Accuracy Consideration by DRP Schemes for DNS and LES of Compressible Flows

H.C. Yee, NASA Ames Research Center
(Joint work: B. Sjogreen, D.V. Kotov, C-W Shu, W. Wang, A.A. Wray & A. Kritsuk)

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Outline

- Objective
- Technical Challenge
- Approach

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- Results
- Summary

Objectives

Show 4 Properties of Our High Order Methods:

- **Improvement in Nonlinear Stability**
  > Methods cater to long time integration of compressible turbulence
- **Improvement in Accuracy** (for a wide spectrum of flow speeds)
  > Efficient Nonlinear Filter methods with adaptive local flow sensors designed to minimize the use of numerical dissipation
- **Prevention of Incorrect Shock Speeds – Stiff Source Terms**
  > Conservative high order subcell resolution method designed to obtain CORECT shock speed using coarse grids
- **Prevention of Unphysical Solutions in Turbulence Simulations**
  Quantify numerical uncertainty via dynamical numerical analysis (Nonlinear Approach)

Important Distinction & Key Points:

> Solutions of the discretized counterparts but NOT solutions of the governing equation
> Numerical chaos/"turbulence" leading to FALSE prediction of transition to turbulence
> Some claims of computed turbulence are NOT turbulence of the governing equation
(e.g., applying time series analysis or shadowing lemma techniques to the computed data)

Challenges in Numerical Method Development

(Long Time Integration of Multiscale Compressible Turbulence)

Nonlinear Instability:

> Existing accurate schemes developed for rapidly developing flows usually SUFFER from nonlinear instability for long time integration

Numerical Stability & Accuracy: Conflicting Requirements for DNS & LES

> Stable schemes usually contain more numerical dissipation than their higher accuracy counterparts

> Numerical dissipation usually smears turbulent fluctuations

> Proper amount of numerical dissipation is required for stability in the vicinity of discontinuities

Difficult to Resolve All Scales: Need efficient methods with extremely fine grids & CPU intensive

Source Terms:

> Well-balanced schemes are needed to preserve physical steady states exactly

> Numerical dissipation & under-resolved grids lead to incorrect shock speeds if source term is stiff

Problems Containing a Wide Spectrum of Flow Speeds & Flow Types:

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

> Cannot be solved accurately with standard numerical methods

Our New Development to address these challenges:
(Yee et al., Yee & Sjogreen, Sjogreen & Yee, Wang et al., Kotov et al., 2009-2018)

Numerical Example

Long Time Integration of Smooth Flows

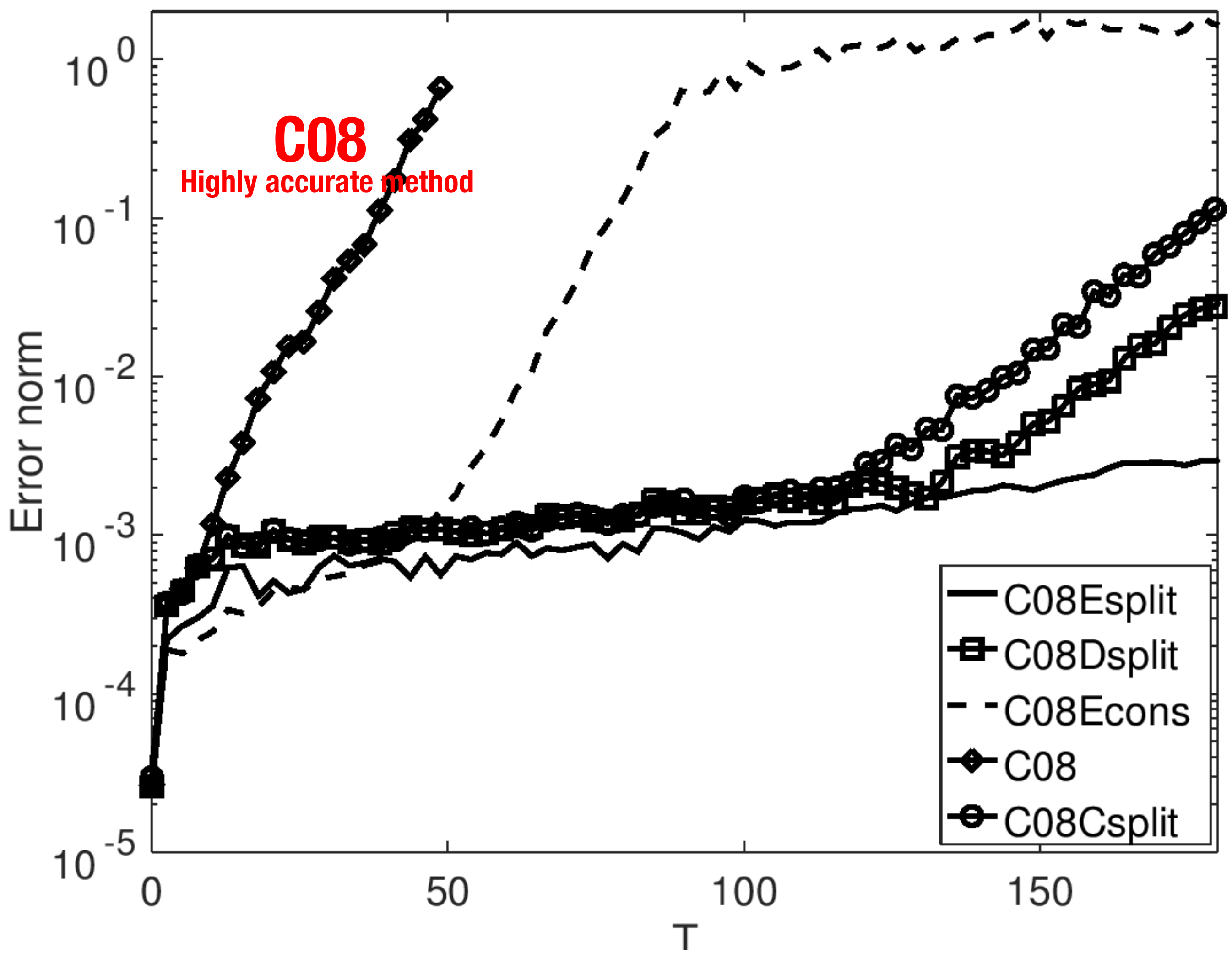
Accurate schemes developed for short time integration (or rapidly developing flows) usually SUFFER from nonlinear instability for long time integration

2D Isentropic Vortex Convection

Exact Solution is Simple Translation

Comparison of High Order Methods
8th order central (C08) vs. 4 different 8th-order skew-symmetric splittings

Norm of Error vs. Time



Improve Stability:
Long time integrations by
4 skew-symmetric splittings
of the inviscid flux derivative
before the application of
non-dissipative C08
Different Accuracy

Spurious Numerics Due to Source Terms

Phenomena occur in simple scalar case – 3D complex systems

By Typical Conservative Schemes

Source Terms: Hyperbolic conservation laws with source terms

- Most high order shock-capturing schemes are NOT well-balanced & produce huge error
- High order WENO/Roe & their nonlinear filter counterparts are well-balanced for certain reacting flows **Our Work:** 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 27 years (Improvement can easily be obtained for a single reacting flow case)
- A New Sub-Cell Resolution Method has been developed for stiff systems on coarse mesh **Our Work:** Wang et al., JCP, 2012 ; CiCP 2016

Nonlinear Source Terms:

- Occurrence of spurious steady-state & discrete standing-wave solutions – by the use of fixed grid spacings & time steps or grid adaptation Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, 1990-2002

Stiff Nonlinear Source Terms with Discontinuities:

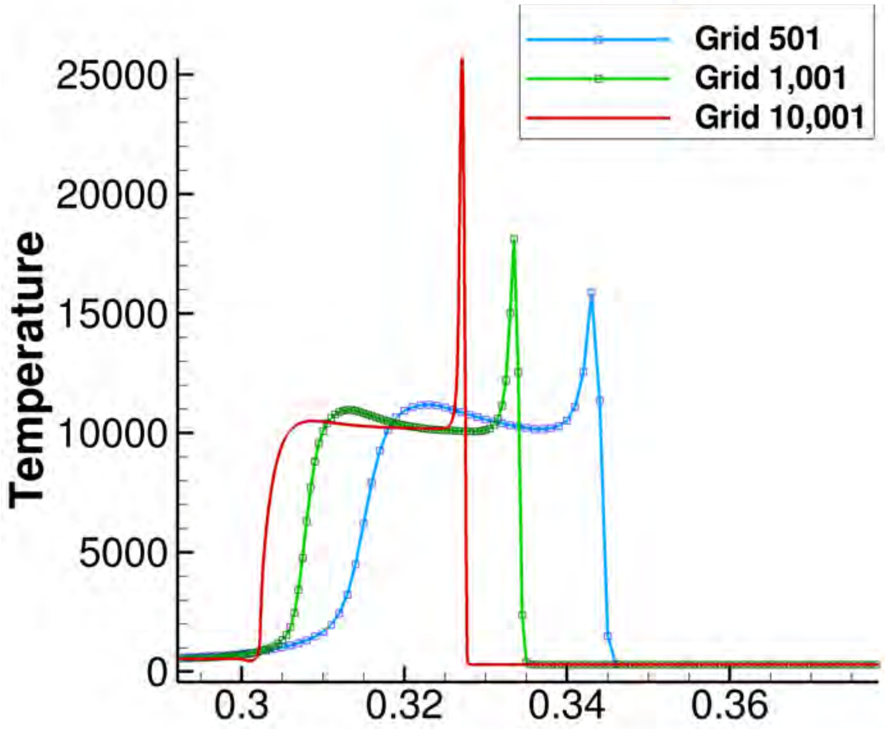
- More complex spurious behavior
- Forced Turbulence, numerical combustion, certain terms in turbulence modeling & reacting flows Yee et al., Yee & Sweby, Griffiths et al., Lafon & Yee, Kotov et al. 1990 – 2017

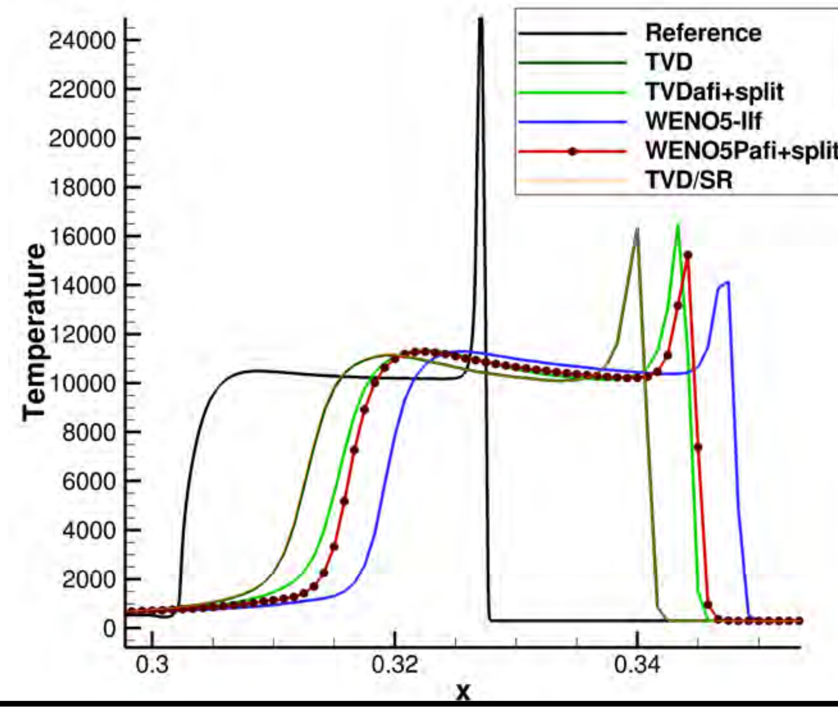
Stiff Source Terms: Wrong Discontinuity Locations

