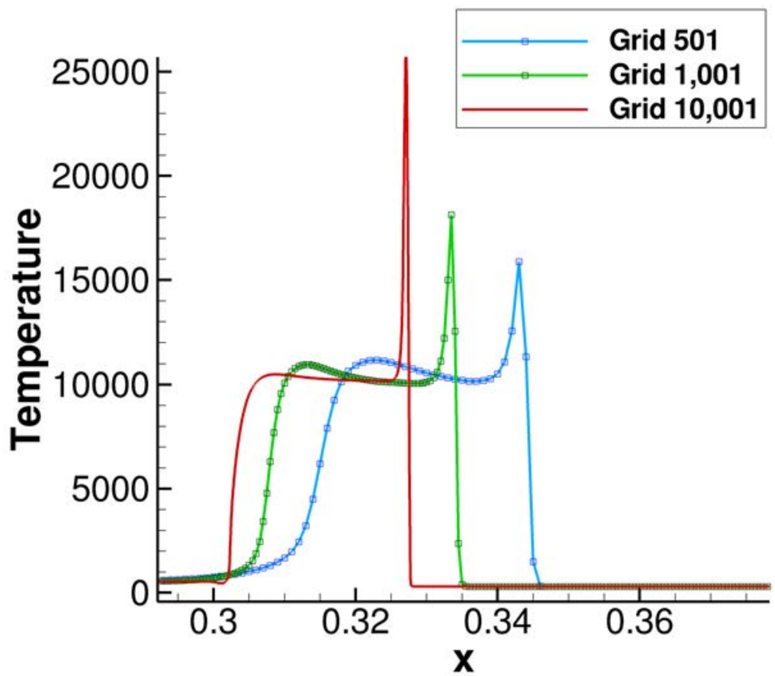
Stiff Nonlinear Source Terms with Discontinuities:

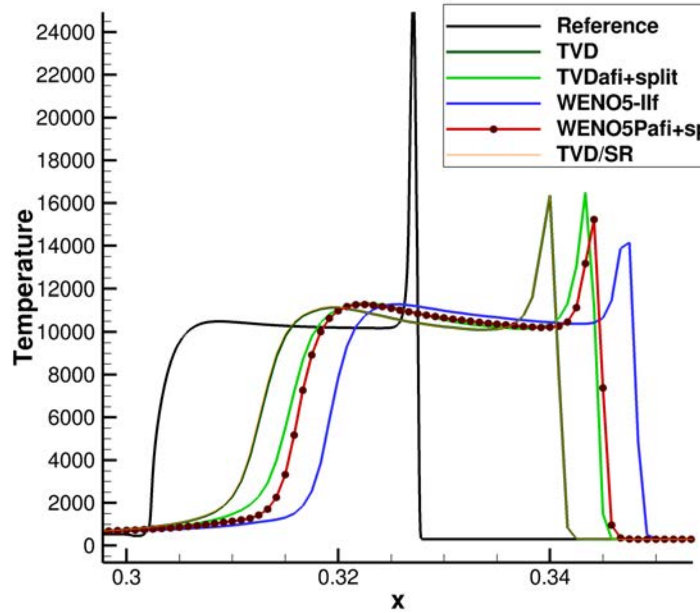
> *More Complex Spurious Behavior*
> *Numerical combustion, certain terms in turbulence modeling & reacting flows*

Stiff Source Terms: Wrong Discontinuity Locations

(E.g., Grid & method dependence of shock & shear locations)

NASA *Electric Arc Shock Tube* (EAST)
- 1D Computation: 13 species(Air+He) using MUTATION library; L = 8.5 m
- Fine grid step h = 0.05mm, 16 times finer than coarse grid





Note: Non-reacting flows - Grid & scheme do not affect locations of discontinuities, only accuracy

Implication: The danger in practical numerical simulation for this type of flow (Kotov et al. JCP, 2015)
(Non-standard behavior observed in non-reacting flows)

Approach

- Schemes that mimic the property of the chosen governing equations
- Schemes that preserve key physical properties
- Schemes that are high order, low dissipation & low dispersive error suitable for a wide range of flow speeds (require flow sensors to adaptively minimize the dissipation and dispersion errors)
- Schemes that are stable, efficient & highly parallelizable
- Schemes with high order stable discrete numerical boundary operators
- Schemes that are applicable for DNS & LES in 3D curvilinear spatial & time varying deforming grids

Yee et al., Yee & Sjogreen, Sjogreen & Yee, Wang et al. and Kotov et al. (1999-2017)

Methods to Improve Nonlinear Stability & Accuracy

(Long Time Wave Propagation & Long Time Integration of Complex Compressible Fluids & Plasma)

- Skew-Symmetric Splitting of the Inviscid Flux Derivative Before the Application of Non-Dissipative Centered Schemes
- DRP (Dispersion Preservation-Relation) Schemes as Alternatives to Classical High Order Central Schemes
- Stable High-Order Entropy Conservative Numerical Fluxes with Entropy Satisfying Properties - Numerical solution satisfies an additional discretized conservation law
- Standard High Order Linear Filters are to be Replaced by High Order Nonlinear Filters
- Smart Flow Sensors to Provide Locations & Amount of Needed Numerical Dissipation
- Nonlinear Dynamics is Utilized to Complement the Traditional Linearized Stability Theory
  - Minimize numerically induced false transition to turbulence
  - Minimize numerical instability due to long time integration of turbulent flows
  - Minimize numerically induced standing wave solutions

Present short talk summaries red arrow methods

Skew-Symmetric Splitting of Inviscid Flux Derivatives

(Improve nonlinear stability for high order central schemes)

Olsson & Oliger 1994, Yee et al. 1999, Ducros et al. 2000, Pirozzoli 2009, Sjogreen et al. 2017

- **Entropy splitting:** Semi-conservative splitting for shock-free turbulence
  (Olsson & Oliger 1994, Yee et al. 1999-2007, Sandham et al. 2002-present)
- **Natural Splitting:** Linearized Euler & Non-conservative Systems
- **Splitting to Preserve Discrete Momentum and/or Energy Conservation:**
  (Arakawa 1966, Blaisdell et al. 1996, Mansour 1980, etc.)
- **Ducros et al. Type Conservative Splitting:** Euler & MHD (Sjogreen et al. 2017)
- **Generalized Skew-Symmetric Splitting:** 3-parameter family
  (Pirozzoli 2009)

Preprocessing Step: Improve stability of classical central scheme

Replacing high order classical central approximation of the inviscid flux derivative ➔
High order approximation of their split form counterpart

➔ **This talk concentrates only on Ducros et al. type conservative splitting**

Ducros et al. Splitting

(Improve nonlinear stability for high order central schemes)

Split the derivative of a product into conservative & non-conservative parts:

$$(ab)_x = \frac{1}{2}(ab)_x + \frac{1}{2}ab_x + \frac{1}{2}a_x b$$

Approximation of the split form can be written in conservative form: e.g.,

$$\frac{1}{2}D_0(ab)_j + \frac{1}{2}a_j D_0 b_j + \frac{1}{2}b_j D_0 a_j = \frac{1}{4}D_+(a_j + a_{j-1})(b_j + b_{j-1})$$

D_0: 2nd-order central, $D_+ u_j = (u_{j+1} - u_j)/\Delta x$

The above can be generalized to 2pth-order accurate: *Ducros et al. 2000*

$$D_{0p}u_j = \sum_{k=1}^{p} \alpha_k^{(p)} D_0(k) u_j \qquad D_0(k)u_j = (u_{j+k} - u_{j-k})/(2k\Delta x)$$

$$\sum_{k=1}^{p} \alpha_k^{(p)} = 1 \qquad \sum_{k=1}^{p} \alpha_k^{(p)} k^{2n} = 0, \;\; n = 1, \ldots, p-1$$

Ducros et al. Splitting (Cont.)

(Improve nonlinear stability for high order central schemes)

Approximation of the 2p^th^-order split form in conservation form:

$$\frac{1}{2}D_p(ab) + \frac{1}{2}D_p(a)b + \frac{1}{2}aD_p(b) =$$

$$\frac{1}{\Delta x}\sum_{k=1}^{p}\frac{1}{2}\alpha_k\left((a_{j+k}b_{j+k} - a_{j-k}b_{j-k}) + a_j(b_{j+k} - b_{j-k}) + (a_{j+k} - a_{j-k})b_j\right)$$

$$= \frac{1}{\Delta x}\sum_{k=1}^{p}\frac{\alpha_k}{2}\left(\sum_{m=0}^{k-1}(a_{j-m} + a_{j+k-m})(b_{j-m} + b_{j+k-m})\right.$$

$$\left.-\sum_{m=0}^{k-1}(a_{j-1-m} + a_{j-1+k-m})(b_{j-1-m} + b_{j-1+k-m})\right) = \frac{1}{\Delta x}(h_{j+1/2} - h_{j-1/2})$$

$2p^{th}$-order Central Ducros et al. Splitting Numerical Flux for 3D Gas Dynamics

3D Inviscid Flux Derivative in x-Direction:

$$\mathbf{f} = ([\rho u, \rho u^2 + p, \rho uv, \rho uw, (e+p)u]^T$$

$2p^{th}$-order Numerical Flux in x-Direction $\mathbf{h}_{j+1/2}$:

$$\mathbf{h}_{j+1/2} =$$

$$\frac{1}{2}\sum_{k=1}^{p}\alpha_k \sum_{m=1}^{k-1}\begin{pmatrix} (\rho_{j-m}+\rho_{j+k-m})(u_{j-m}+u_{j+k-m}) \\ (\rho_{j-m}u_{j-m}+\rho_{j+k-m}u_{j+k-m})(u_{j-m}+u_{j+k-m})+p_{j-m}+p_{j+k-m} \\ (\rho_{j-m}v_{j-m}+\rho_{j+k-m}v_{j+k-m})(u_{j-m}+u_{j+k-m}) \\ (\rho_{j-m}w_{j-m}+\rho_{j+k-m}w_{j+k-m})(u_{j-m}+u_{j+k-m}) \\ (e_{j-m}+p_{j-m}+e_{j+k-m}+p_{j+k-m})(u_{j-m}+u_{j+k-m}) \end{pmatrix}$$

High Order Entropy Conservative Methods

(One way to improve numerical stability & minimize added numerical dissipation)

- Numerical solutions satisfy additional discretized conservation law
- Low order entropy conservative methods with linear numerical dissipation for shock-capturing require further accuracy improvement
  (Tadmor 1984 – gas dynamics; Janhunen 2000 – MHD; Winters & Gassner 2016 – MHD)
- High order entropy conservative methods for central schemes
  (Fjordholm et al. (2012) – ENO; Sjogreen & Yee 2016, 2017– central + nonlinear filter, gas dynamics & MHD)

MHD:

Four forms of the MHD equations to be considered

> Conservative form
> Godunov/Powell symmetrizable form (non-conservative)
> Janhunen form: (Div B) terms not included in the gas dynamics part of the equations)
> Brackbill & Barnes form

Three forms of the entropy fluxes to be considered

> Winter & Gassner (2016), Chandrasheka & Klingenbery (2016), Sjogreen & Yee (2016)

Well-Balanced High Order Nonliner Filter Schemes
Non-Reacting & Reacting Flows

Yee et al., *1999-2017, Sjogreen &Yee, 2004-2017,* **Wang et al.**, *2009-2010. Kotov et al., 2012-2016*

Preprocessing step

Condition (equivalent form) the governing equations by, e.g., *Yee et al. Entropy Splitting & Ducros et al. Splitting* to improve numerical stability

High order low dissipative base scheme step (Full time step)

- High order **Central, DRP, or Entropy Conser. Num. Flux** scheme
- SBP numerical boundary closure, matching spatial & temporal order conservative metric evaluation *Vinokur & Yee, Sjögreen & Yee, Yee & Vinokur* (2000-2014)

Nonlinear filter step

- Filter the base scheme step solution by a dissipative portion of **any** positive high-order shock capturing scheme, e.g., **7th-order positive WENO**
- Use local flow sensor to control the amount & location of the nonlinear numerical dissipation to be employed

Well-balanced scheme: preserve certain non-trivial physical steady state solutions of reactive eqns exactly

Note: "Nonlinear Filter Schemes" not to be confused with "LES filter operation"

Nonlinear Filter Step $(U_t + F_x(U) = 0)$

- **Denote the solution by the base scheme (e.g. 6^{th} order central, $4th$ order RK)**

$$U^* = L^*(U^n)$$

- **Solution by a nonlinear filter step**

$$U_j^{n+1} = U_j^* - \frac{\Delta t}{\Delta x}\left[H_{j+1/2} - H_{j-1/2}\right]$$
$$H_{j+1/2} = R_{j+1/2}\overline{H}_{j+1/2}$$

$\overline{H}_{j+1/2}$ **- numerical flux,** $R_{j+1/2}$ **- right eigenvector, evaluated at the Roe-type averaged state of** U_j^*

- **Elements of** $\overline{H}_{j+1/2}$**:**

$$\overline{h}_{j+1/2} = \frac{\kappa_{j+1/2}^m}{2}\left(s_{j+1/2}^m\right)\left(\phi_{j+1/2}^m\right)$$

$\phi_{j+1/2}^m$ ***- Dissipative portion of a shock-capturing scheme***
$s_{j+1/2}^m$ ***- Local flow sensor (indicates location where dissipation needed)***
$\kappa_{j+1/2}^m$ ***- Controls the amount of*** $\phi_{j+1/2}^m$

Improved High Order Filter Method

Form of nonlinear filter

$$\bar{h}_{j+1/2} = \frac{\kappa^m_{j+1/2}}{2} \left(s^m_{j+1/2} \right) \left(g^m_{j+1/2} - b^m_{j+1/2} \right)$$

