Recent Developments in Accuracy and Stability Improvement of Nonlinear Filter Methods for DNS and LES of Compressible Flows

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Numerical Techniques in MHD Simulations

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Objectives

(Construction of Accurate High Order Shock-Capturing Methods)

Yee et al. (1999-2017), Yee & Sjogreen (2004-2017), Kotov et al. (2013-2016)

Ultimate Goal:

Develop an integrated approach for stable, accurate & reliable yet efficient DNS & LES computations

Remarks:

- Low dissipative schemes that were designed for rapidly developing flows might suffer from nonlinear instability for long time integration of turbulence computations
- Dissipative stable schemes usually smear turbulent fluctuations to an unrecognizable state

Outline

- Objectives
- Technical Challenge
- Approach
- Significance
- Results
- Future Plan

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
- Stable & Accurate Temporal & Spatial Low Dissipative & Dispersive methods applicable to long time integration are required
- 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 existing tools
- 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

Recent developments:

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

Approach

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

- 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 sensor 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

Key Ingredients in Numerical Construction

(Tools to Improve Predictability & Reliability of Turbulence Simulations)

- **Nonlinear simulations of data limited complex multiscale flows**

  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*

- **Post-processer step**

  Conditioned the governing equations to an equivalent form before discretization
  (Discrete momentum/entropy conservation; discrete kinetic energy preservation, etc.)

- **Highly accurate non-dissipative base scheme**

- **Nonlinearly filter the solution to remove spurious oscillations**
  - *Device flow sensors to delineate:*
    Shock-free turbulence, low speed turbulence, and turbulence with strong shocks
  - *Utilized adaptive flow sensor to control locations & amount of numerical dissipation to be employed for maximum accuracy & stability consideration*

Five Methods to Improve Nonlinear Stability & Accuracy

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

Under the Yee et al. nonlinear filter approach framework:

- 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
- 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*

All methods are included in our 3D overset grid code ADPDIS3D

Yee & collaborators published work (2009-2017)

Remark

Present numerical method development for gas dynamics
***with* Modification**
can carry over to MHD for short time & long time integration

Yee et al., 2000-2013, Yee & Sjogreen, 2007-20017, Sjogreen & Yee, 2016-2017, Wang et al., 2009-2015, Kotov et al., 2011-20016

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* 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. WENO5*)

High order central numerical flux (*e.g. 6^{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)*

Performance of High Order Nonlinear Filter Scheme

(A wide range of Compressible Flow Types)

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)
- ➔ > *Dual & Direct Cascade Study of 2D Forced Compressible Turbulence*

  (Aeronautical & Astrophysical Applications, Kritsuk et al. 2016)

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)

Study the role of compressibility in turbulent mixing layers

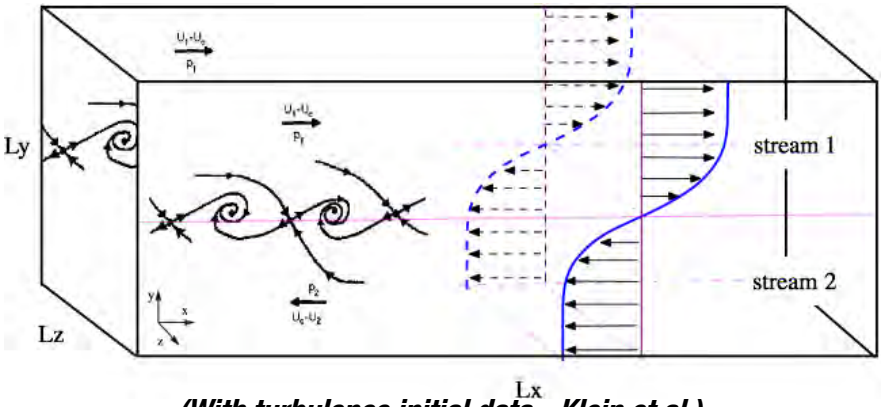
LES computations are carried out up to dimensionless time $\tau = t\Delta U / \delta_{\theta 0} \simeq 3000$ for the higher M_c cases & $\tau \simeq 1200$ for the quasi-incompressible cases

Grid

Case	M_c	Re_{θ_0}	Re_{ω_0}	Grid
DNS [37]	0	800	1370	
DNS [33]	0.3	160	640	
LES-C1	0.1	200	800	512 x 211 x 65
LES-C2	0.3	200	800	512 x 211 x 121
LES-C3	0.8	200	800	
LES-C4	1.0	200	800	512 x 211 x 131
LES-C5	1.5	200	800	