(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





Flows without stiff source term: Computed locations of discontinuities are independent of the grid size or high-resolution shock-capturing methods

Implication: The danger in trusting numerical simulation for problems with stiff source terms

Non-standard behavior of numerics observed in non-reacting flows

(Yee et al., Griffith et al., Wang et al., Kotov et al., 1990 - 2016)

Our Approach
(To Address the Various Numerical Method Challenges)

Schemes that

- **Mimic & preserve properties** of the chosen governing equations
  (e.g., Discrete momentum conservation, discrete kinetic energy preservation, positivity preserving of computed pressure & density, etc.)
- Are **high order, low dissipative & low dispersive** and **suitable for a wide range of flow speeds**
  (e.g., develop local flow sensors to adaptively minimize numerical dissipation & dispersion errors)
- Are **nonlinear stable, efficient & highly parallelizable**
- Possess **high order stable** numerical boundary operators -- SBP Boundary operators
- Are applicable for 3D **spatial & time varying deforming grids with** geometric conservation law property **(GCL)**
- **Quantify numerical uncertainty** via dynamical numerical analysis – **A nonlinear approach**

Yee et al., Yee & Sjogreen, Sjogreen & Yee, Wang et al. and Kotov et al. (1999-2018)

Methods to Improve Nonlinear Stability & Accuracy

(Long Time Wave Propagation & Long Time Integration of Compressible Turbulence)

- **Skew-Symmetric Splitting** of the inviscid flux derivative (before the application of non-dissipative centered schemes for nonlinear stability) Yee & Sjogreen, Sjogreen & Yee, 2016-2018
- **DRP** (Dispersion Preservation-Relation) schemes as **alternatives** to split version of classical high order central schemes Yee & Sjogreen, 2017
- **High-Order Entropy Conservative Numerical Fluxes** with entropy satisfying properties - Numerical solution satisfies an additional discretized conservation law Sjogreen & Yee, 2016-2018
- Standard high order **Linear Filters** are to be **replaced by** high order **Nonlinear Filters**

  Yee et al., Yee & Sjogreen, Sjogreen & Yee, Kotov et al. (1999-2017)
- **Smart Flow Sensors** to provide locations & appropriate amount of numerical dissipation needed Yee & Sjogreen, Kotov et al. (2009-2016)
- **Nonlinear Dynamics** is utilized to complement the traditional linearized stability theory (Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, Wang et al., Kotov et al. 1990- 2015)
  - Minimize numerically induced false transition to turbulence
  - Minimize numerical instability due to long time integration of turbulent flows
  - Minimize numerically induced standing wave solutions
  - Minimize wrong shock speeds

Yee et al. high-order nonlinear filter schemes with smart local flow sensors

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:** (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, Kennedy & Gruber 2008

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

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*

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

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

==================================

General splitting: $(ab)_x = \alpha(ab)_x + \gamma ab_x + \beta a_x b$ Pirozzoli 2009, Kennedy & Gruber 2008

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 nonlinear 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, Carpenter et al. 2013-2016,
  Sjogreen & Yee 2016, 2017– central + nonlinear filter, gas dynamics & MHD)

Plasma (Hypersonic Flows):

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 2016-2017)

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., **7^{th}-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. 8^{th} 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)*

Examples of Improved Nonlinear Stability & Accuracy

Selected Illustrations:

3D DNS Taylor & Green and Isotropic Turbulence

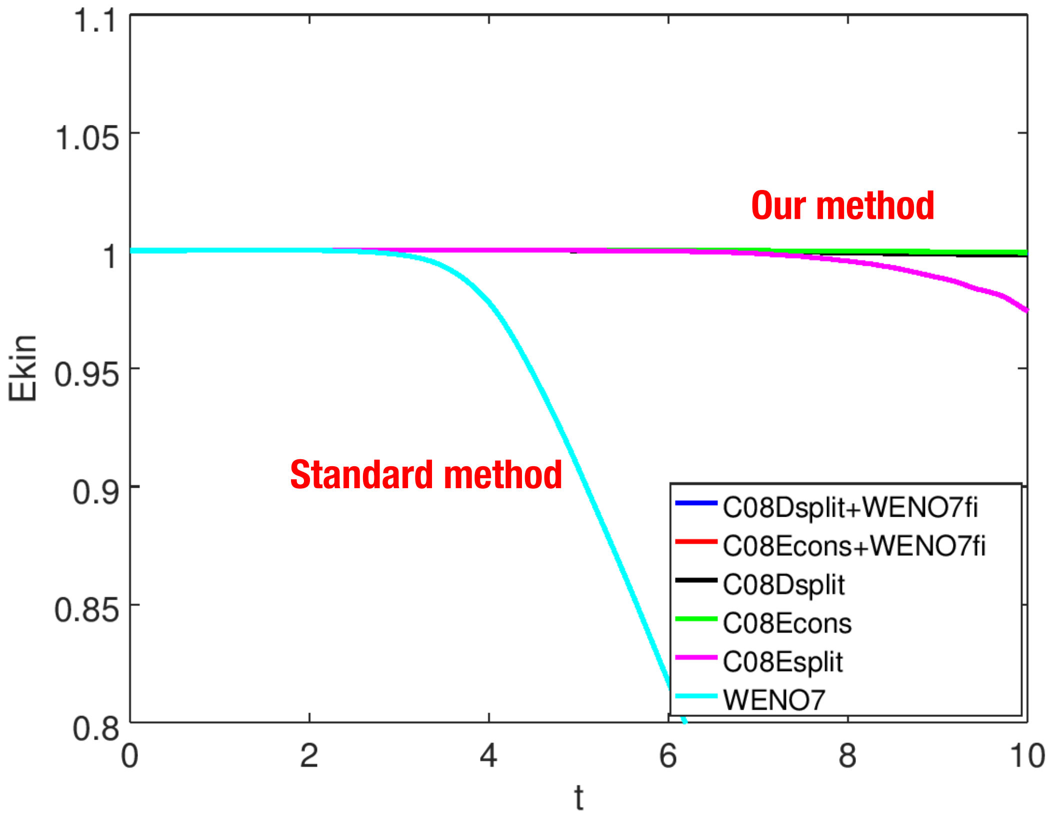
More Complicated Flows, Supersonic DNS & LES:

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

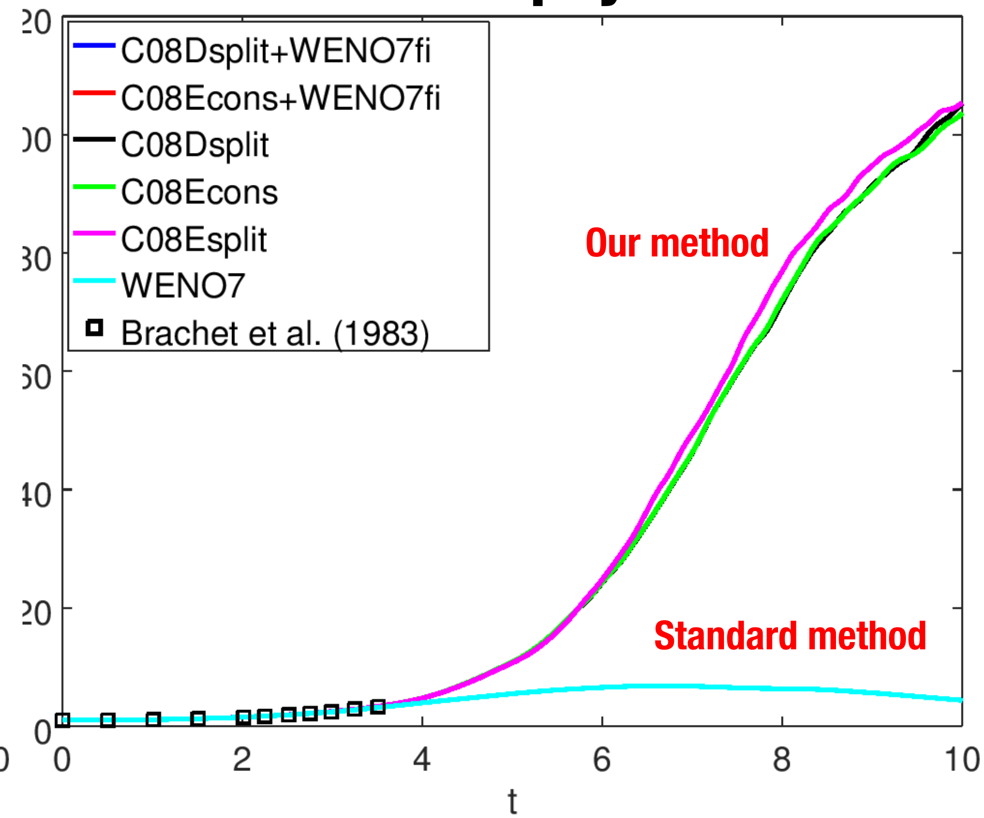
3D Taylor-Green Vortex (Compressible & Inviscid)

(Skew-Symmetric Splitting vs. Entropy Conservative Methods, 64^3 grids)

Kinetic Energy



Enstrophy

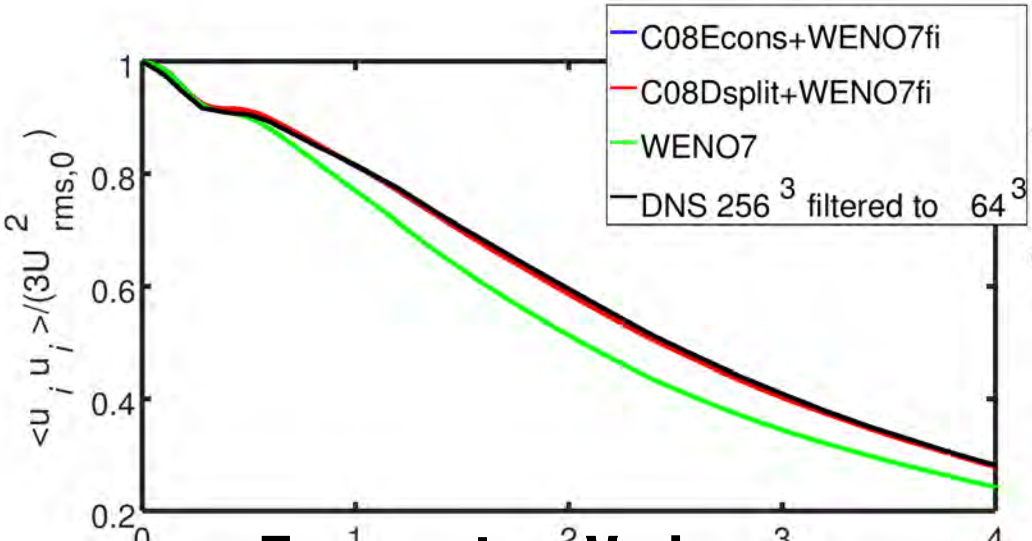


C08Dsplit+WENO7fi: 8th-order central + Ducros et al. split + WENO7fi
C08Econs+WENO7fi: 8th-order central entropy conservative flux + WENO7fi
C08Dsplit: 8th-order central + Ducros et al. split
C08Econs: 8th-order central + Entropy conservative flux
C08Esplit: 8th-order central + Entropy split
WENO7: Standard WENO7