Control amount of dissipation based on local flow condition

Local flow sensor *(Shock Sensor, ACM (Harten), Ducros et al, Multiresolution wavelet, etc.)*

Any High Order Shock capturing numerical flux *(e.g. WENO7)*

High order central numerical flux *(e.g. 8th order central)*

2007 – κ = global constant
2009 – $\kappa_{j+1/2}$ = local, evaluated at each grid point
Simple modification of κ *(Yee & Sjögreen, 2009)*

$$\kappa = f(M) \cdot \kappa_0$$

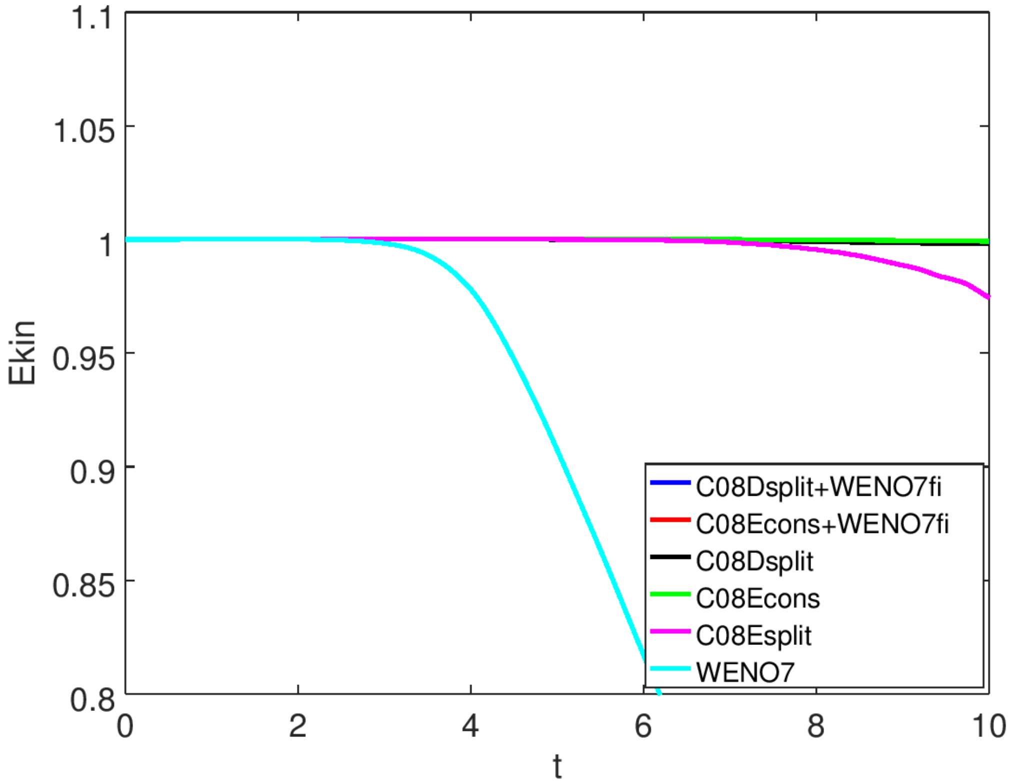
$$f(M) = min\left(\frac{M^2}{2} \frac{\sqrt{4 + (1 - M^2)^2}}{1 + M^2}, 1 \right)$$

For other forms of $\kappa_{j+1/2}, s_{j+1/2}$, see *(Yee & Sjögreen, 2009)*

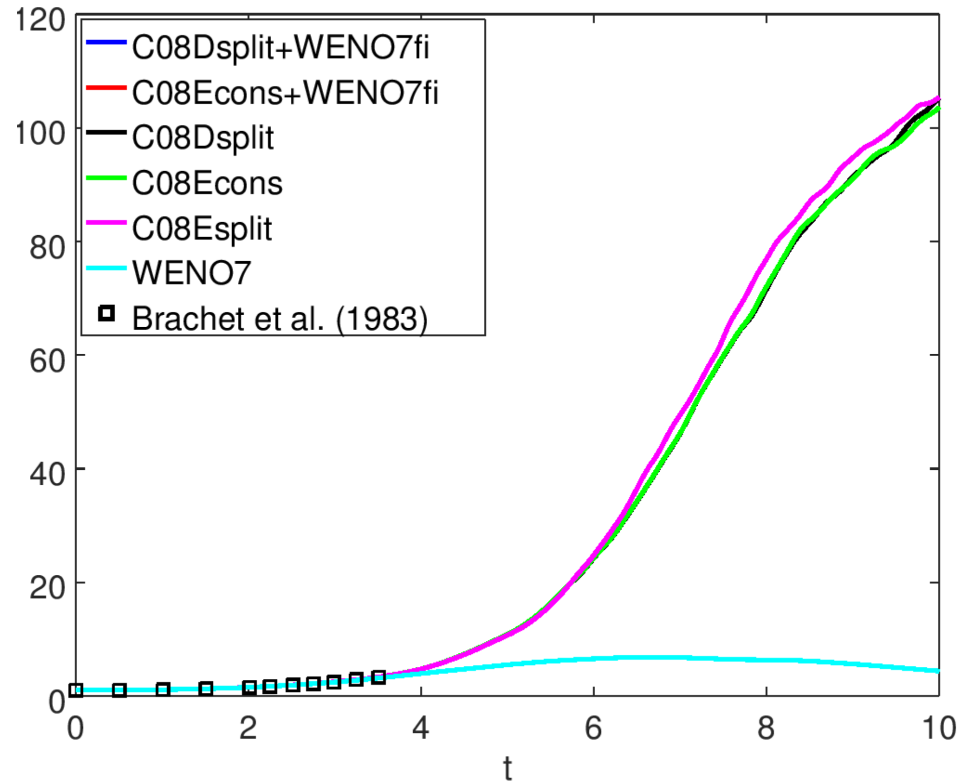
3D Taylor-Green Vortex (Compressible & Inviscid)

(Comparison of Skew-Symmetric splitting & Entropy Conservative Methods, 64^3 grids)

Kinetic Energy



Enstrophy



C08Dsplit+WENO7fi: 8^{th}-order central + Ducros et al. split +WENO7fi

C08Econs+WENO7fi: 8^{th}-order central entropy conservative flux + WENO7fi

C08Dsplit: 8^{th}-order central + Ducros et al. split

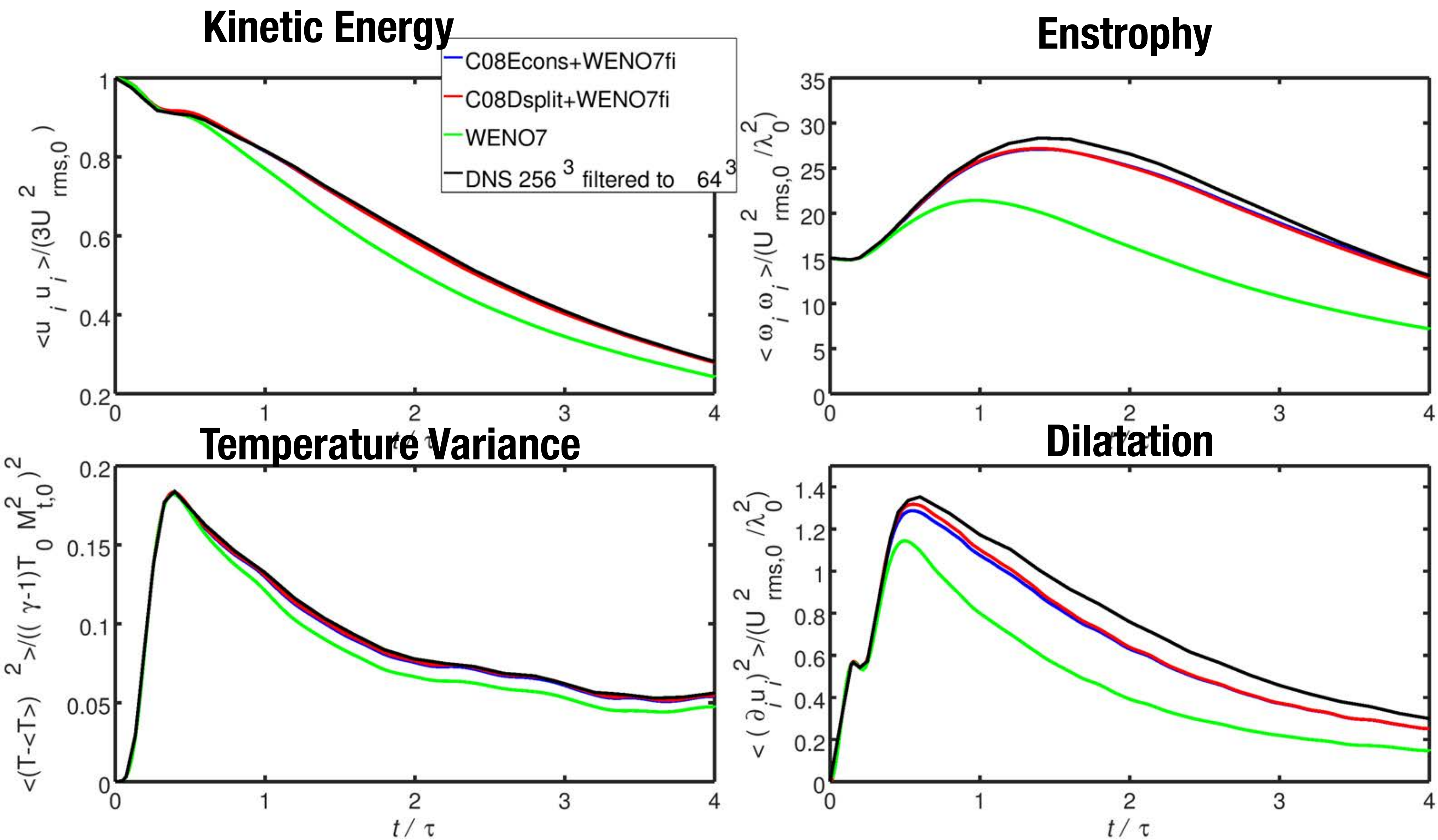
C08Econs: 8^{th}-order central Entropy conservative flux

C08Esplit: 8^{th}-order central + Entropy split

WENO7: Standard WENO7

3D Isotropic Turbulence with Shocklets

(Comparison of Skew-Symmetric splitting & Entropy Conservative Methods, 64^3 grids)

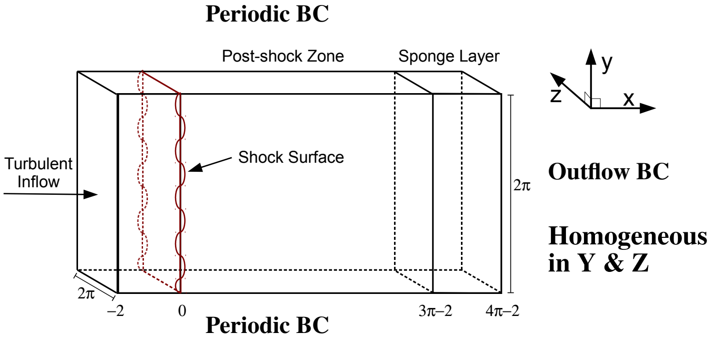


3D Shock-Turbulence Interaction Test Case

(Amplification of Turbulence Across a Supersonic Shock Wave: Supersonic flow over wings, fins, control surfaces & inlets)

What is needed:

- **Inflow BC:** **DNS of isotropic turbulence** *(from Larsson & Lele, Phys. Fluid, 2009)*
- **Sponge layer** **reduce domain size**
- **Compute back pressure** **to obtain mean stationary shock**



Sponge source term: $W = -\frac{k_0 u_0}{2\pi}\left(\frac{x - x_{sp}}{x_{max} - x_{sp}}\right)(f - <f>_{yz})$

(Gently drive the flow towards a laminar state)

Turbulence Across a Supersonic Shock Wave

(Turbulent eddies are compressed & amplified upon passing though a stationary shock)

Problem parameters:

$M = 1.5$ **or** $M = 3.0$

$M_t = 0.16$

$Re_\lambda = 40$ (Taylor microscale Re)

$Pr = 0.7$

$k_0 = 4$ (Inflow peak energy wavenumber)