LES Model: Germano-Lilly dynamic procedure

Initial profile: $u(y) = (\Delta U / 2) \tanh [y/(2\delta)]$
v=0, w=0

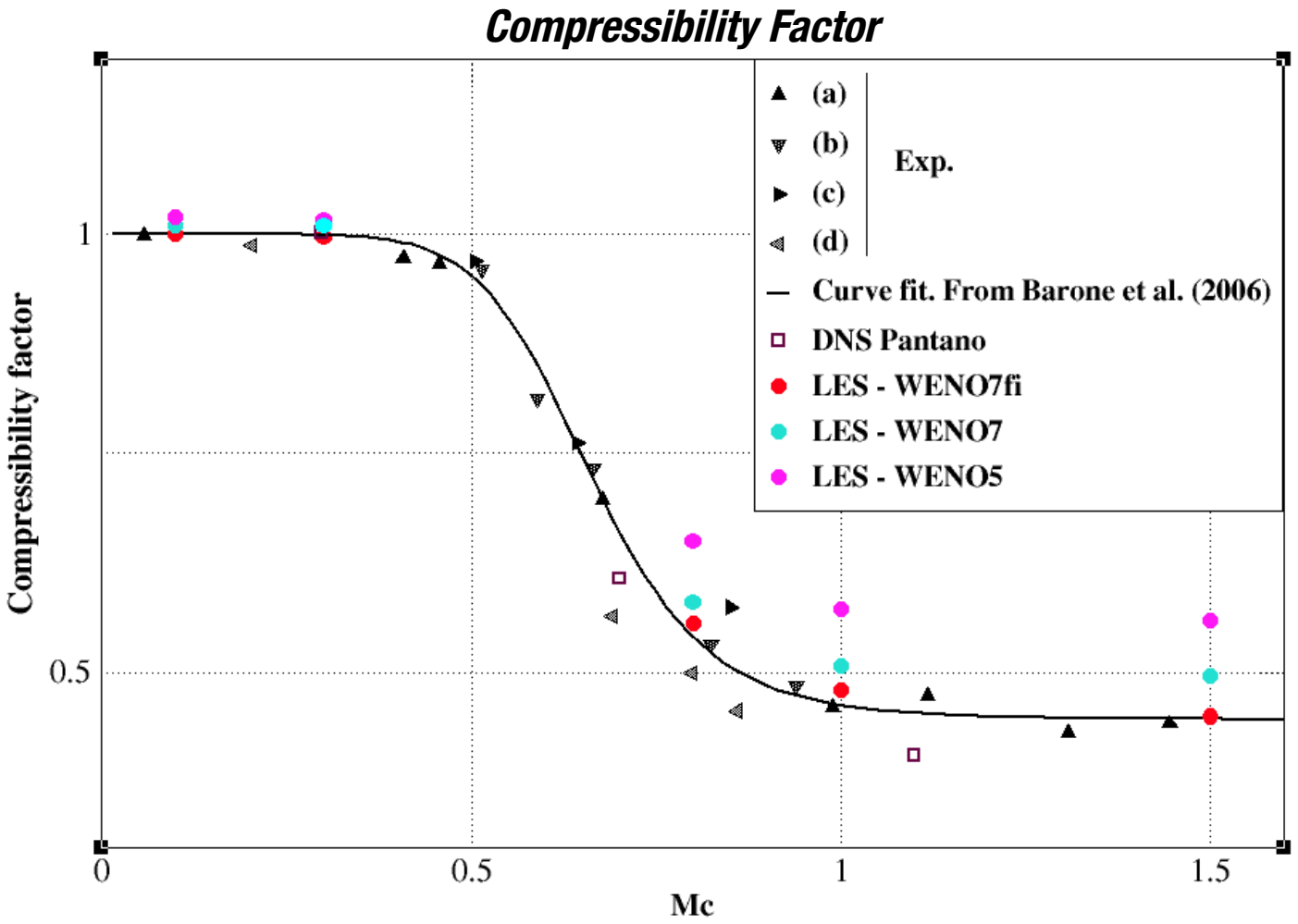


(With turbulence initial data - Klein et al.)