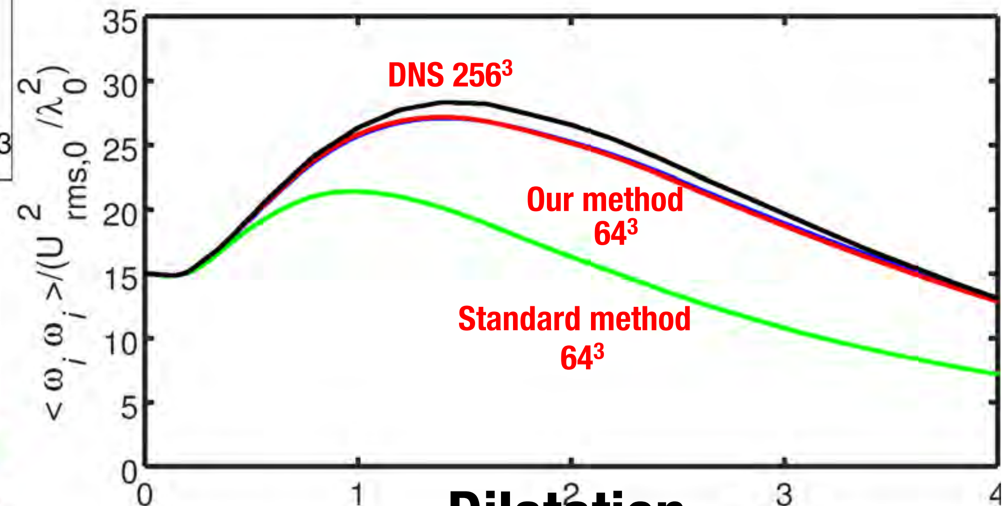
3D Isotropic Turbulence with Shocklets

(Skew-Symmetric Splitting vs. Entropy Conservative Methods, 64^3 grids)

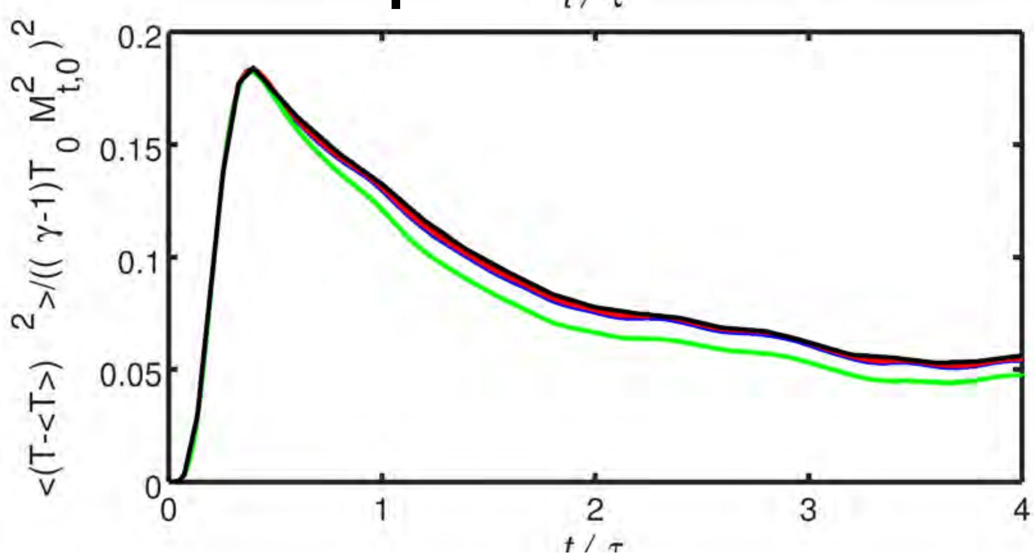
Kinetic Energy



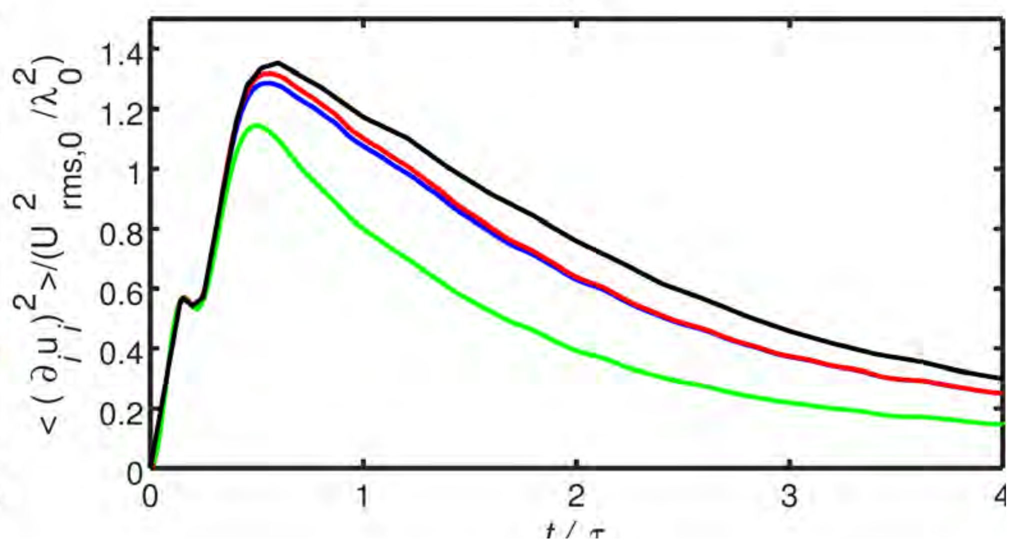
Enstrophy



Temperature Variance

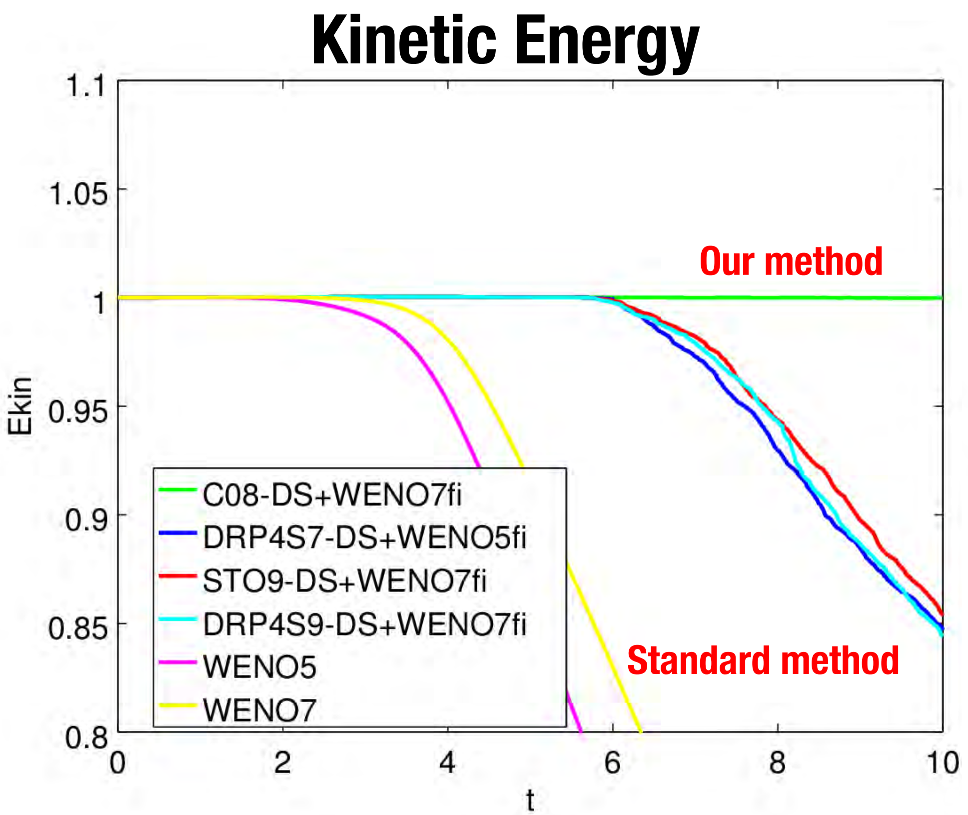


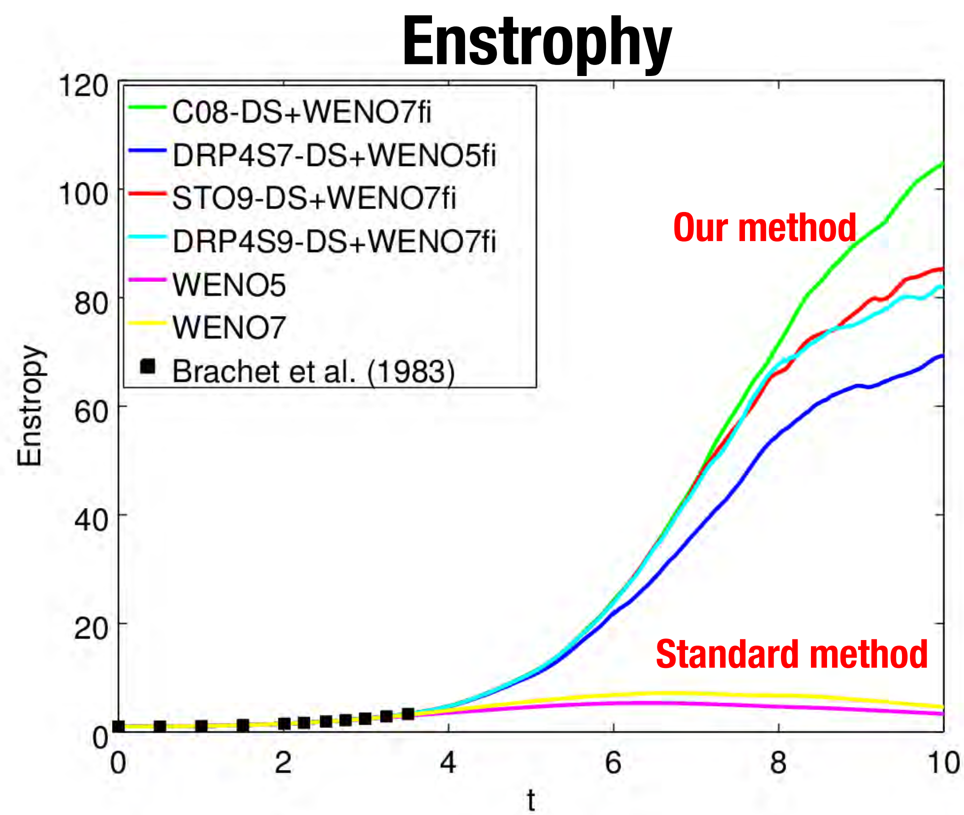
Dilatation



3D Taylor-Green Vortex (Shock-Free Turbulence)

(Comparison of 6 Methods, 64^3 grids)