DNS grid: 1553×256^2

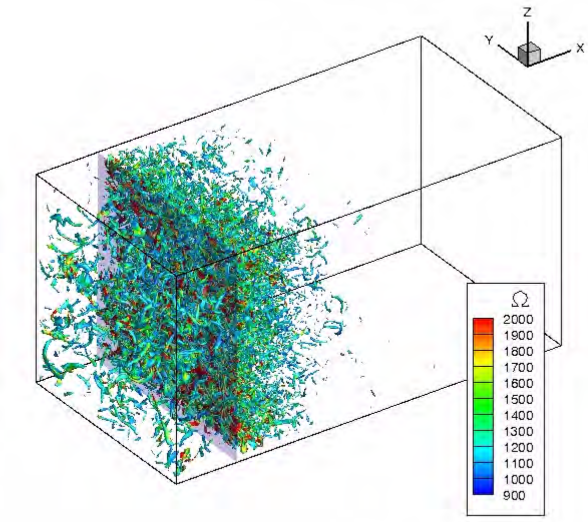
LES grid 1/2: 777×128^2

LES grid 1/4: 389×64^2

$\Delta_Z = \Delta_Y = 3\Delta_X$

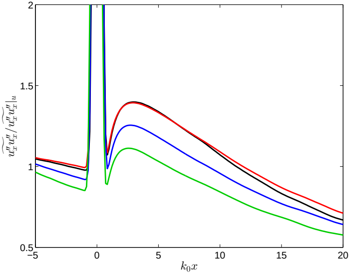
Num. Method: **WENO7fi+split**

Q-criterion isosurface, colored by vorticity magnitude

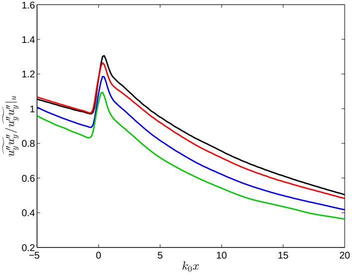


CDNS: Scheme Comparison, 389×64^2, $M = 1.5$

Streamwise Reynolds Stress



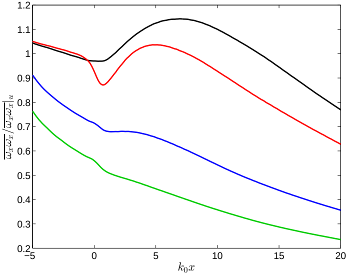
Streamwise Vorticity



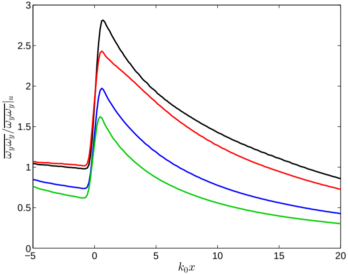
- Filtered DNS
- WENO7fi+split
- WENO7
- WENO5

All: No LES Model

Streamwise Vorticity



Transverse Vorticity



WENO7fi+splt:

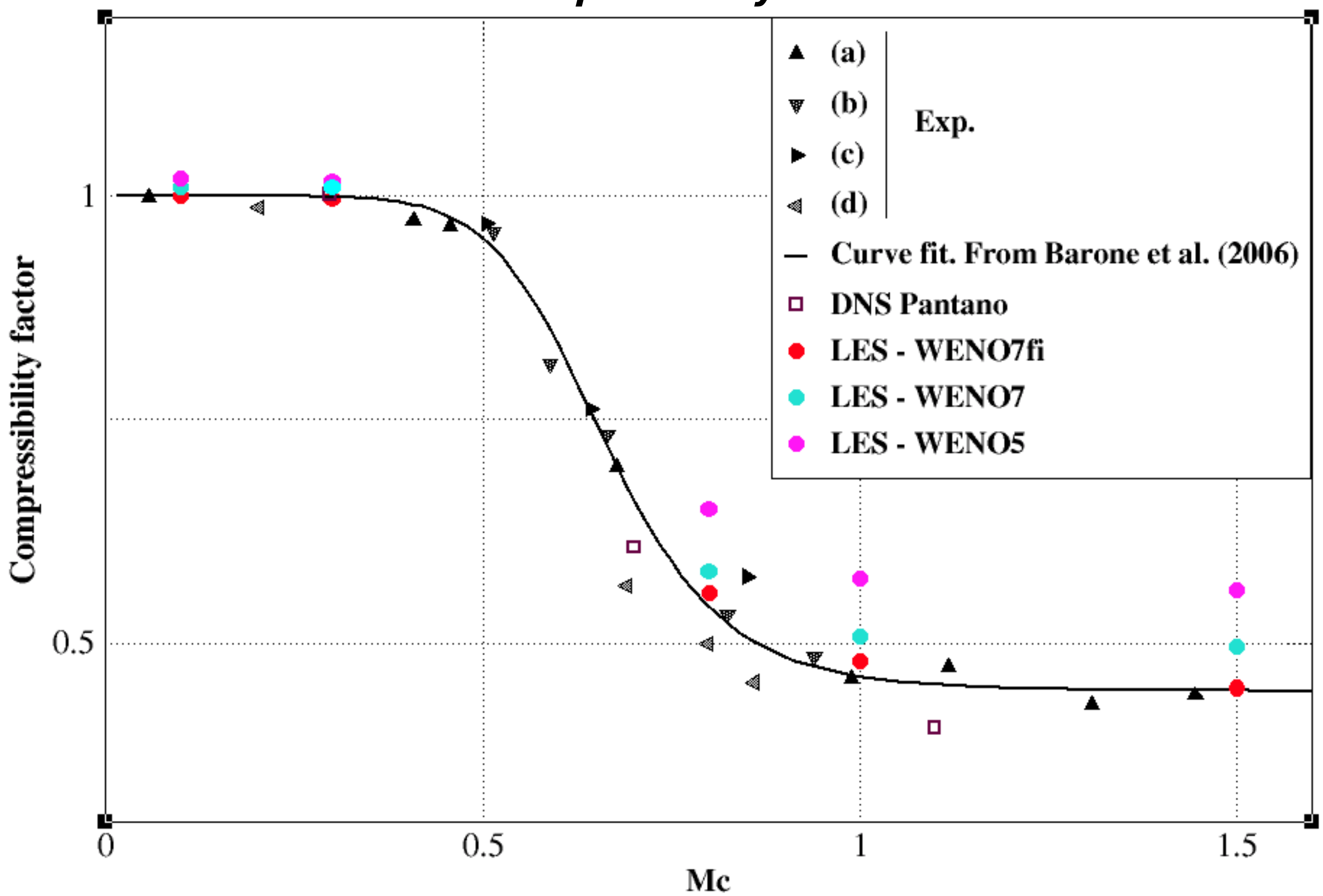
- 8^{th}-order central & Ducros split
- 7^{th}-order WENO filter, **diss. in 3D**
- Ducros et al. sensor, **D = 0.01**

LES of 3-D Temporal Mixing Layer with Shocks

(Mach # up to hypersonic speed; M_C = 0.1, 0.8. 1.0, 1.5 & 2.0)

Final Re is as large as 30,000; **SGS Model: Germano-Lilly dynamic procedure**

Compressibility Factor



Solving Reactive Governing Equations

(Different Procedures in solving the Governing Eqs. produce different spurious behavior)

Consider two typical procedures:

- **Fully coupled sysytem**
  - Consistent
  - Small time step due to numerical instability
- **Fractional method using the Strang Splitting of the system**
  - Commonly used in combustion for over 30 years
  - Can extend the valid CFL range but exhibits more complex spurious behavior

Strang Splitting (1968)

Split equations into convective & reactive parts

$$U_t + F(U)_x + G(U)_y = S(U)$$

Convective step

$$U_t + F(U)_x + G(U)_y = 0$$

A – Convective difference operator
(Full time step of WENO5 or WENO7, RK4)

Reactive step

$$\frac{dU}{dt} = S(U)$$

R – Reactive difference operator
(RK1, RK2, RK3, RK4)

Numerical solution: $U^{n+1} = A\left(\frac{\Delta t}{2}\right) R(\Delta t) A\left(\frac{\Delta t}{2}\right) U^n$
(At the next time level)

OR: $U^{n+1} = A\left(\frac{\Delta t}{2}\right) R\left(\frac{\Delta t}{N_r}\right) \cdots R\left(\frac{\Delta t}{N_r}\right) A\left(\frac{\Delta t}{2}\right) U^n$

N_r – number of subiterations

Subcell Resolution (SR) Method

Wang, Shu, Yee, & Sjögreen, 2012, JCP

Basic Approach

- Any high resolution shock capturing operator can be used in the convection step

  Test case: **WENO5, WENO7,** Roe flux, **RK4**
- Any standard shock-capturing scheme produces a few transition points in the shock

  ⇒ Solutions from the convection operator step, if applied directly to the reaction operator step, result in wrong shock speed

New Approach

Apply Subcell Resolution *(Harten 1989; Shu & Osher 1989)* **to the solution from the convection operator step before the reaction operator step**

Note: if $N_r > 1$ apply SR at each subiteration

High Order Methods with Subcell Resolution

Strang Splitting + Subcell Resolution (SR)

$$U_t + F(U)_x + G(U)_y = S(U)$$

Convective step

$$U_t + F(U)_x + G(U)_y = 0$$

$$A \rightarrow U^*$$

Convective difference operator

(Full time step of WENO5 or WENO7, RK4)

SR step

$$SR \rightarrow U^{**}$$

SR operator

(No time involved)

Reactive step

$$\frac{dU}{dt} = S(U)$$

$$R \rightarrow U^{n+1}$$

Reaction difference operator

(RK1, RK2, RK3, RK4)

Numerical solution: $U^{n+1} = A^*\left(\frac{\Delta t}{2}\right) R(\Delta t) A^*\left(\frac{\Delta t}{2}\right) U^n$
(At the next time level)

OR: $U^{n+1} = A^*\left(\frac{\Delta t}{2}\right) R\left(\frac{\Delta t}{N_r}\right) \cdots R\left(\frac{\Delta t}{N_r}\right) A^*\left(\frac{\Delta t}{2}\right) U^n$

A^* operator includes SR step correction at shocks
N_r – number of subiterations

Subcell Resolution Step

New Approach: **Apply Subcell Resolution** *(Harten 1989; Shu & Osher 1989)* **to the solution from the convection operator step before the reaction operator**

I. **Locate the shock by examining the mass fraction z_{ij} in X (Harten's indicator)**

x-direction: $s^x_{ij} = minmod(z_{i+1,j} - z_{ij}, z_{ij} - z_{i-1,j})$

Shock present in the cell I_{ij} if

$$|s^x_{i,j}| \geq |s^x_{i,j-1}| \text{ and } |s^x_{i,j}| \geq |s^x_{i,j+1}|$$

y-direction: $s^y_{ij} = minmod(z_{i,j+1} - z_{ij}, z_{ij} - z_{i,j-1})$

II. **Apply subcell resolution in the direction for which a shock has been detected. If both directions require subcell resolution – choose the largest jump**

$$s^x_{ij} \text{ or } s^y_{ij}$$

Subcell Resolution Step *(Cont.)*

For I_{ij} with shock present, $I_{i-q,j}$ and $I_{i+r,j}$ without shock present:

- **Compute ENO interpolation polynomials P_{i-q} and P_{i+r}**
- **Modify points in the vicinity of the shock (mass fraction z_{ij}, temperature T_{ij} and density ρ_{ij})**

$$\begin{pmatrix} \tilde{z}_{ij} \\ \tilde{T}_{ij} \\ \tilde{\rho}_{ij} \end{pmatrix} = \begin{pmatrix} P_{i-q,j}(x_i, z) \\ P_{i-q,j}(x_i, T) \\ P_{i-q,j}(x_i, \rho) \end{pmatrix}, \ \theta \geq x_i \qquad \begin{pmatrix} \tilde{z}_{ij} \\ \tilde{T}_{ij} \\ \tilde{\rho}_{ij} \end{pmatrix} = \begin{pmatrix} P_{i+r,j}(x_i, z) \\ P_{i+r,j}(x_i, T) \\ P_{i+r,j}(x_i, \rho) \end{pmatrix}, \ \theta < x_i$$

θ Determined by the conservation of energy E:

$$\int_{x_{i-1/2}}^{\theta} p_{i-s,j}(x;E)dx + \int_{\theta}^{x_{i+1/2}} p_{i+r,j}(x;E)dx = E_{ij}\Delta x$$

III. Reaction Step: Apply Reaction difference operator on SR solution to obtain U^{n+1}

$$(\rho z)_{ij}^{n+1} = (\rho z)_{ij}^{n} + \Delta t S(\tilde{T}_{ij}, \tilde{\rho}_{ij}, \tilde{z}_{ij})$$ **– e.g. explicit Euler**

I_{ij} – shock center location,
$I_{i-q,j}$ & $I_{i+r,j}$ – closest points to the shock (to the left and to the right)

1D C-J Detonation Wave

(Helzel et al. 1999; Tosatto & Vigevano 2008)

Left state (totally burned gas)

Right state (totally unburned gas)

$$\begin{pmatrix} \rho_b \\ u_b \\ p_b \end{pmatrix} = \begin{pmatrix} \rho_u \dfrac{[p_b(\gamma+1)-p_u]}{\gamma p_b} \\ S_{CJ}-(\gamma p_b/\rho_b)^{1/2} \\ -b+(b^2-c)^{1/2} \end{pmatrix}$$

$$\begin{pmatrix} \rho_u \\ u_u \\ p_u \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$S_{CJ}=[\rho_u u_u+(\gamma p_b \rho_b)^{1/2}]/\rho_u$$

$$b=-p_u-\rho_u q_0(\gamma-1) \qquad c=p_u^2+2(\gamma-1)p_u\rho_u q_0/(\gamma+1)$$

Ignition temperature $T_{ign}=25$

Heat release $q_0=25$

Rate parameter $K_0=16418$

$$K(T)=K_0 \exp\left(\frac{-T_{ign}}{T}\right)$$

Wrong Propagation Speed of Discontinuities

(Standard Shock-Capturing Schemes: TVD, WENO5, WENO7)

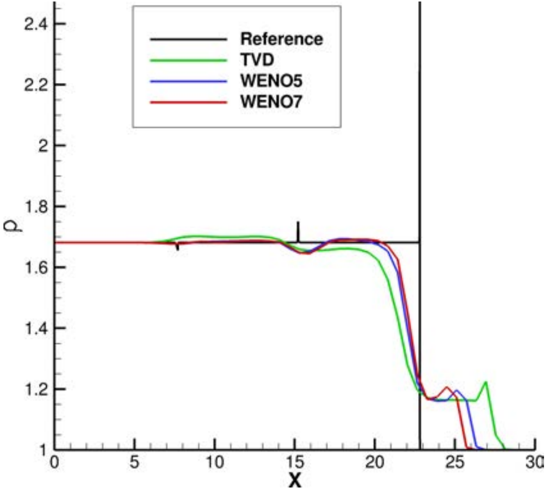
Chapman-Jouguet (C-J) 1D detonation wave

Arrhenius reaction rate:

$$K(T) = K_0 \exp\left(\frac{-T_{ign}}{T}\right)$$

K_0 can be large (stiff coeff.)