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**



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: $t = 10$

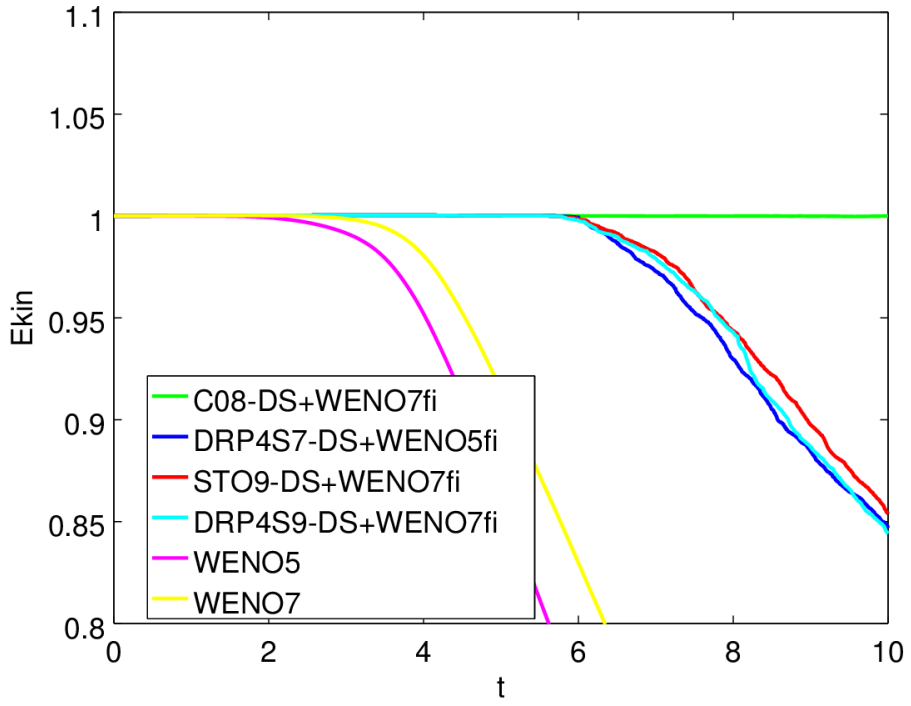
Viscous case

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

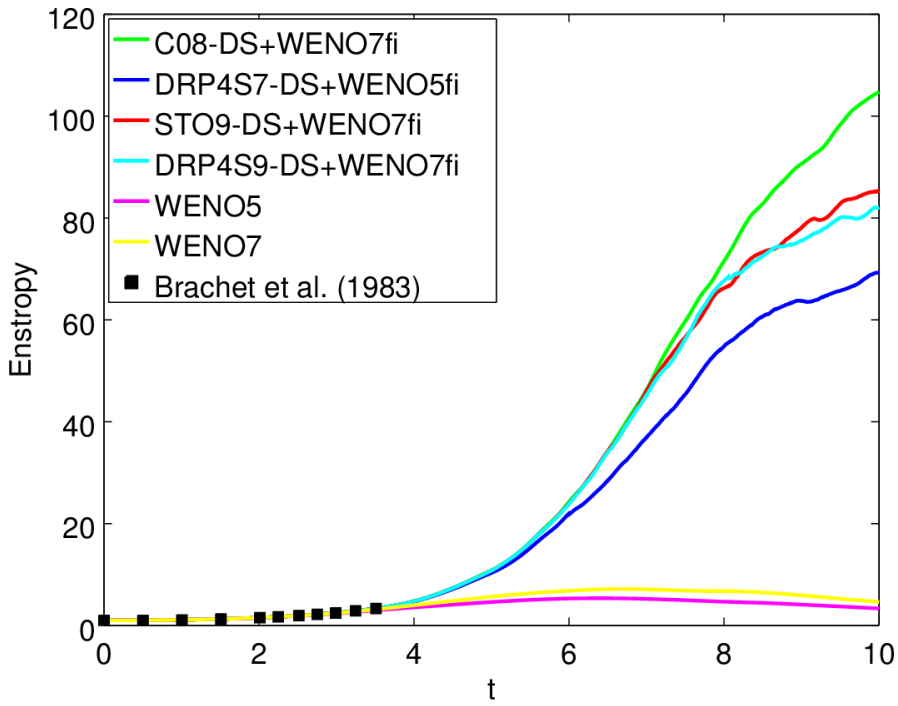
3D Taylor-Green Vortex (Compressible & Inviscid)