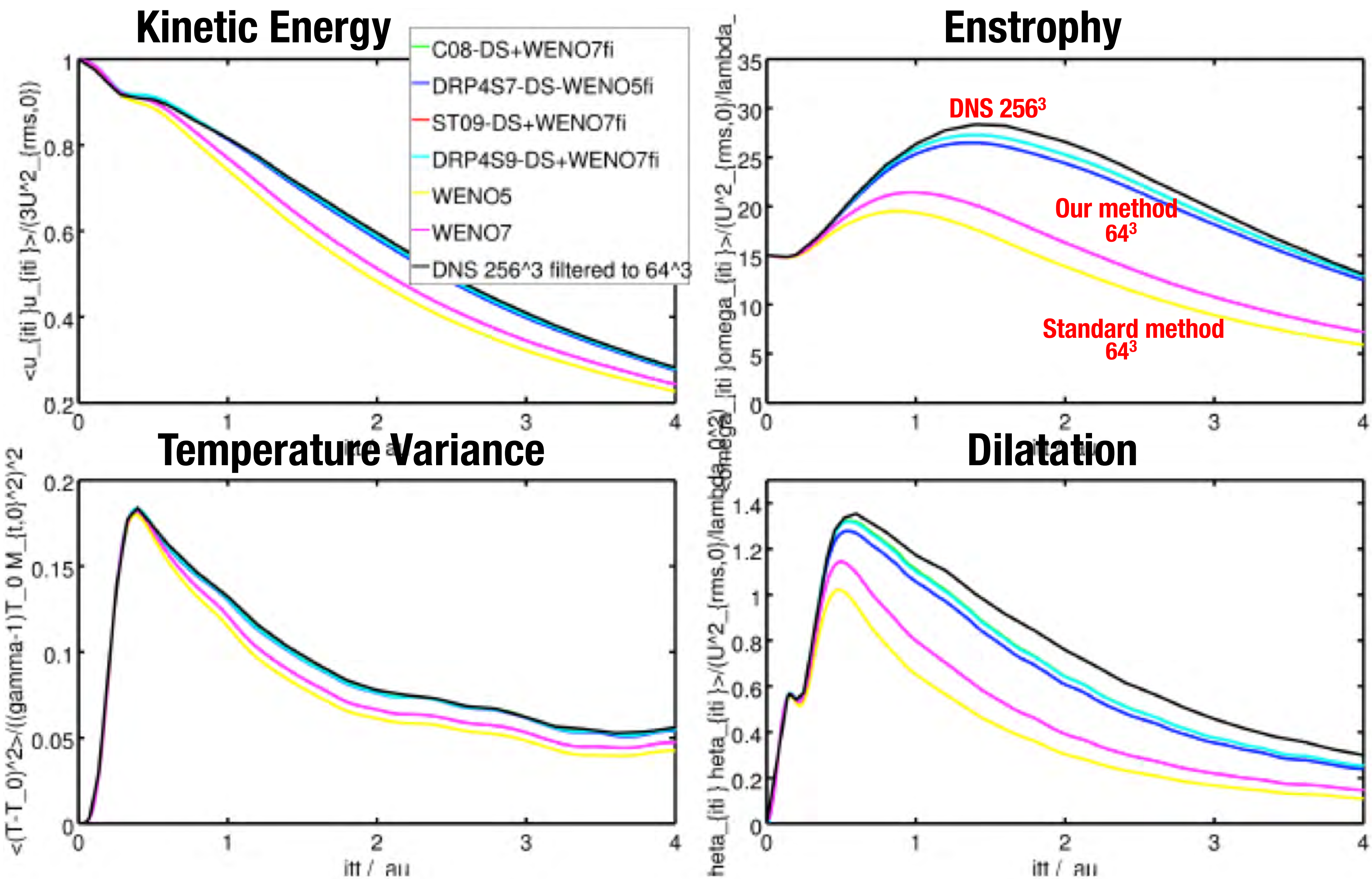


C08-DS+WENO7fi: 8^{th}-order central + Ducros et al. split +WENO7fi
DRP4S7-DS+WENO5fi: Tam & Webb 4^{th}-order DRP, 7pt grid stencil + Ducros et al. split + WENO5fi
ST09-DS+WENO7fi: Bogey & Bailly 4^{th}-order DRP, 9pt grid stencil + Ducros et al. split + WENO7fi
DRP4S9-DS+WENO7fi: Tam & Webb 4^{th}-order DRP, 9pt grid stencil + Ducros et al. split + WENO7fi

3D Isotropic Turbulence with Shocklets

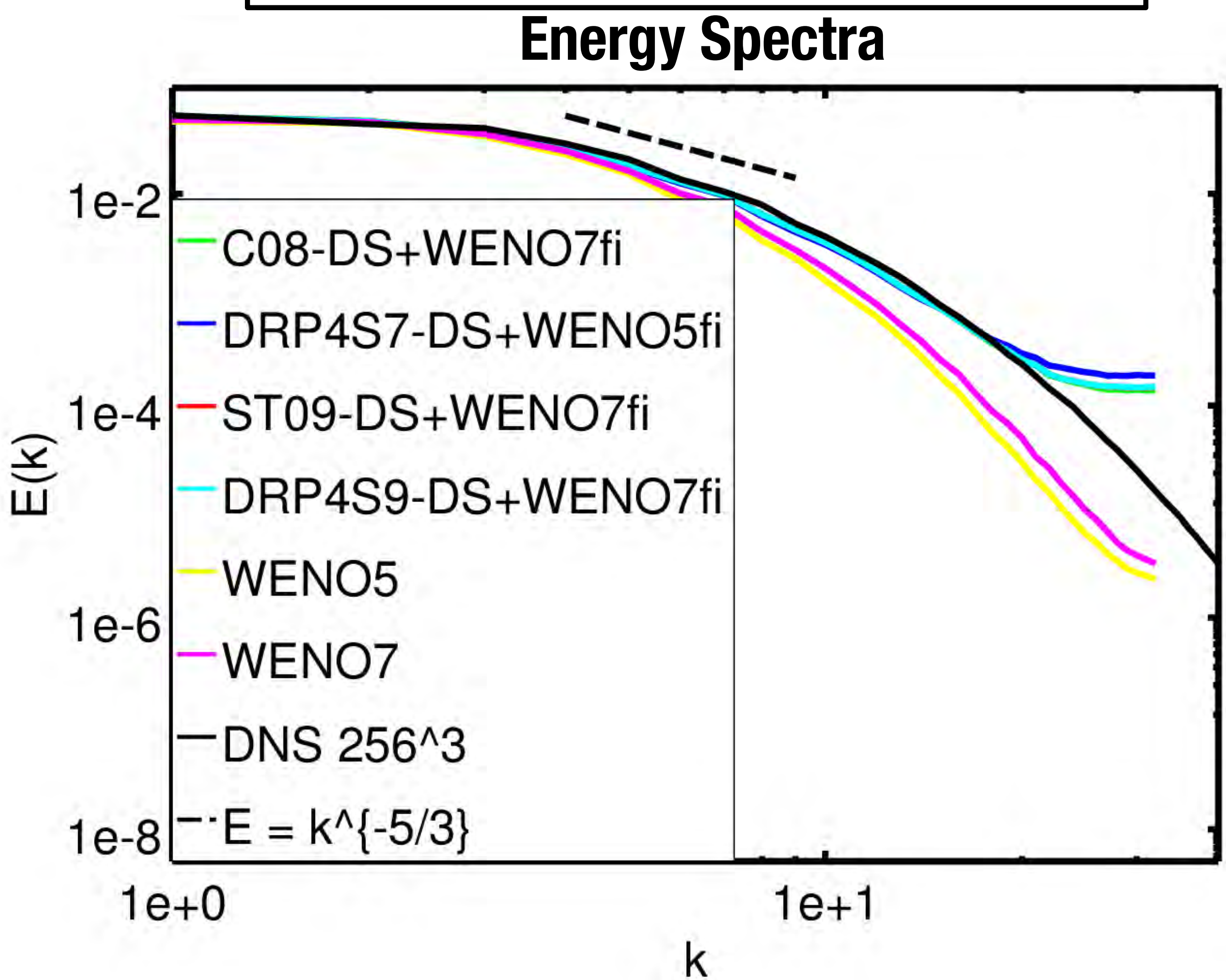
(Comparison of 6 Methods, 64^3 grids)

TACP - Transformational Tools & Technologies Project



3D Isotropic Turbulence with Shocklets
(Compressible & Inviscid)

Comparison of 6 Methods, 64^3 grids

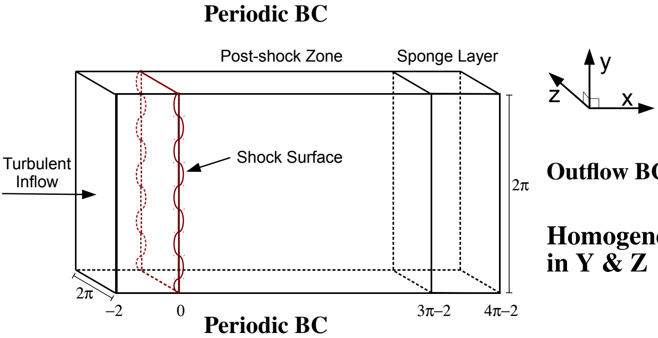


3D Shock-Turbulence Interaction Test Case

(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



Outflow BC

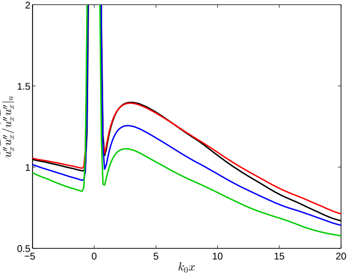
Homogeneous in Y & Z

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

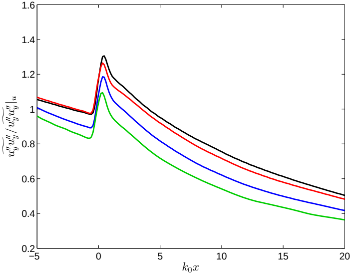
(Gently drive the flow towards a laminar state)

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

Streamwise Reynolds Stress



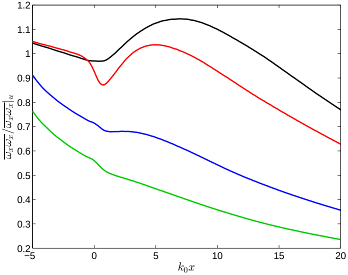
Streamwise Vorticity



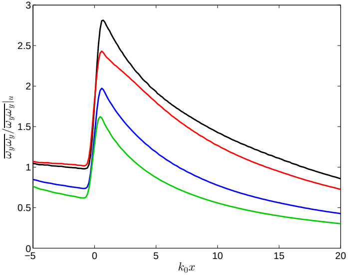
- Filtered DNS
- WENO7fi+split
- WENO7
- WENO5

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**

New Approach: Subcell Resolution Method for Stiff Source

(Obtaining Correct Shock/Contact/Shear Locations)

Selected Illustration: Detonation

More Complicated Examples & Minimizing Spurious Numerics:

Yee et al., Wang et al. and Kotov et al. (2002-2016)

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: Subcell resolution methods can be used for LES using dynamic SGS model with shocks by locating the shock location & solve left & right problems