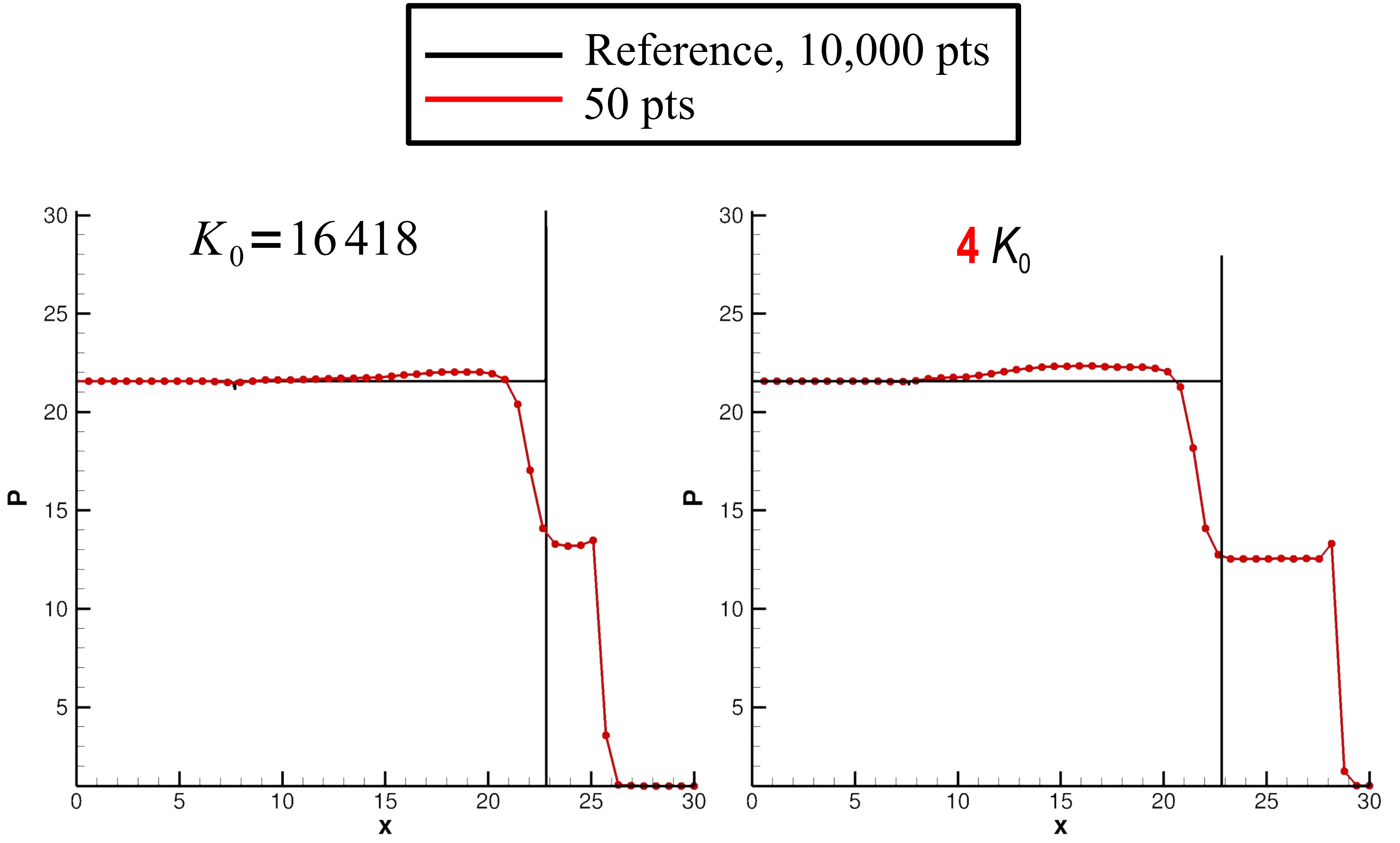
50 pts *(Ref. 10,000 pts)*, $K_0 = 16,418$



Note: Wrong propagation speed becomes more pronounced as K_0 increases

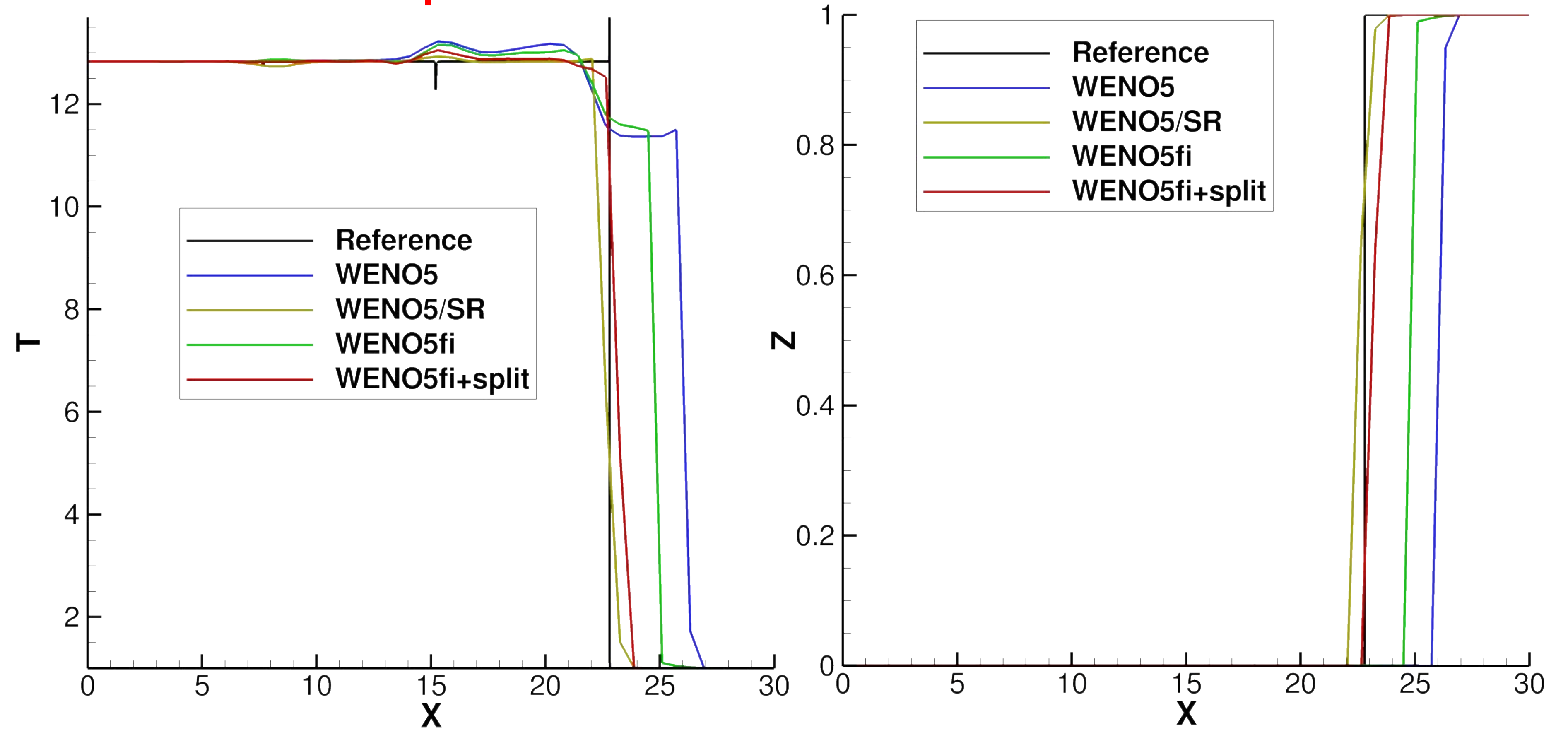
Wrong Propagation Speed of Discontinuities

(WENO5, Two Stiff Coefficients, 50 pts)



1D C-J Detonation (K_0 = 16418, 50 pts)

tend = 1.7



Standard Meth. – WENO5: Standard 5th order WENO (WENO7, TVD)

Improved Meth. –
- WENO5/SR: WENO5 + subcell resolution
- WENO5fi: filter version of WENO5
- WENO5fi+split: WENO5fi + preprocessing (Ducros splitting)

Reference: WENO5, 10,000 points

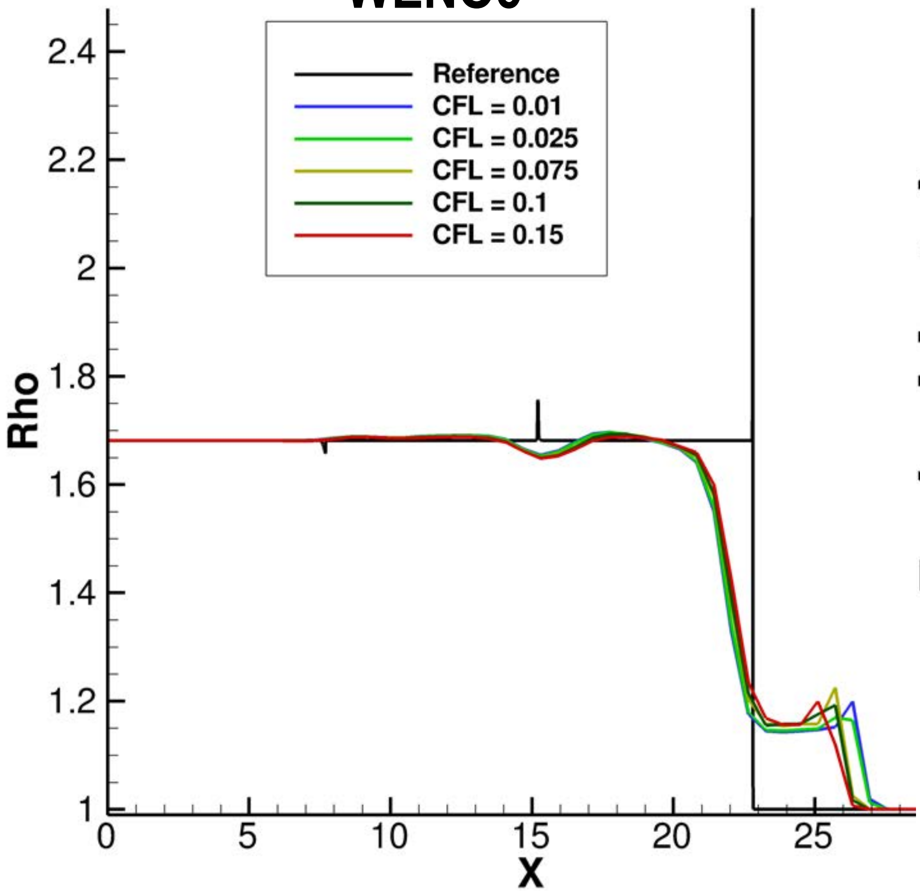
(Strang Splitting & Safeguard)

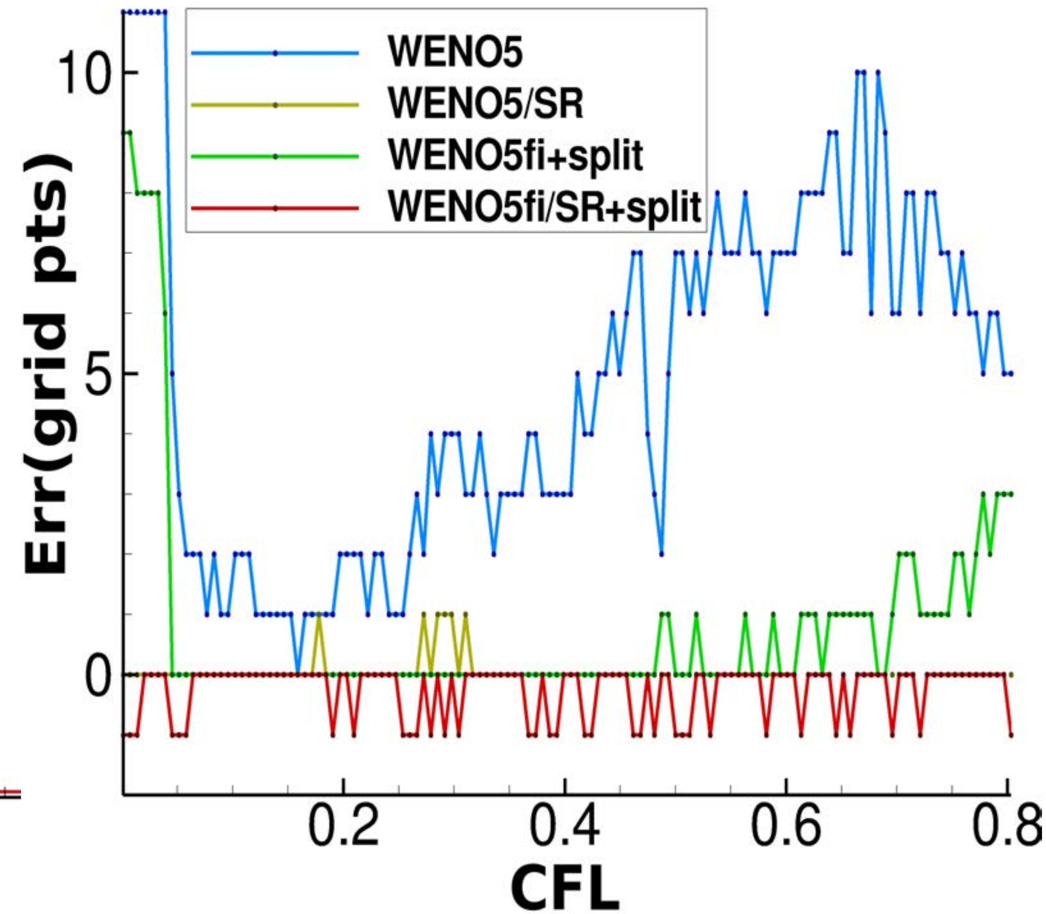
Behavior of the schemes below CFL limit

(Allowable Δt below CFL limit, consists of disjoint segments)