(Comparison of 6 Methods, 64^3 grids)

Kinetic Energy



Enstrophy



C08-DS+WENO7fi: 8^{th}-order central + Ducros split +WENO7fi

DRP4S7-DS+WENO5fi: Tam & Webb 4^{th}-order DRP, 7pt grid stencil + Ducros split +WENO5fi

ST09-DS+WENO7fi: Bogey & Bailly 4^{th}-order DRP, 9pt grid stencil + Ducros split +WENO7fi

DRP4S9-DS+WENO7fi: Tam & Webb 4^{th}-order DRP, 9pt grid stencil + Ducros split +WENO7fi

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

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

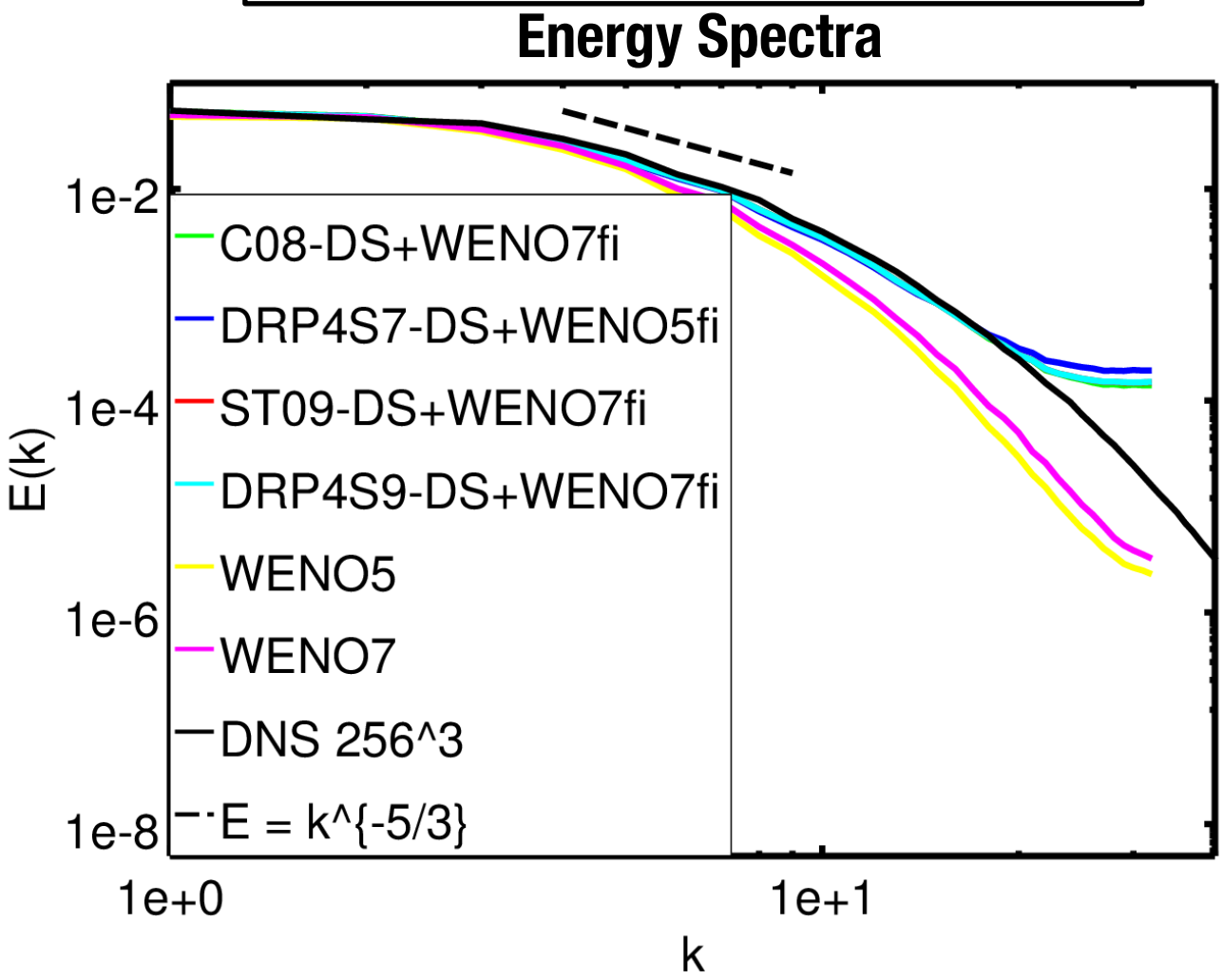
$\frac{3}{2} u_{rms,0}^2 = \frac{\langle u_{i,0} u_{i,0} \rangle}{2} = \int_0^\infty E(k) dk$