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

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 $T_{ign}=25$

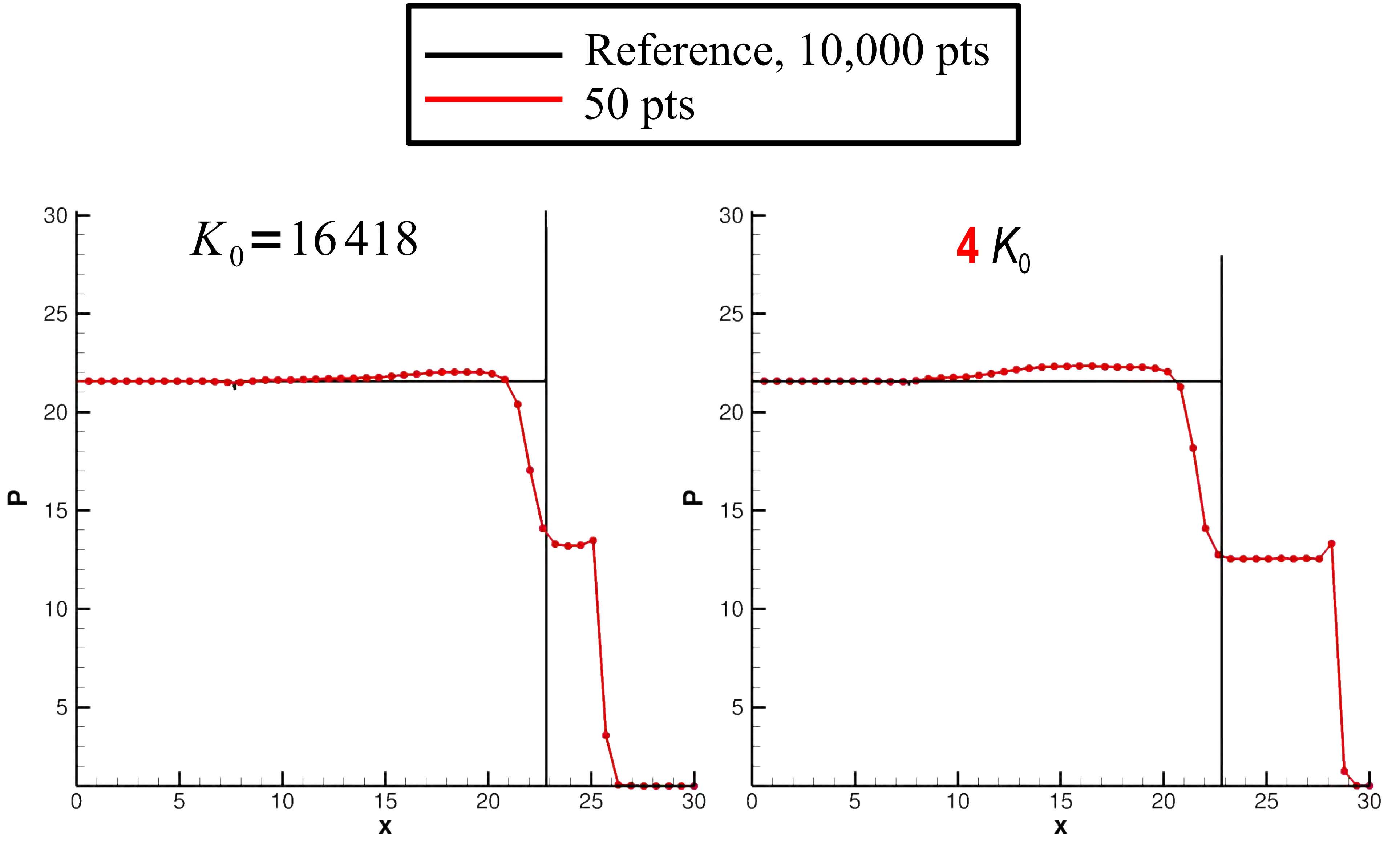
Heat release $q_0=25$

Rate parameter $K_0=16418$

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

Wrong Propagation Speed of Discontinuities

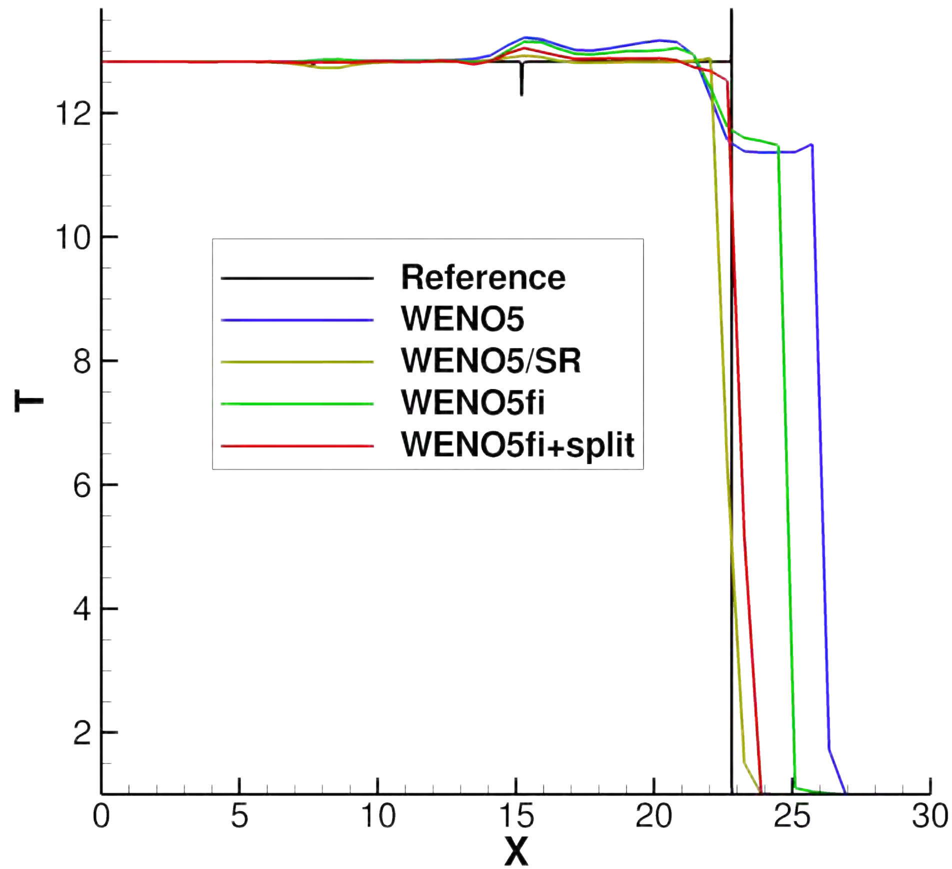
(Standard Method: WENO5, Two Stiff Coefficients, 50 pts)



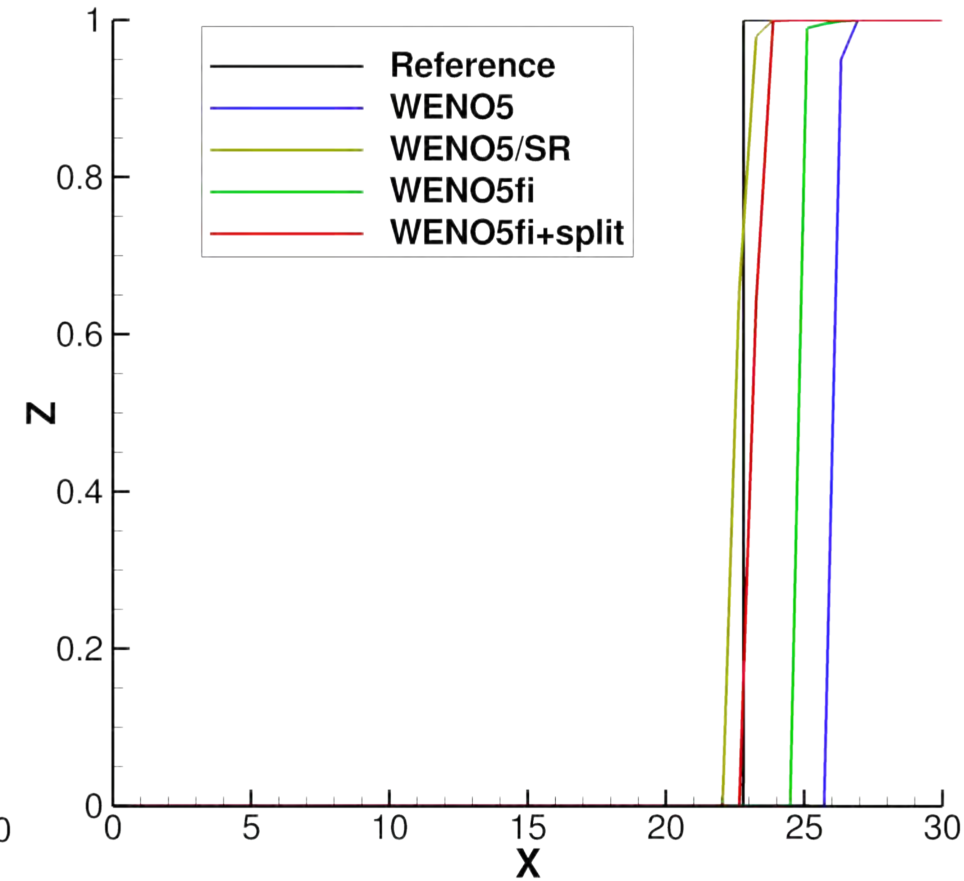
1D C-J Detonation (K_0 = 16418, 50 pts)

tend = 1.7

Temperature



Mass Fraction



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

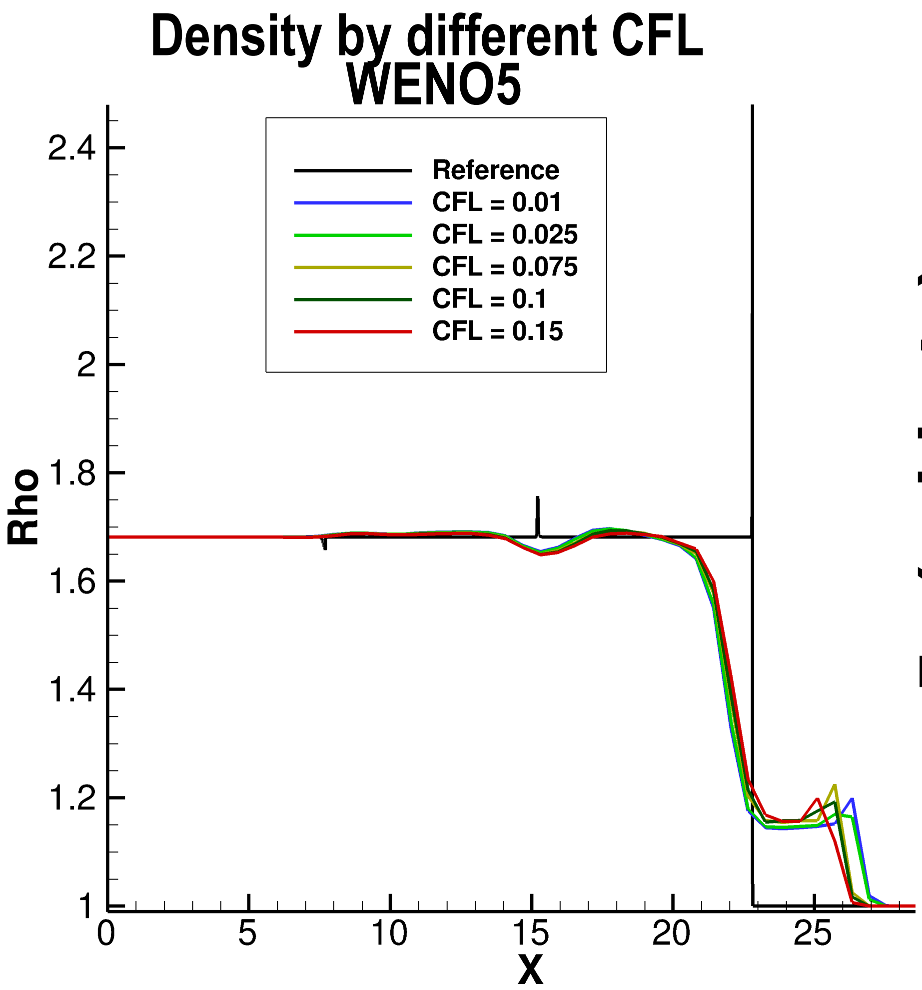
Our Meth. –
- WENO5/SR: WENO5 + subcell resolution
- WENO5fi: filter version of WENO5
- WENO5fi+split: WENO5fi + preprocessing (Ducros splitting)