Strang Splitting & Safeguard, 50 pts, 100 K_0

Density by different CFL
WENO5





- ***Incorrect or diverged solution may occur for Δt below CFL limit.***
- ***CFL limit based on the convection part of PDEs***
- ***Confirms the study by Lafon & Yee and Yee et al. (1990 - 2000)***

MHD (Four Forms)
(Conservative, Godunov/Powell, Janhunen, Brackbill & Barnes)

1D MHD:

$$\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ B^{(x)} \\ B^{(y)} \\ B^{(z)} \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p + \frac{1}{2}|\mathbf{B}|^2 - B^{(x)}B^{(x)} \\ \rho uv - B^{(x)}B^{(y)} \\ \rho uw - B^{(x)}B^{(z)} \\ u(e + p + \frac{1}{2}|\mathbf{B}|^2) - B^{(x)}\mathbf{u}^T\mathbf{B} \\ 0 \\ uB^{(y)} - vB^{(x)} \\ uB^{(z)} - wB^{(x)} \end{pmatrix}_x + \mathbf{e}_G B_x^{(x)} = \mathbf{0}$$

Variants: replace $\mathbf{e}_G = (0,\ B^{(x)},\ B^{(y)},\ B^{(z)},\ \mathbf{u}^T\mathbf{B},\ u,\ v,\ w)^T$ by

$$\mathbf{e}_J = (0,\ 0,\ 0,\ 0,\ 0,\ u,\ v,\ w)$$

or

$$\mathbf{e}_B = (0,\ B^{(x)},\ B^{(y)},\ B^{(z)},\ 0,\ 0,\ 0,\ 0)$$

or by $\mathbf{0}$. $B_x^{(x)}$ is divergence of $\mathbf{B}$ in 3D.

3-D Compressible MHD (Ideal)

$$\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ B_x \\ B_y \\ B_z \end{pmatrix}_t + \mathrm{div} \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u}\mathbf{u}^T + (p + \frac{1}{2}B^2)I - \mathbf{B}\mathbf{B}^T \\ \mathbf{u}(e + p + \frac{1}{2}B^2) - \mathbf{B}(\mathbf{u}^T\mathbf{B}) \\ \mathbf{u}\mathbf{B}^T - \mathbf{B}\mathbf{u}^T \end{pmatrix} = 0$$

Conservative

$$\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ B_x \\ B_y \\ B_z \end{pmatrix}_t + \mathrm{div} \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u}\mathbf{u}^T + (p + \frac{1}{2}B^2)I - \mathbf{B}\mathbf{B}^T \\ \mathbf{u}(e + p + \frac{1}{2}B^2) - \mathbf{B}(\mathbf{u}^T\mathbf{B}) \\ \mathbf{u}\mathbf{B}^T - \mathbf{B}\mathbf{u}^T \end{pmatrix} = -(\nabla \cdot \mathbf{B}) \begin{pmatrix} 0 \\ B_x \\ B_y \\ B_z \\ \mathbf{u}^T\mathbf{B} \\ u \\ v \\ w \end{pmatrix}$$

Non-conservative (Symmetrizable - *Godunov, Powell*)

$$\mathbf{u} = (u, v, w)^T$$

$$\mathbf{B} = (B_x, B_y, B_z)^T$$

$$B^2 = B_x^2 + B_y^2 + B_z^2$$

$$p = (\gamma - 1)(e - \frac{1}{2}\rho(u^2 + v^2 + w^2) - \frac{1}{2}(B_x^2 + B_y^2 + B_z^2))$$

Non-uniqueness of Ducros et al. Splitting for MHD

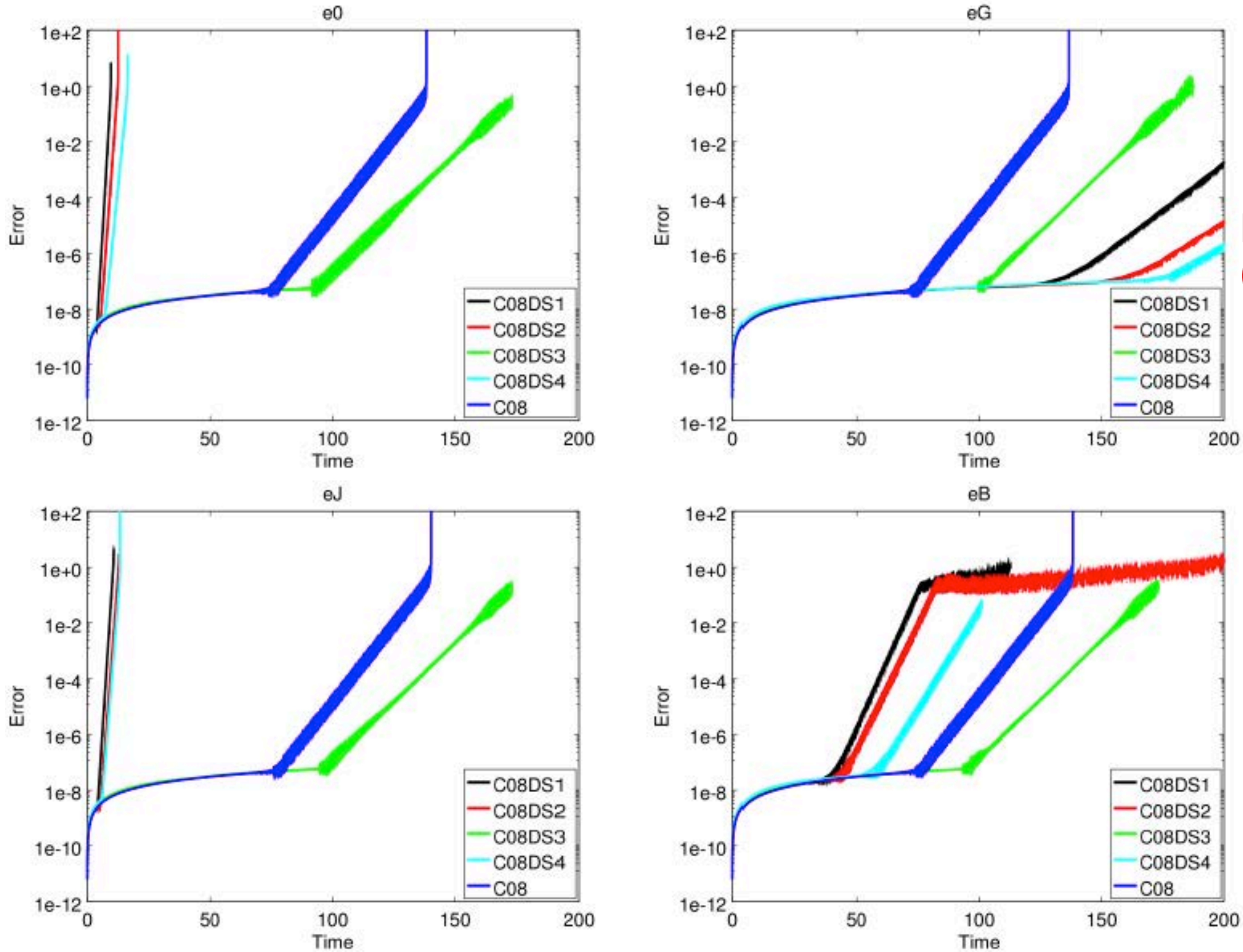
(Minimize the use of numerical dissipation for high order central schemes)

- **MHD inviscid (ideal) flux derivatives consist of triple products of conservative variables & their derivatives**
- **No unique guidelines in splitting triple products of derivatives (more choices than their gas dynamics counterparts)**
  (See Sjogreen & Yee, ICOSAHOM-2016 & Journal version for the chosen forms)
- **4-Forms: Split all 8 flux derivatives, partial or just the gas dynamic portion (all recover to split form of gas dynamics when MHD not present)**
  (Results compare with no splitting)
- **Four forms of the MHD Equations to be solved:**
  - > Conservative form (no split)
  - > Godunov/Powell symmetrizable form (non-conservative)
  - > Janhunen form: (Div B) terms not included in the gas dynamics part of the equations)
  - > Brackbill & Barnes form

The above consists of 12 combinations for the current study

Alfven Wave Smooth Flow Test Case (Max. Norm Errors vs. Time)

(4 MHD & 4 Ducros et al. 8th-order Split Method Comparison with 8th-order Classical central)



Best:
C08DS4 by eG

Four MHD: e0, eG, eJ & eB
Four Split Methods: DS1, DS2, DS3 & DS4

Compressible Orszag-Tang Vortex $(\gamma = 5/3)$

I.C.

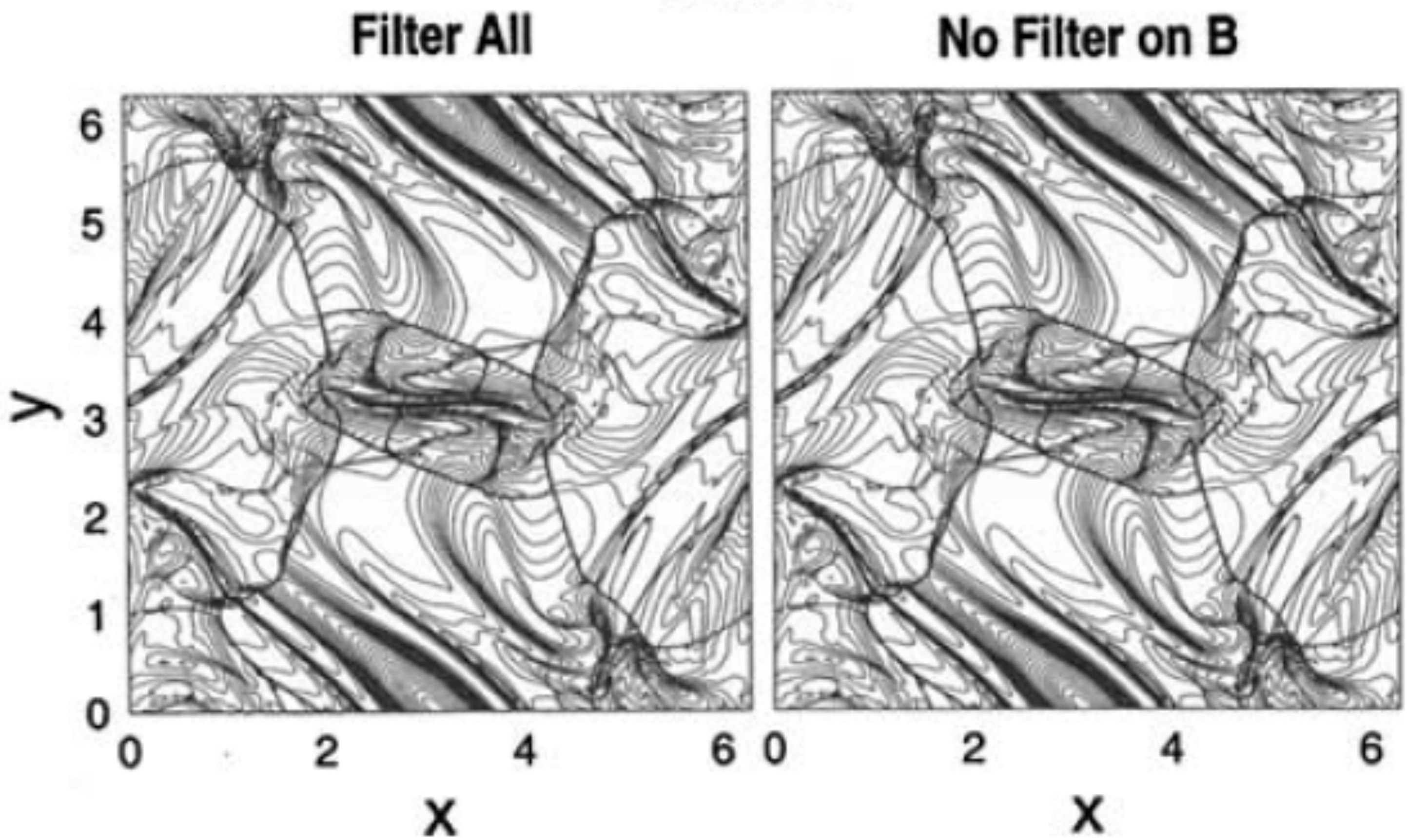
$$\begin{pmatrix} \rho \\ u \\ v \\ w \\ p \\ B_x \\ B_y \\ B_z \end{pmatrix} = \begin{pmatrix} 25/9 \\ -\sin y \\ \sin x \\ 0 \\ 5/3 \\ -\sin y \\ \sin 2x \\ 0 \end{pmatrix}$$