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

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

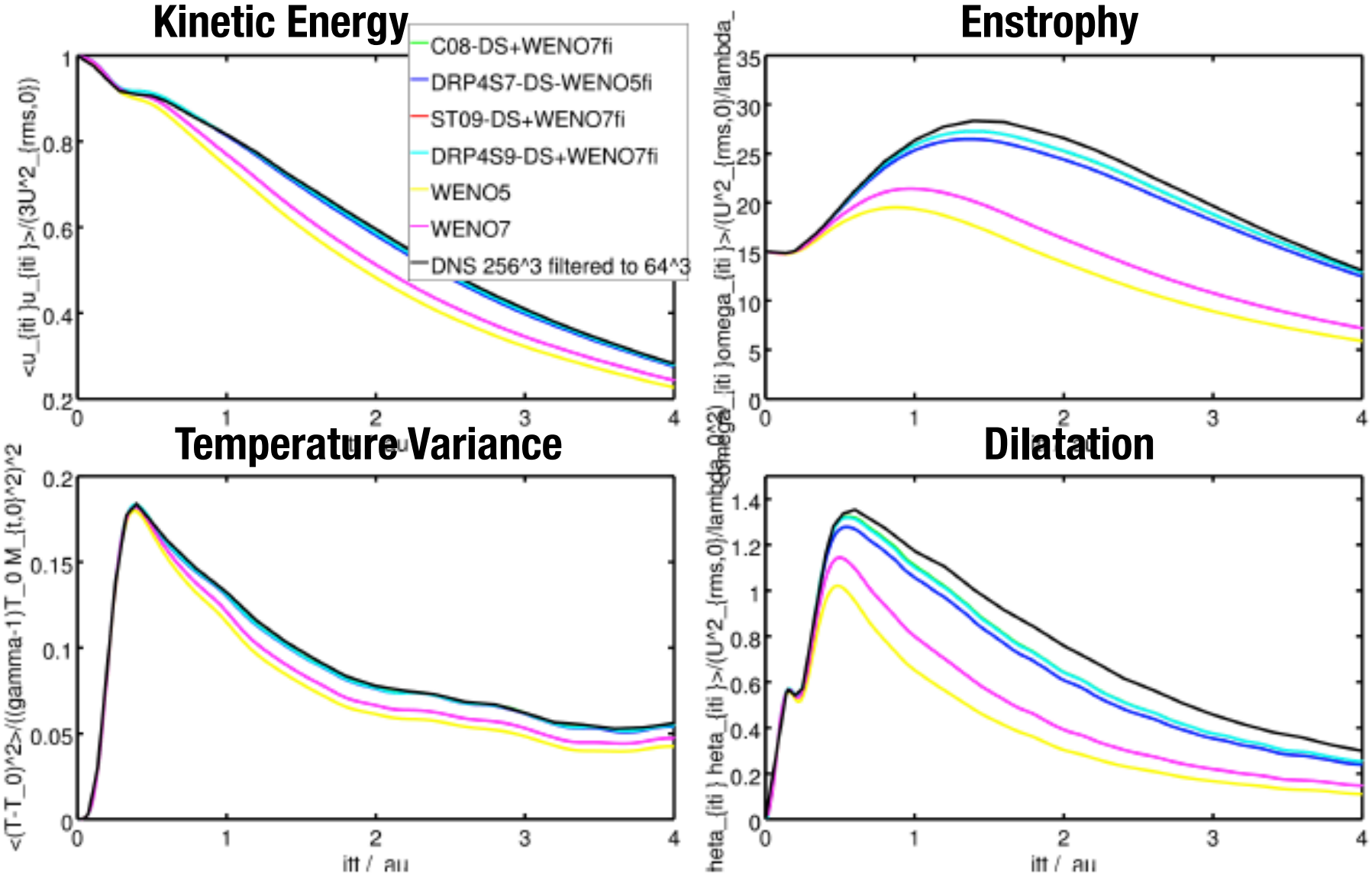
3D Isotropic Turbulence with Shocklets
Compressible & Inviscid