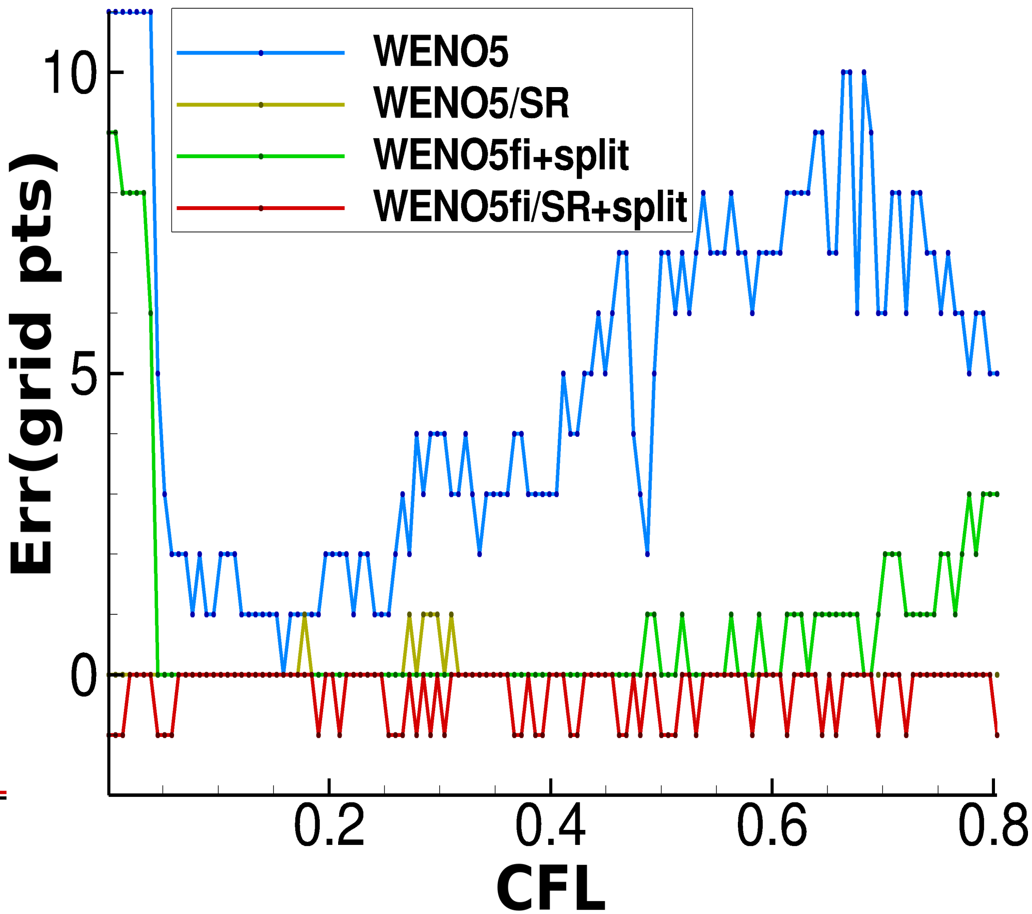
Reference: WENO5, 10,000 points

Behavior of the schemes below CFL limit

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

Strang Splitting & Safeguard, 50 pts, 100 K_0





- ***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)***

Summary
(Split Classical Central vs. Split DRP Central)

GAS dynamics: Classical central & DRP central

- Both Split central schemes can improve nonlinear stability for smooth flows in general
- Both nonlinear filter version of split schemes can improve stability & accuracy for DNS & LES
- Both split schemes provide similar stability & accuracy improvement

Plasma: Classical central

- Split centered schemes can improve nonlinear stability in general for smooth flows but MHD equations 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

DRP schemes for plasma study - in progress

Backup Slides

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

Plasma:

- Split centered schemes can improve nonlinear stability in general for smooth flows but MHD equations 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

Performance of High Order Nonlinear Filter Scheme
(Skew-Symmetric Splitting of Inviscid Flux Derivative)

Rapidly Developing Flows: (subsonic, transonic, supersonic & hypersonic)

> Smooth flows Yee et al., 1999

> Flows with discontinuities Yee et al., Sjogreen & Yee, Sandham et al., 2000-2004

> Supersonic Mixing & Richtmyer-Meshkov Instability Yee & Sjogreen, 2004, 2012

> Extreme Flows - positivity-preserving nonlinear filter scheme Kotov et al., 2014

> Flows with stiff source terms – Wrong shock speed
High order well-balanced subcell resolution schemes Wang et al., Yee et al., Kotov et al., 2009-2015

Long Time Integrations, DNS & LES:

> Shock Free Compressible Turbulence (Kotov et al., 2016)

> Low Speed Turbulence with Shocklets (Kotov et al., 2016)

> LES of Temporally Evolving Mixing Layers (Yee et al., 2012)

> DNS & LES of Turbulence Interacting with a Stationary Supersonic Shock --
One-sided SGS model & subcell resolution to locate the shock within one grid cell (Kotov et al., 2016)

> 3D Forced Turbulence (Time Varying Forcing) (Sjogreen et al., 2016)

> Dual & Direct Cascade Study of 2D Turbulence with Random Forcing
(Astrophysical Applications, Kritsuk et al., 2016)

Astrophysical Applications: 2D Turbulence

(Joint work with Alexei G. Kritsuk, U.C. San Diego)

Application: *Energetics of the ISM in Galactic Disks*

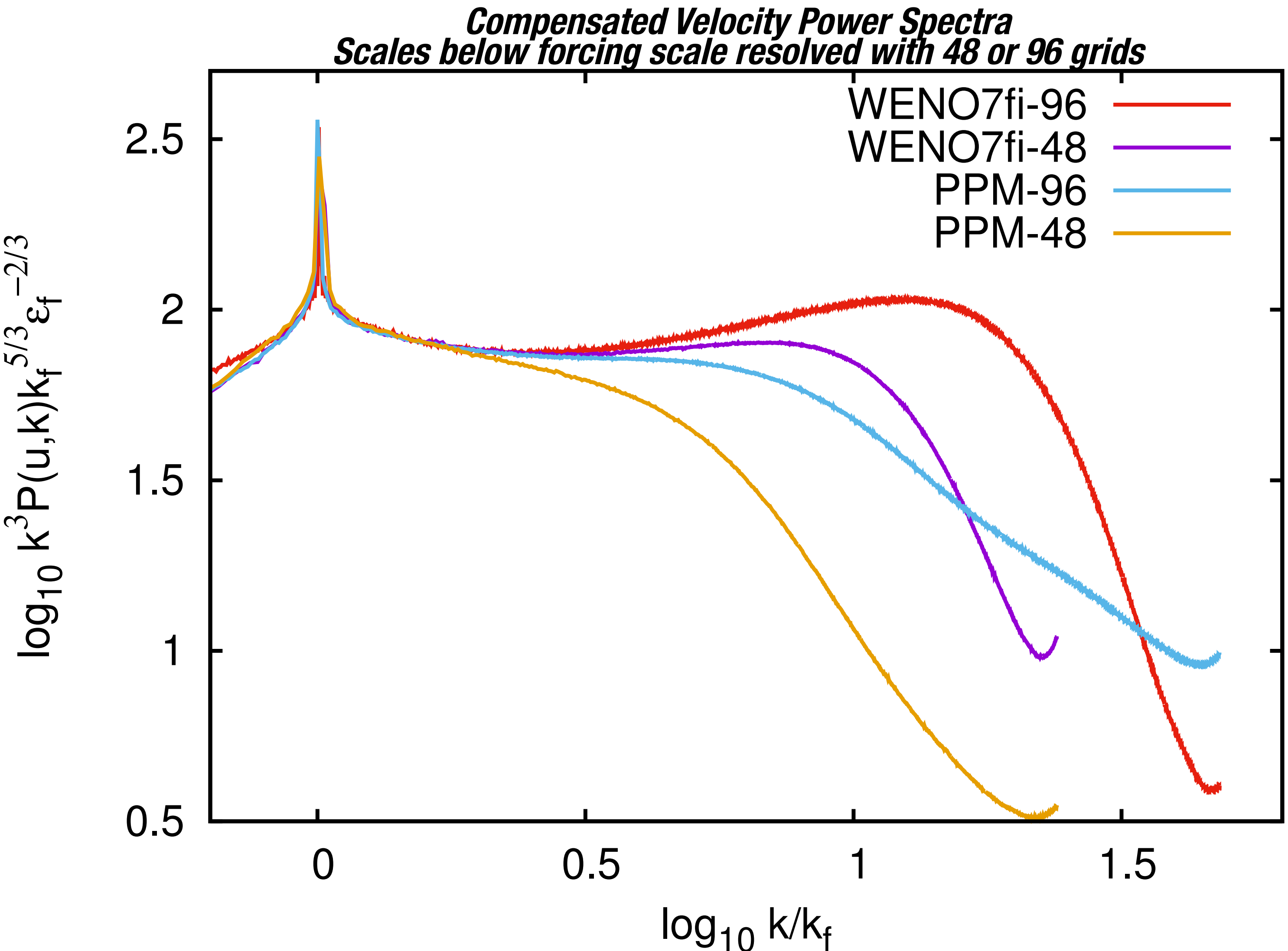
- *Dual energy cascade study*
- *Does the inverse energy cascade work in the compressible case?*
- *What are the corresponding scaling relations?*

Grid size:

- *Physics Study:* 512^2, $2{,}048^2$, $8{,}192^2$, $16{,}384^2$
- *Computation Grid Resolutions:* $2{,}048^2$, $8{,}192^2$, $16{,}384^2$

Scheme Comparison: PPM vs WENO7fi+split

2D Compressible Turbulence: Isothermal γ=1.001, periodic BCs
Flow determined by grid N, energy injection rate & energy injection scale