BC: Periodic

Domain: $0 < x < 2\pi$
$0 < y < 2\pi$

Density at T=3.14
WAV66+AD8

801 x 801



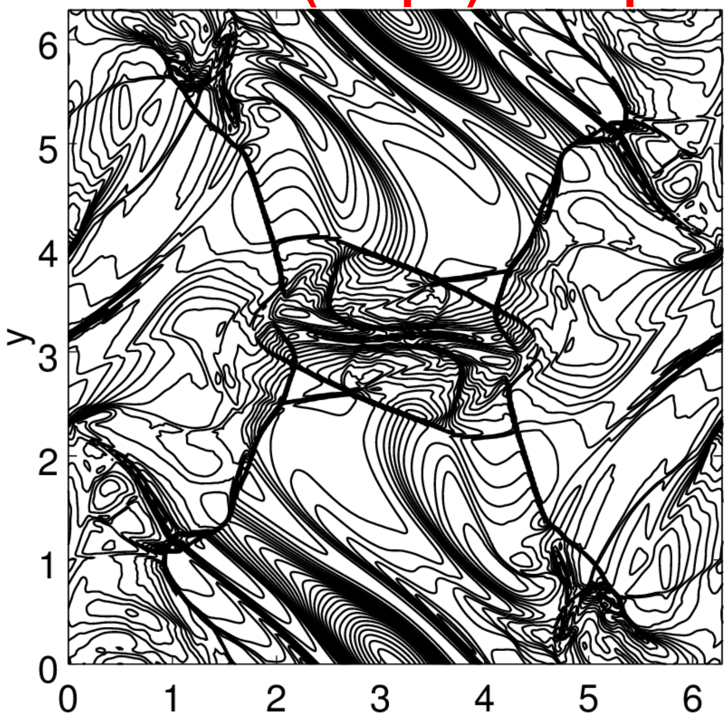
Ducros et al. Splitting *- Orszag-Tang Vortex Test case*

(Only on the Gas Dynamic Variables)

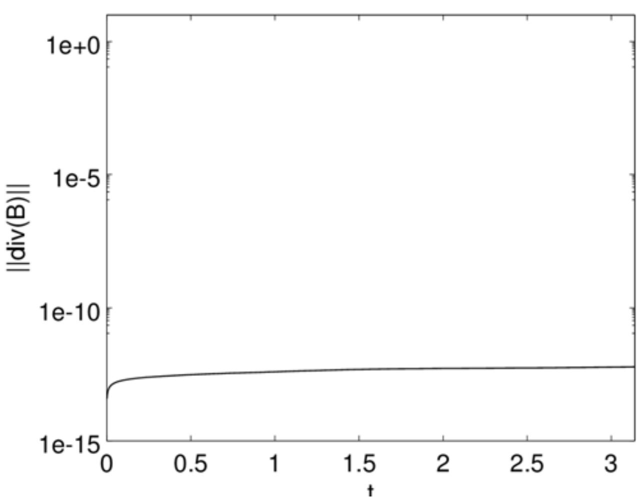
WENO5fi (no split) + Dissp

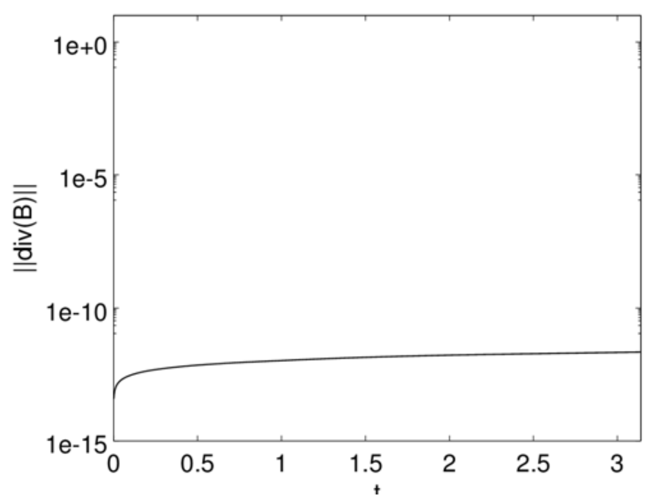
WENO5fi+split

Density



divB History





Summary

(Split Centered Schemes & Entropy Conservative centered (EC) Methods)

GAS dynamics:

- Split centered schemes can improve nonlinear stability for smooth flows in general
- Nonlinear filter version of split schemes can improve stability & accuracy for DNS & LES
- High order entropy conserving methods (centered or nonlinear filter version) provide similar stability & accuracy improvement as split schemes

MHD:

- Split centered schemes can improve nonlinear stability in general for smooth flows but MHD equation dependent
- Nonlinear filter version of split schemes can improve stability & accuracy for flows with discontinuities but MHD equations dependent
- High order entropy conserving methods (centered or nonlinear filter version) can provide different stability & accuracy improvement, depending on the forms of the MHD equations & the choice of entropy fluxes

Concluding Remarks

(Compressible Gas Dynamics of a Wide Spectrum of Flow Types)

Stability Improvement by Skew-Symmetric Splitting

Smooth Flows: *Stable without added high order linear numerical dissipation*

> Semi-Conservative Entropy Splitting with summation-by-part (SBP) boundary closure energy norm bound *(Yee et al. 1999-2007, Sandham et al. 2002-present)*

- *Most accurate & stable among the considered three splittings*

> Ducros et al. splitting

- *Improved stability*
- *Smaller improvement than Entropy Splitting*

Flows with shocks: *Under the Yee et al. nonlinear filter framework*

Ducros et al. Splitting Employs Two Types of Central Scheme:

> *Classical high order central (6th-order & 8th-order)*

> *Three DRP (4th-order, 7-point & 9-point grid stencils)*

Among studied test cases

Classical central schemes provide slightly more improvement than DRP

Significance

- The key advantage of the adaptive flow sensor is that no a priori knowledge of the flow structure of the entire evolution is needed, even for compressible shock-free turbulence & low speed turbulence with shocklets.
- The proposed developments provide an improved predictability & reliability of CFD turbulent computations containing both low speed and high speed regimes that can be compromised by standard high order shock-capturing schemes without a proper numerical dissipation control.

High Order Numerical Method Development in MHD

(Added Issues Beyond Compressible Gas Dynamics Developments)

MHD Equations:

> *Conservative Form* - *non-strictly hyperbolic system w/ degenerate identical eigenvalues*
> *Godunov/Powell Form (1972, 1994)* - *symmetrizable hyperbolic non-conservative system*
> *Janhunen Form (2000)*
> *Brackbill & Barnes (1980)*

Skew-symmetric Splitting of Inviscid Flux Derivatives: *Improve Stability & Minimize Num. Dissipation*

> *Yee et al. Entropy Splitting (2000) – Only for the gas dynamics portion*
> *Ducros et al. Splitting (2000) & Pirozzoli Generalization (2010) – Not unique*
> *High Order Extension of Tadmor Entropy Conservative Numerical Fluxes (Sjogreen & Yee, 2009) – can be viewed as a splitting*

Discrete Conservation Methods: *FV vs. FD & DG, etc; Low Order vs. High Order*

> *Entropy stable conservative numerical fluxes*
– *Low Order: Janhunen (2000), Winters & Gassner (2016), Chandrasekar-Klingenberg (2015)*
– *High Order: Sjogreen & Yee (2009) - Central, Fjordholm, Mishra & Tadmor (2012) - ENO, etc.*
> *Momentum conservation, Kinetic energy preservation, etc.*

Approximate Riemann Solver: *Extension of Roe's Average States*

> *Gallice average states (1997)*
> *Ismail & Roe (2009) – Logarithmic mean for entropy (not square root mean)*
. . .

Eigenvector Scaling: *(Roe & Balsara, 1996)*

3D Taylor-Green vortex
(Inviscid & Viscous Shock-Free Turbulence)

Computational Domain: 2π square cube, 64^3 grid.
(Reference solution on 256^3 grid)

Initial condition

$\rho = 1,$
$p = 100 + ([\cos(2z) + 2][\cos(2x) + \cos(2y)] - 2)/16,$
$u_x = \sin x \cos y \cos z$
$u_y = -\cos x \sin y \cos z$
$u_z = 0.$
Initial turbulent Mach number: $M_{t,0} = 0.042$
Final time: $t = 10$

Viscous case

$\mu/\mu_{ref} = (T/T_{ref})^{3/4}$
$\mu_{ref} = 0.005, T_{ref} = 1, Re_0 = 2040$

Compressible Isotropic Turbulence

(Low Speed Turbulence with Shocklets)

Computational Domain: 2π square cube, 64^3 grid.
(Reference solution on 256^3 grid)

Problem Parameters

Root-mean-square velocity: $u_{rms} = \sqrt{\frac{\langle u_i u_i \rangle}{3}}$

Turbulent Mach number: $M_t = \frac{\sqrt{\langle u_i u_i \rangle}}{\langle c \rangle}$

Taylor-microscale: $\lambda = \sqrt{\frac{\langle u_x^2 \rangle}{\langle (\partial_x u_x)^2 \rangle}}$

Taylor-microscale Reynolds number: $Re_\lambda = \frac{\langle \rho \rangle u_{rms} \lambda}{\langle \mu \rangle}$

Eddy turnover time: $\tau = \lambda_0 / u_{rms,0}$

Initial Condition: **Random solenoidal velocity field with the given spectra**

$E(k) \sim k^4 \exp(-2(k/k_0)^2)$

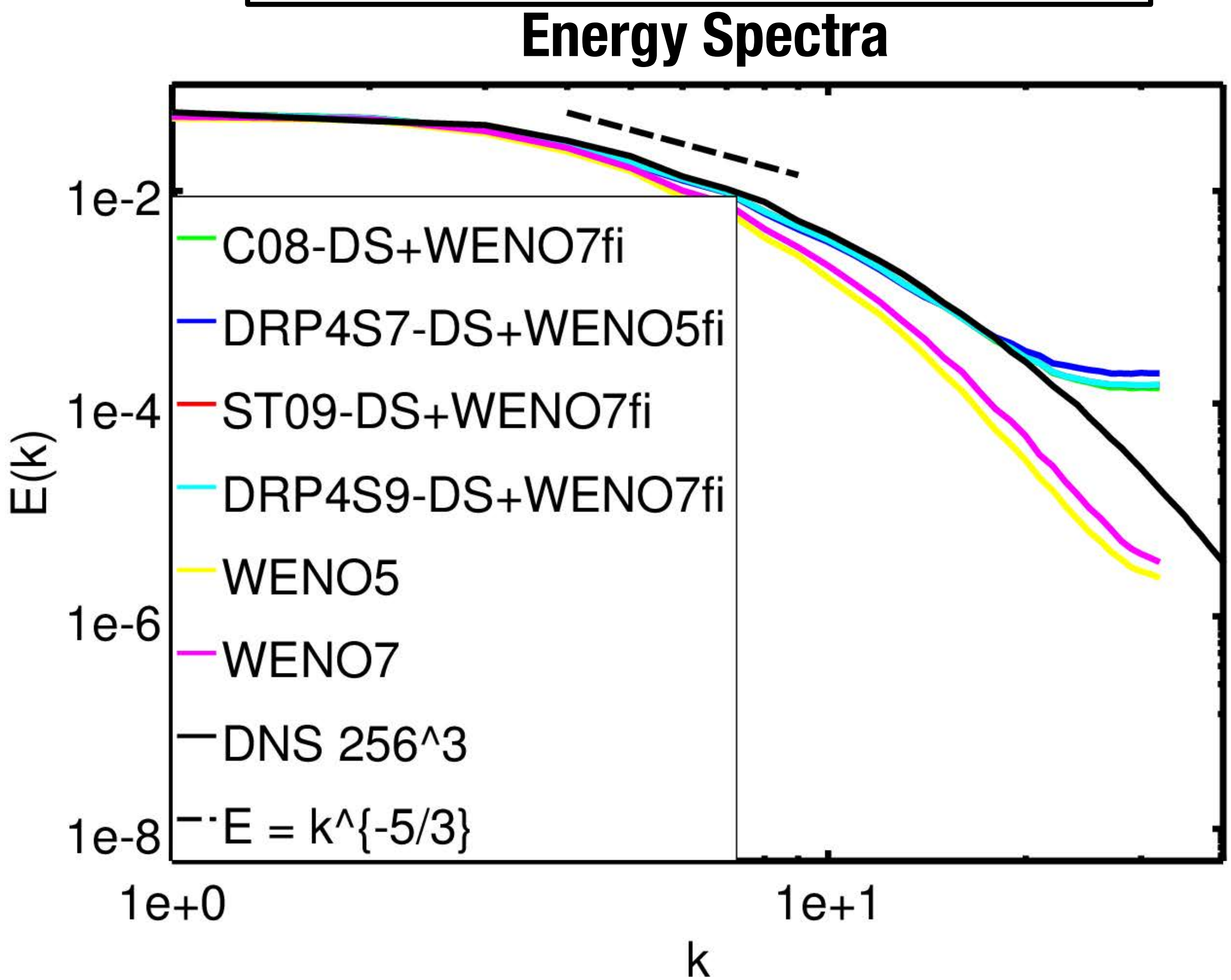
$\frac{3}{2} u_{rms,0}^2 = \frac{\langle u_{i,0} u_{i,0} \rangle}{2} = \int_0^\infty E(k) dk$

$u_{rms,0} = 1$, $k_0 = 4$, $\tau = 0.5$, $M_{t,0} = 0.6$, $Re_{\lambda,0} = 100$

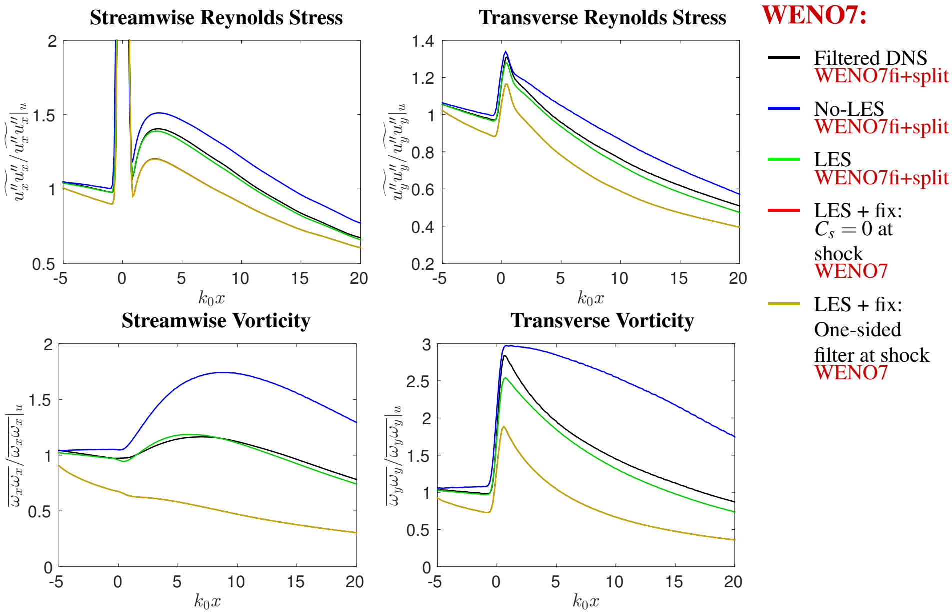
Final time: $t = 2$ **or** $t/\tau = 4$

3D Isotropic Turbulence with Shocklets
Compressible & Inviscid

Comparison of 6 Methods, 64^3 grids



LES: Filtering Procedures Comparison, 389×64^2, $M = 1.5$



Behavior of the Schemes Below CFL Limit

The examples on the next slides indicate different spurious behavior by following different numerical procedures for solving the governing equations:

- Strang splitting **with** Safeguard procedure
- Strang splitting **without** Safeguard procedure
- **No-**Strang splitting **with** Safeguard procedure
- **No-**Strang splitting **without** Safeguard procedure

Scalar Case Behavior of WENO5 & WENO5/SR below CFL limit

(Obtaining the Correct Discontinuity Speed)

Source term:

$S = K_0(1-u)(u-0.5)u$

$K_0 = 10{,}000$

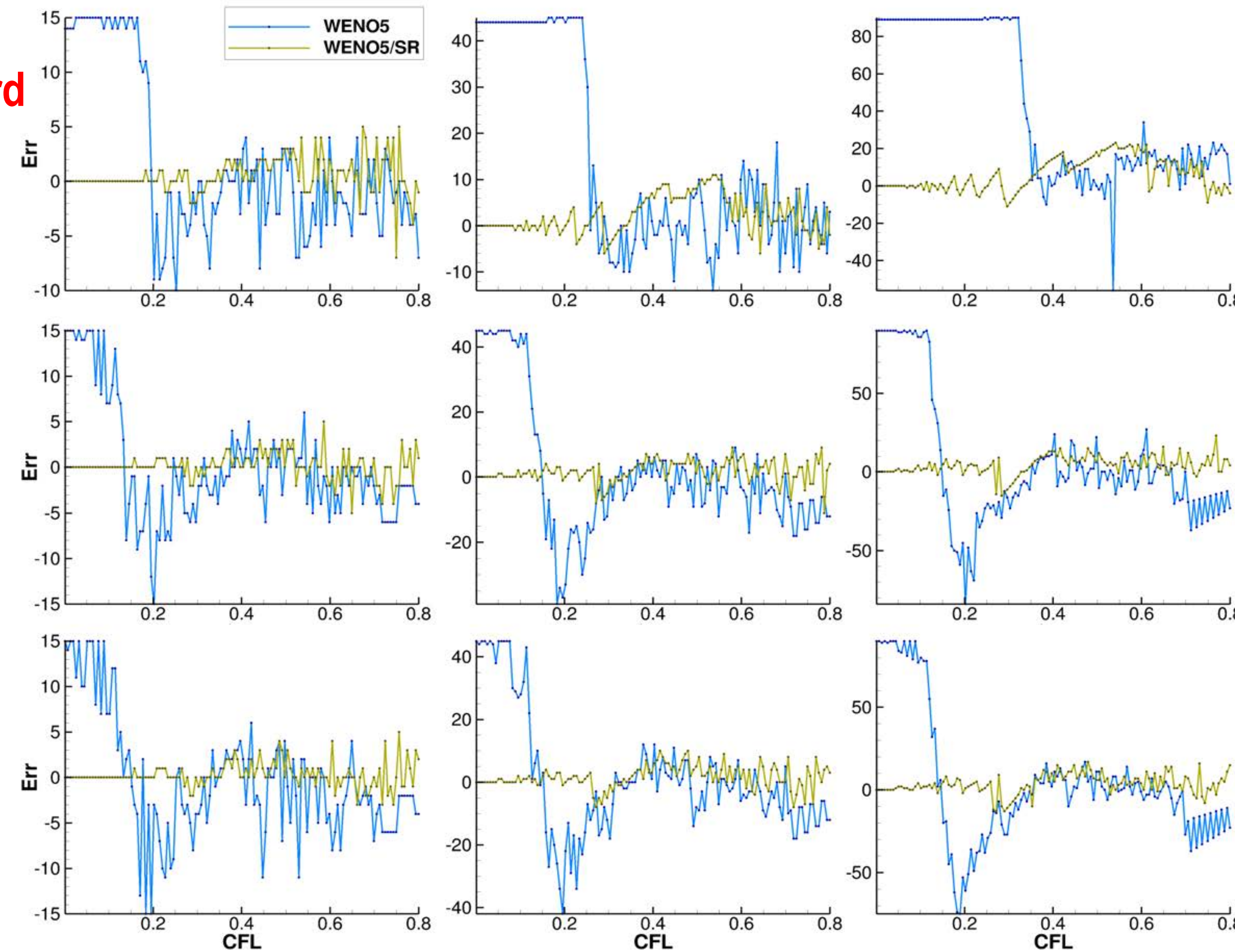
Strang/Safeguard

Grid 50 | **Grid 150** | **Grid 300**

Stiff. K_0

Stiff. 100 K_0

Stiff. 1000 K_0



Note: CFL limit based on the convection part of PDE

Behavior of Improved Schemes Below CFL Limit

(Different Procedures: Num. Dissip. Control Schemes)

1D C-J Detonation

Strang/Safeguard

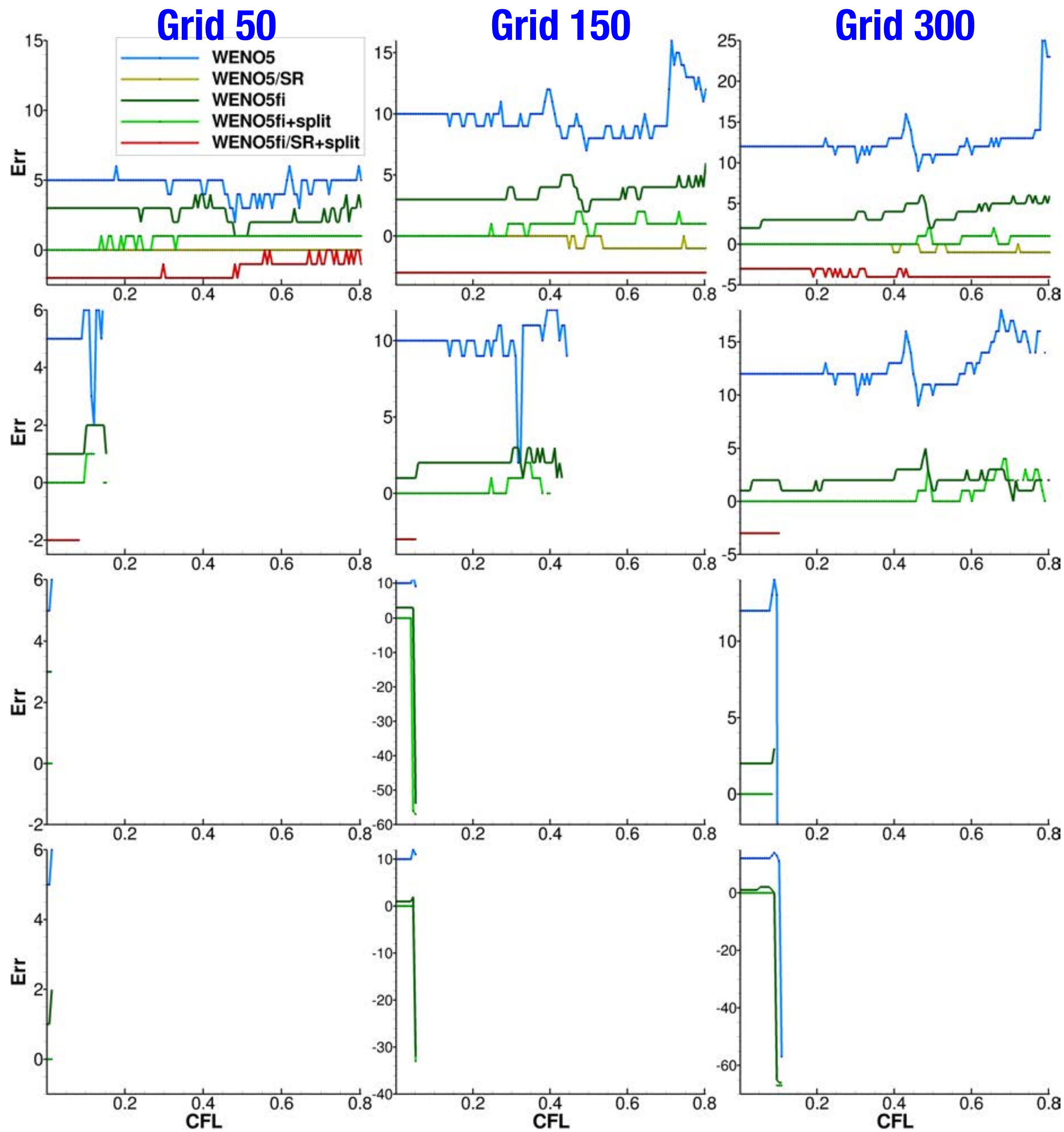
Strang/No-Safeguard

No-Strang/Safeguard

(Stable for small CFL)

No-Strang/No-Safeguard

(Stable for small CFL)



Summary

Same spatial & temporal schemes for the convection operator

(1D C-J Detonation, K_0 , and 50, 150 & 300 grid points)

(a) Strang/Safeguard, $N_r > 4$

Can extend the valid CFL range & with more complex spurious behavior

(b) Strang/No-Safeguard, $N_r > 4$

Less spurious behavior than Strang/Safeguard

(c) No-Strang/Safeguard *(Small CFL)*

(d) No-Strang/no-safeguard *(Small CFL; similar to (c))*

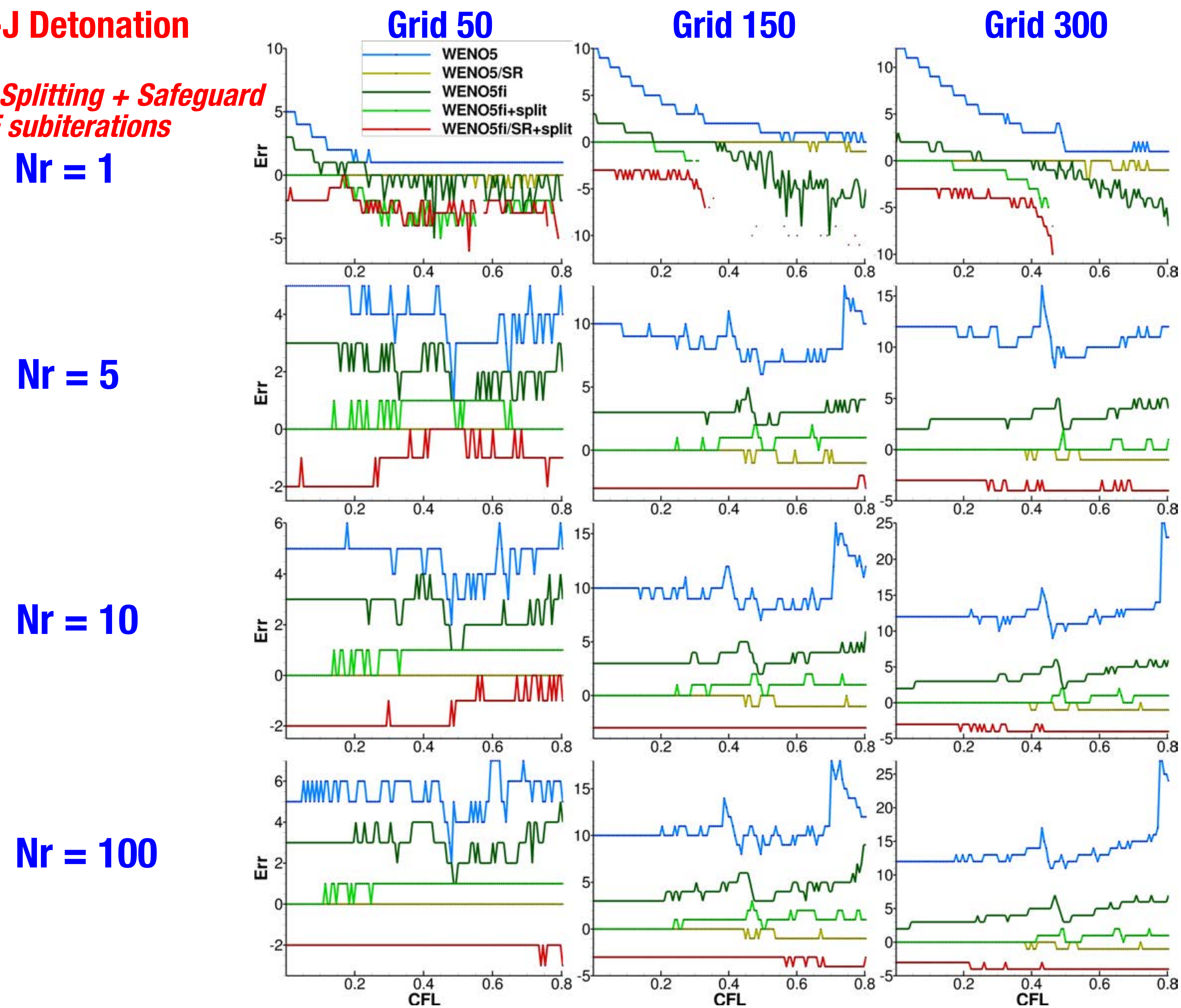
General:

> *(b) - (d) exhibit a similar CFL range with less spurious behavior than (a).*
> *No-Strang splitting + Safeguard or No-Safeguard procedures are constrained by a similar CFL range.*
> *Over all, WENO5/SR & WENO5fi+split in certain cases can improve the results in terms of reducing spurious numerics.*

Behavior of Improved Schemes Below CFL Limit
(Effect of # sub-iteration: Reaction Step Time Integrator, RK1)

1D C-J Detonation

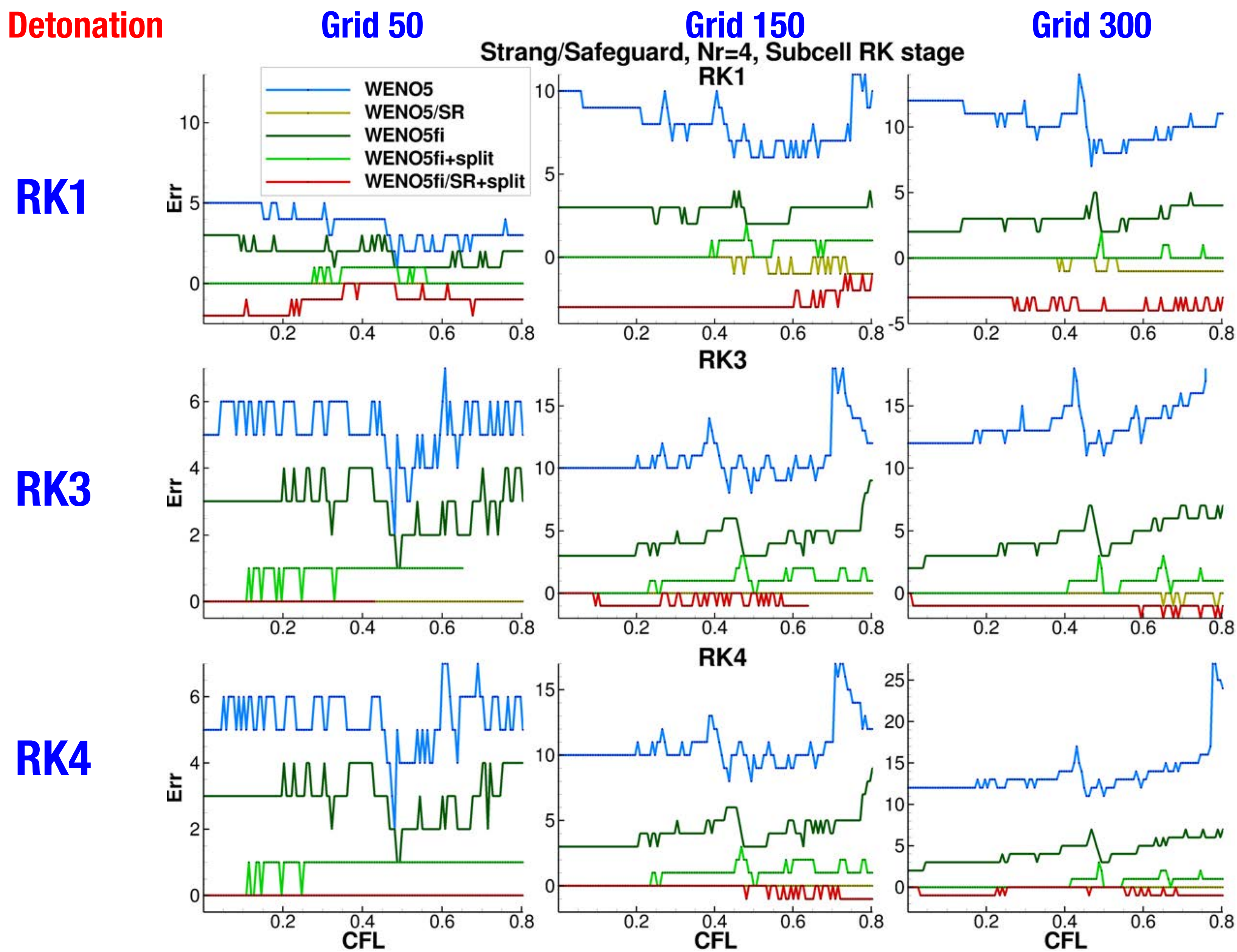
Strang Splitting + Safeguard ODE subiterations



Effort of Different Time Integrator -- Reaction Step

(*Strang Splitting/Safeguard, Nr=4, SR at every RK stage*)

1D C-J Detonation



Summary

Same spatial & temporal schemes for the convection operator

(1D C-J Detonation, K_0 , and 50, 150 & 300 grid points)

Explicit Euler (RK1) for the reaction operator:

(a) **Strang/Safeguard**, $N_r > 1$, SR at every subiteration

Can extend the valid CFL range & with more complex spurious behavior

(b) **Strang/No-Safeguard**, $N_r > 1$

Less spurious behavior than Strang/Safeguard

RK2, RK3 & RK4 for the reaction operator:

(a) **Strang/Safeguard**, $N_r > 1$, SR at every subiteration

> *Can extend the valid CFL range & with complex spurious behavior*
> *SR at every RK stage – minor different*

(b) **Strang/No-Safeguard**, $N_r > 1$, SR at every subiteration

> *Less spurious behavior than Strang/Safeguard*
> *No need at every RK stage*

General:

> *Over all, WENO5/SR & WENO5fi+split improve the results in terms of reducing spurious numerics*

> *Higher order RK improve spurious behavior only slightly*

MHD Splittings

- Splitting 1: Gas dynamics 2, split $B^{(x)}B^{(y)}$-terms, split $uB^{(y)}$-terms as $\rho u \bullet B^{(x)}/\rho$
- Splitting 2: Gas dynamics 2, split $B^{(x)}B^{(y)}$-terms, split $uB^{(y)}$-terms as $u \bullet B^{(x)}$
- Splitting 3: Gas dynamics 2, no splitting of magnetic field variables.
- Splitting 4: Gas dynamics 2, as Splitting 3, but one split term in the magnetic field equations.

Example EC flux, 2nd order ([2])

$$
\mathbf{h}_{j+1/2} = \begin{pmatrix} \rho^{ln}\{u\} \\ \rho^{ln}\{u\}^2 + p_1 + \frac{1}{2}(\{(B^{(x)})^2 + (B^{(y)})^2 + (B^{(z)})^2\} - \{(B^{(x)})^2\} \\ \rho^{ln}\{u\}\{v\} - \{B^{(x)}B^{(y)}\} \\ \rho^{ln}\{u\}\{w\} - \{B^{(x)}B^{(z)}\} \\ h_5' \\ 0 \\ \frac{1}{\{\rho/p\}}(\{\rho u/p\}\{B^{(y)}\} - \{\rho v/p\}\{B^{(x)}\}) \\ \frac{1}{\{\rho/p\}}(\{\rho u/p\}\{B^{(z)}\} - \{\rho w/p\}\{B^{(x)}\}) \end{pmatrix}
$$

$$
h_5' = (\frac{1}{\gamma - 1}p_2 + p_1)\{u\} + \rho^{ln}\{u\}(\{u\}^2 + \{v\}^2 + \{w\}^2 - \frac{1}{2}\{u^2 + v^2 + w^2\}) + \frac{\{\rho u/p\}}{\{\rho/p\}}(\{B^{(y)}\}^2 + \{B^{(z)}\}^2) - \frac{\{\rho v/p\}}{\{\rho/p\}}\{B^{(x)}\}\{B^{(y)}\} - \frac{\{\rho w/p\}}{\{\rho/p\}}\{B^{(x)}\}\{B^{(z)}\} \quad (1)
$$

$$
\{u\} = \frac{u_{j+1} + u_j}{2} p_1 = \frac{\{\rho\}}{\{\rho/p\}} \qquad p_2 = \frac{\rho^{ln}}{(\rho/p)^{ln}} \qquad \rho^{ln} = \frac{\rho_{j+1} - \rho_j}{\ln \rho_{j+1} - \ln \rho_j}
$$

Extension to High Order is Straightforward

High order f.d. by Richardson extrapolation. Example, 4th order

$$f_x \approx Df_j = (-f_{j+2}+8f_{j+1}-8f_{j-1}+f_{j-2})/12\Delta x = \frac{4}{3}\frac{f_{j+1}-f_{j-1}}{2\Delta x} - \frac{1}{3}\frac{f_{j+2}-f_{j-2}}{4\Delta x}$$

If the flux $h_{j+1/2} = h(u_{j+1}, u_j)$ is second order, and have symmetry property so that error expansion has only even terms,

$$\frac{h_{j+1/2} - h_{j-1/2}}{\Delta x} = f_x + \phi_2 \Delta x^2 + \phi_4 \Delta x^4 + \ldots$$

same extrapolation can be used. Example, fourth order

$$\frac{4}{3}\frac{h(u_{j+1}, u_j) - h(u_j, u_{j-1})}{\Delta x} - \frac{1}{3}\frac{h(u_{j+2}, u_j) - h(u_j, u_{j-2})}{2\Delta x}$$

Entropy conservation condition

$$(\mathbf{v}_{j+1} - \mathbf{v}_j)^T \mathbf{h}(\mathbf{u}_{j+1}, \mathbf{u}_j) = \psi_{j+1} - \psi_j$$

can be applied to each term, replacing $j+1$ by $j+2$ for the second term.

MHD Splitting 1

$$\begin{pmatrix} \rho \bullet u \\ \rho u \bullet u + p + \frac{1}{2}|\mathbf{B}|^2 - B^{(x)} \bullet B^{(x)} \\ \rho v \bullet u - B^{(x)} \bullet B^{(y)} \\ \rho w \bullet u - B^{(x)} \bullet B^{(z)} \\ (e + p + \frac{1}{2}|\mathbf{B}|^2) \bullet u - \rho \mathbf{u}^T \mathbf{B} \bullet B^{(x)}/\rho \\ u \bullet B^{(x)} - \rho u \bullet B^{(x)}/\rho \\ u \bullet B^{(y)} - \rho v \bullet B^{(x)}/\rho \\ u \bullet B^{(z)} - \rho w \bullet B^{(x)}/\rho \end{pmatrix}$$

MHD Splitting 2

$$\begin{pmatrix} \rho \bullet u \\ \rho u \bullet u + p + \frac{1}{2}|\mathbf{B}|^2 - B^{(x)} \bullet B^{(x)} \\ \rho v \bullet u - B^{(x)} \bullet B^{(y)} \\ \rho w \bullet u - B^{(x)} \bullet B^{(z)} \\ (e + p + \frac{1}{2}|\mathbf{B}|^2) \bullet u - \mathbf{u}^T \mathbf{B} \bullet B^{(x)} \\ u \bullet B^{(x)} - u \bullet B^{(x)} \\ u \bullet B^{(y)} - v \bullet B^{(x)} \\ u \bullet B^{(z)} - w \bullet B^{(x)} \end{pmatrix}$$

MHD Splitting 3

$$\begin{pmatrix} \rho \bullet u \\ \rho u \bullet u + p + \frac{1}{2}|\mathbf{B}|^2 - B^{(x)} B^{(x)} \\ \rho v \bullet u - B^{(x)} B^{(y)} \\ \rho w \bullet u - B^{(x)} B^{(z)} \\ (e + p + \frac{1}{2}|\mathbf{B}|^2) \bullet u - B^{(x)} \mathbf{u}^T \mathbf{B} \\ 0 \\ u B^{(y)} - v B^{(x)} \\ u B^{(z)} - w B^{(x)} \end{pmatrix}$$

MHD Splitting 4

$$\begin{pmatrix} \rho \bullet u \\ \rho u \bullet u + p + \frac{1}{2}|\mathbf{B}|^2 - B^{(x)} B^{(x)} \\ \rho v \bullet u - B^{(x)} B^{(y)} \\ \rho w \bullet u - B^{(x)} B^{(z)} \\ (e + p + \frac{1}{2}|\mathbf{B}|^2) \bullet u - B^{(x)} \mathbf{u}^T \mathbf{B} \\ 0 \\ u \bullet B^{(y)} - v B^{(x)} \\ u \bullet B^{(z)} - w B^{(x)} \end{pmatrix}$$

- Four schemes, three source terms, gives 12 different methods.
- Source term $\mathbf{e}_j(B_{j+1} - B_{j-1})$ can use with either of $\mathbf{e}_G$, $\mathbf{e}_J$, $\mathbf{e}_B$.
- $\mathbf{e}_{j+1/2}$ needs to be adapted to each case $\mathbf{e}_G$, $\mathbf{e}_J$, $\mathbf{e}_B$.
- Many possible variants, different $\mathbf{z}$, different entropy, ...