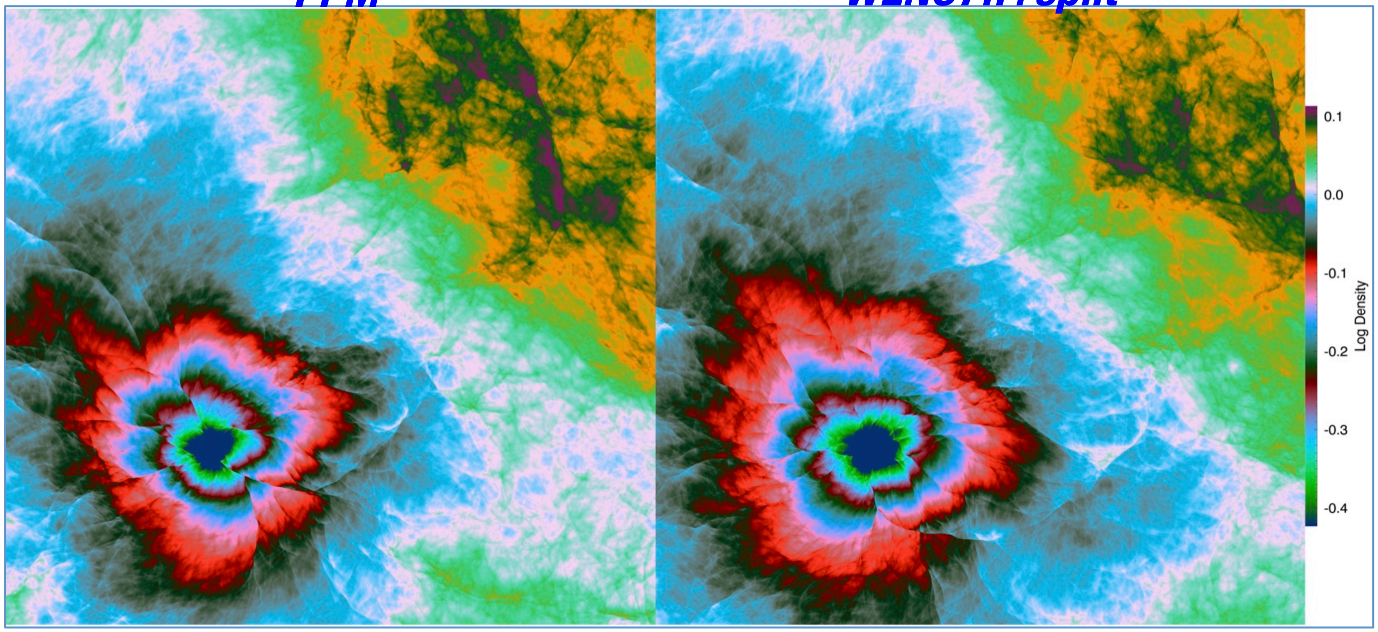


Spectral Bandwidth: **WENO7fi+split 2.2 X > PPM; ~4 times less CPU in 2D for same resolution** (assume 25%)

Note: If P(k) is a spectrum and $P(k) \sim k^n$, then the compensated spectrum is $k^{-n}P(k)$

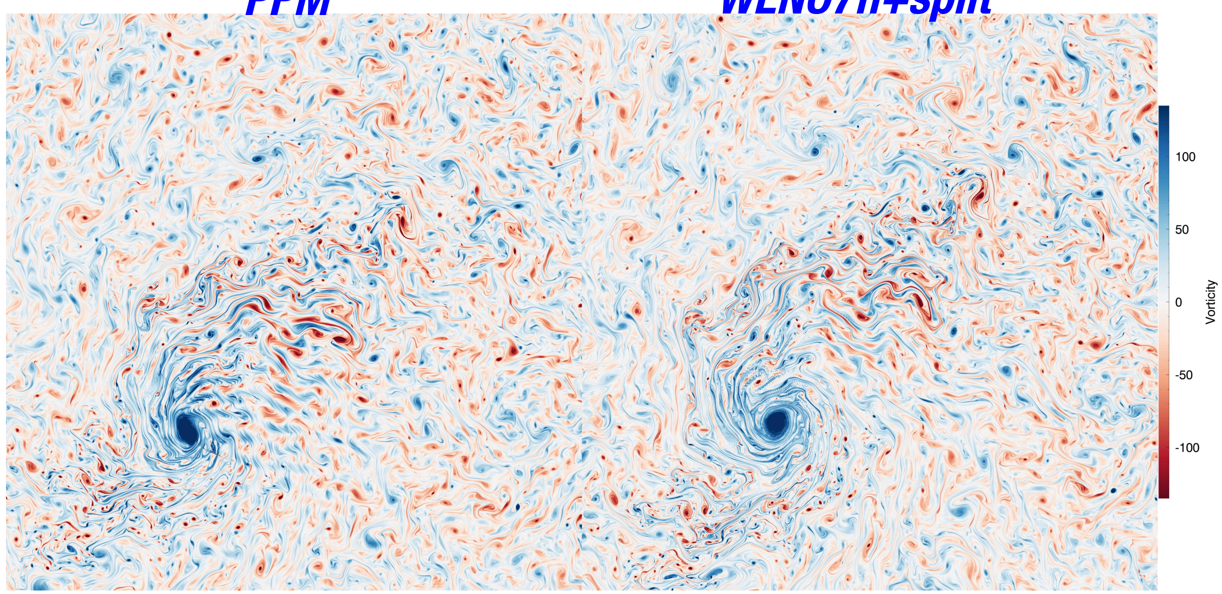
Instantaneous Density Comparison

PPM *WENO7fi+split*



Instantaneous Vorticity Comparison

PPM *WENO7fi+split*

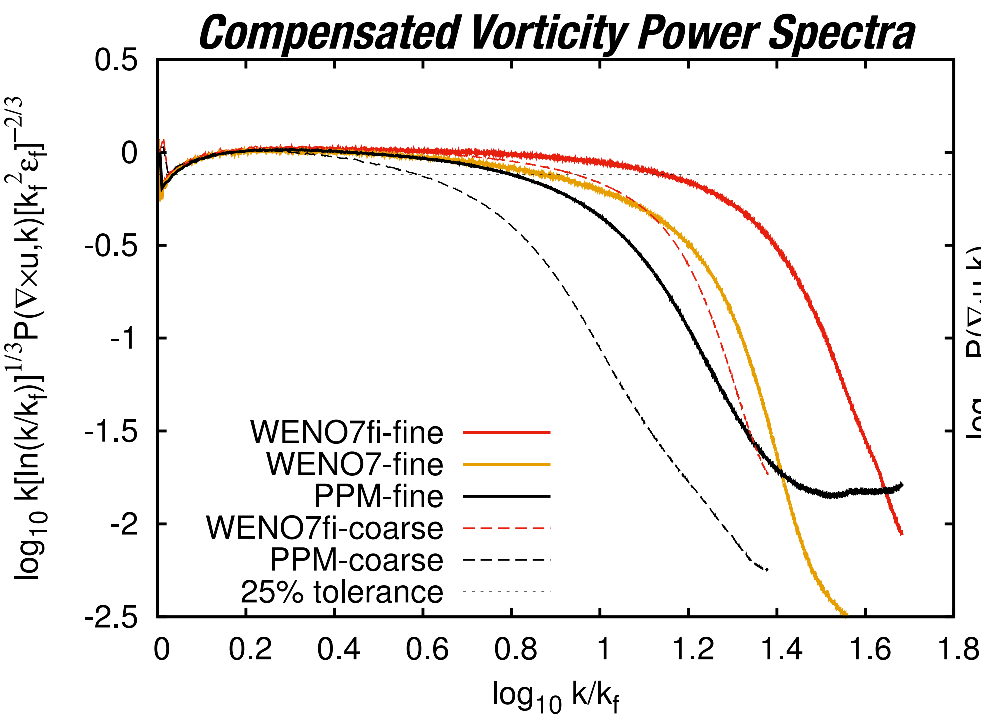


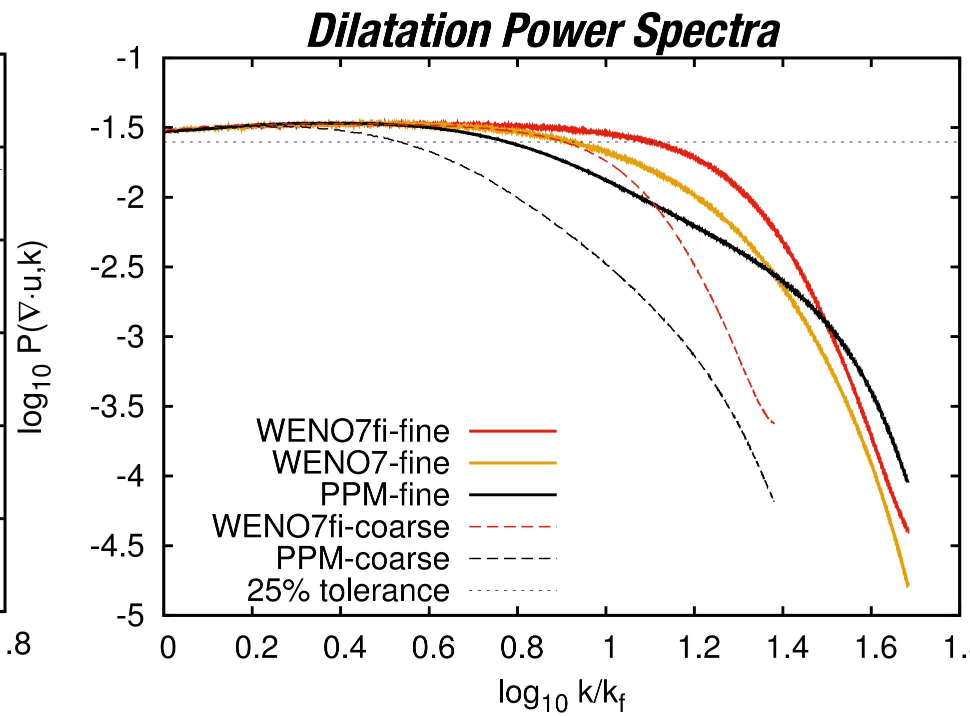
Scheme Comparison: PPM, WENO7, WENO7fi+split

2D Compressible Turbulence: Isothermal γ=1.001, periodic BCs

Flow determined by grid N, energy injection rate & energy injection scale

Direct Cascade study: Coarse vs. fine grids





Conclusion:

- **Vorticity bandwidth:** WENO7/PPM=1.2; WENO7fi/WENO7=1.8; WENO7fi/PPM=2.2
- **Dilatation bandwidth:** WENO7/PPM=1.5; WENO7fi/WENO7=1.5; WENO7fi/PPM=2.2
- **Absolute WENO7fi bandwidth:** for vorticity 68%; for dilatation 66%

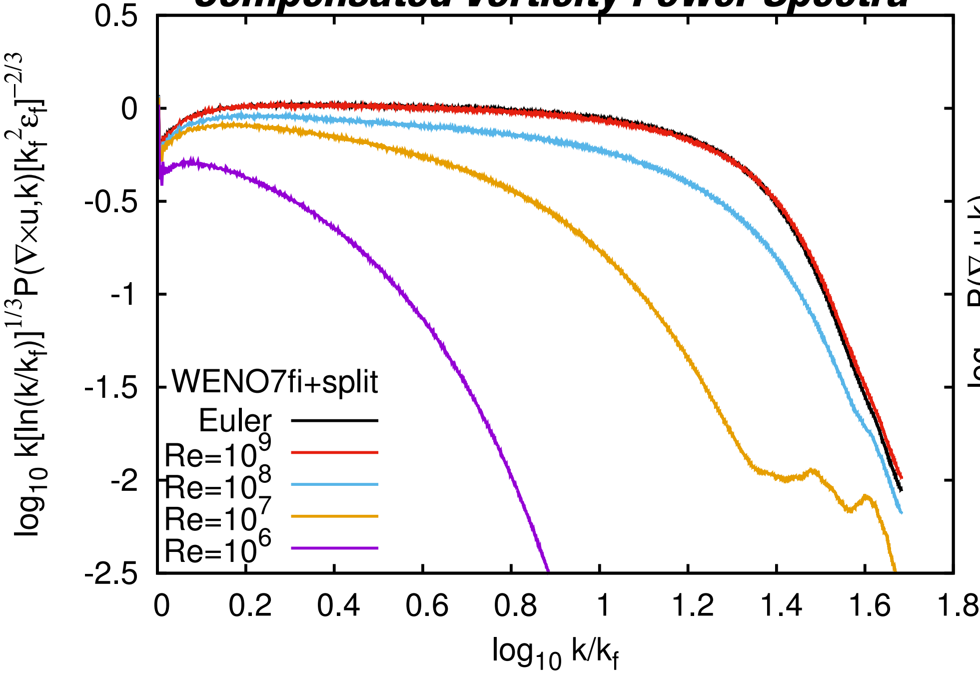
Euler vs. NS Comparison: WENO7Fi+split

2D Compressible Turbulence: Isothermal γ=1.001, periodic BCs

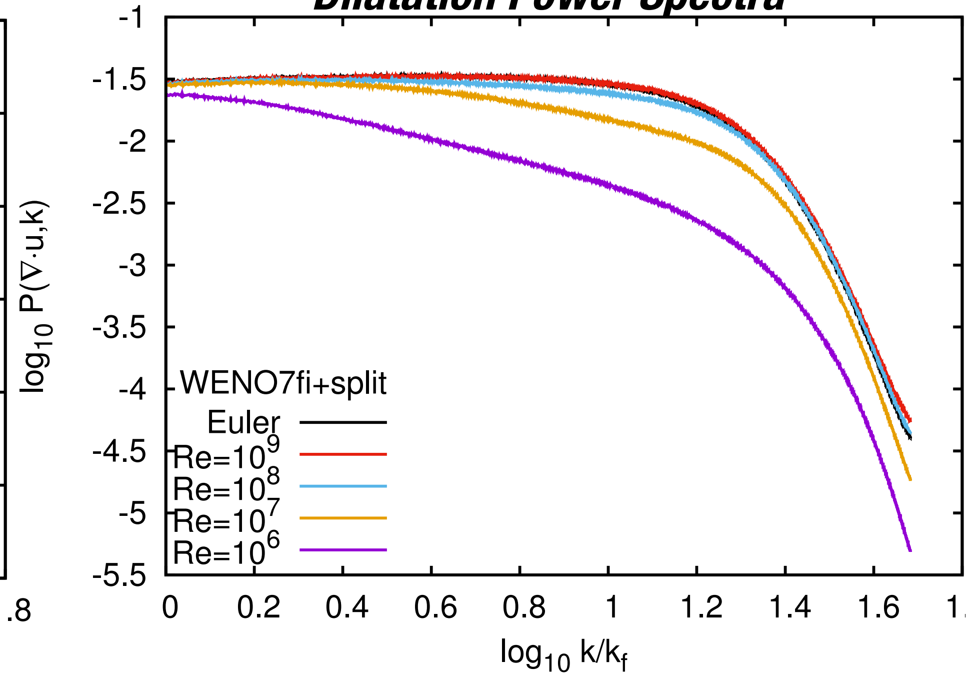
Flow determined by grid N, energy injection rate & energy injection scale

Isothermal Fluids: $T=T_0$ Constant Dynamic Viscosity, $Re=10^6, 10^7, 10^8, 10^9$

Compensated Vorticity Power Spectra



Dilatation Power Spectra



Summary:

WENO7fi+split correctly captures theoretically predicted spectra for both incompressible & compressible diagnostics in the limit of vanishing controlled numerical dissipation

3-D Compressible MHD (Ideal)

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

Conservative

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

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

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

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

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

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

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)*

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)
- **3-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**
  - > **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 16 combinations for the current study

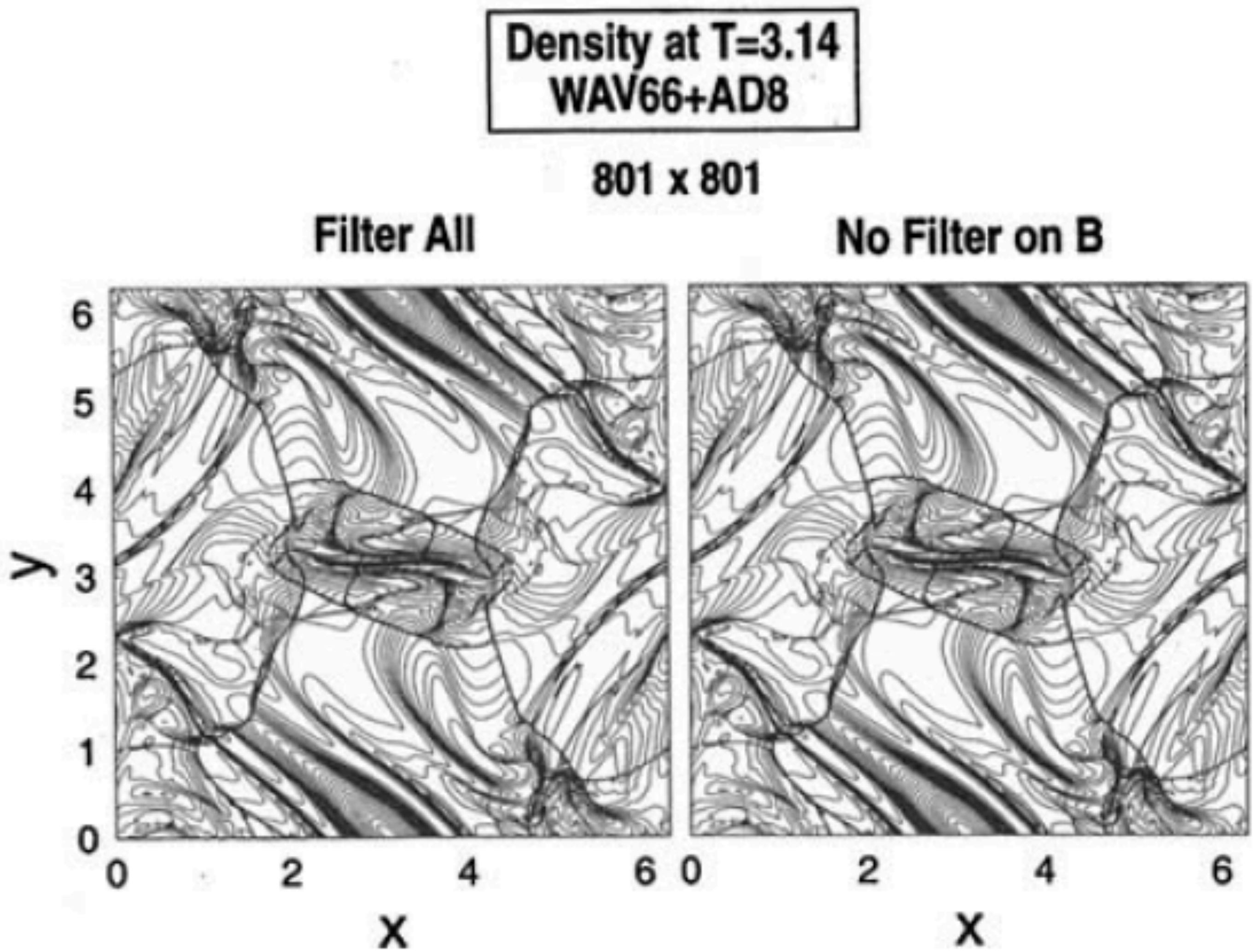
Compressible Orszag-Tang Vortex $(\gamma = 5/3)$

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

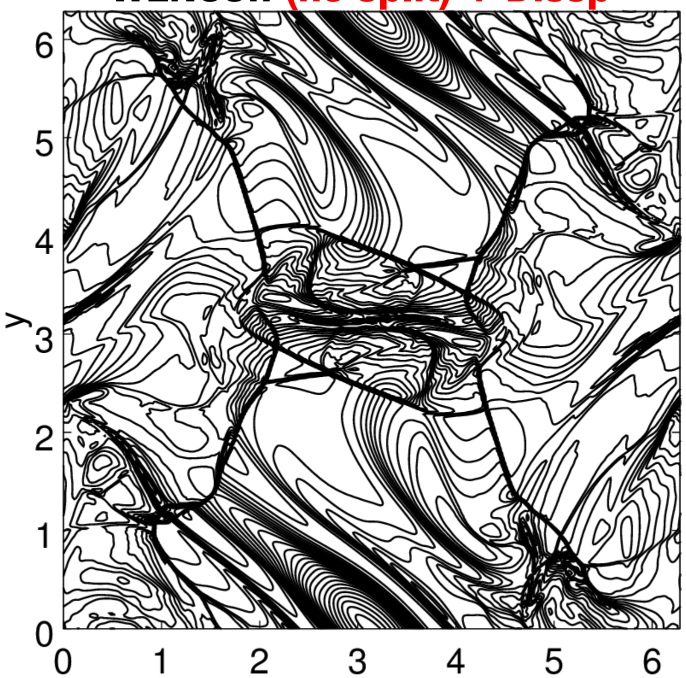


Ducros et al. Splitting *- Orszag-Tang Vortex Test case*

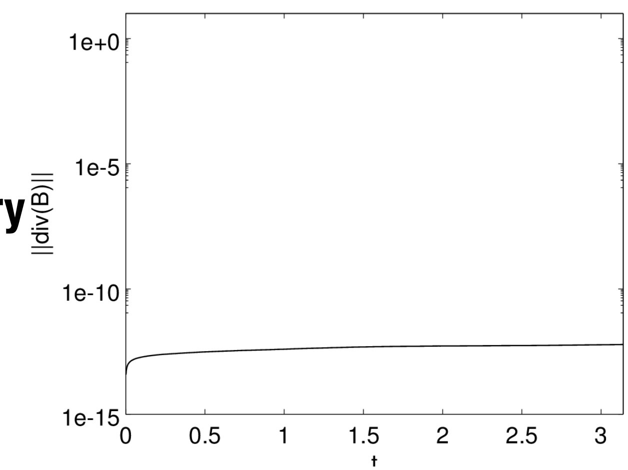
(Only on the Gas Dynamic Variables)

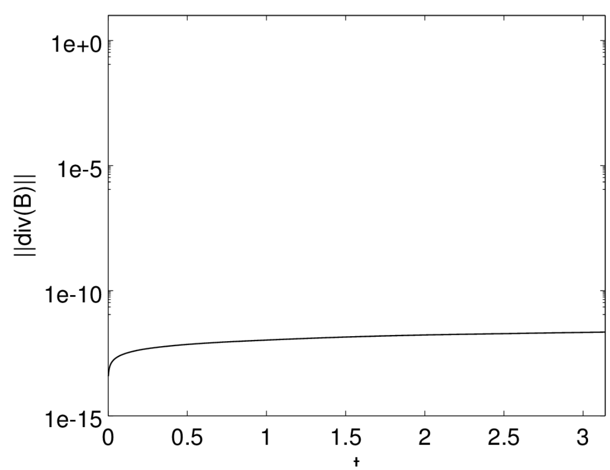
WENO5fi (no split) + Dissp | **WENO5fi+split**

Density



divB History





Numerical Examples

3D DNS Computations of Shock-Free Turbulence & Turbulence with Shocklets

- Standard shock-capturing methods are too diffusive for long time integration
- Careful design of appropriate nonlinear numerical dissipations with flow sensors can improve accuracy

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** $t/\tau = 4$