Comparison of 6 Methods, 64^3 grids



3D Isotropic Turbulence with Shocklets

Comparison of 6 Methods, 64^3 grids



Test Cases

(3D DNS & LES)

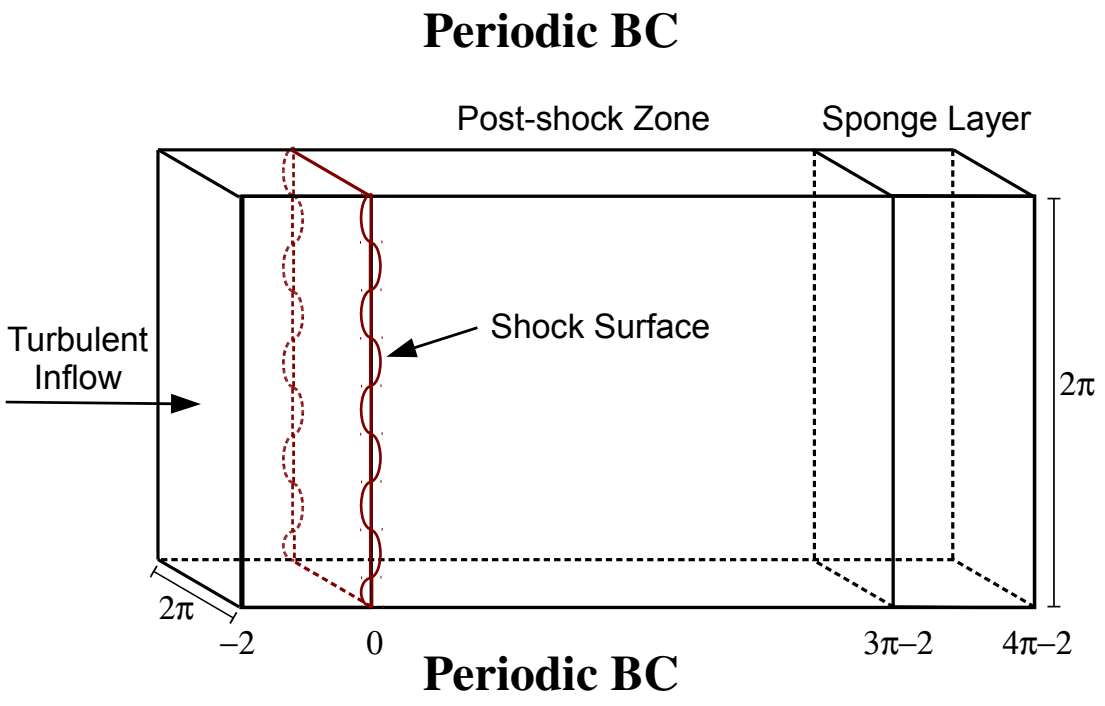
Turbulence Interacting with a Strong Shock

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

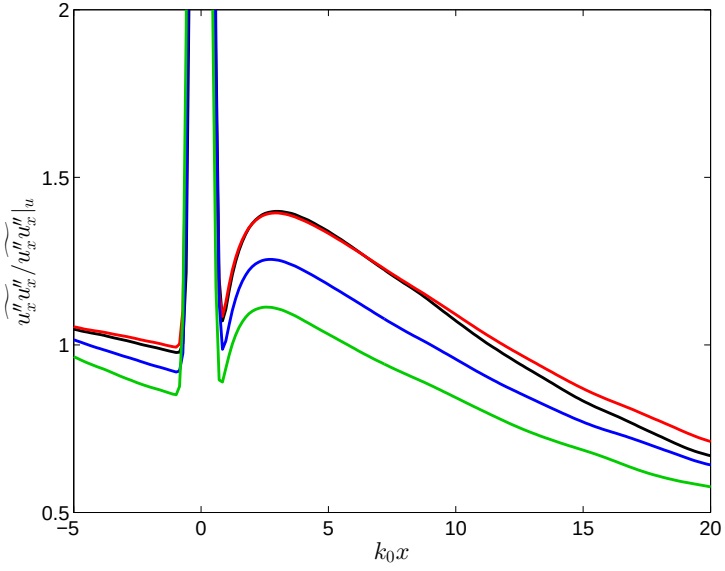


Sponge source term: $$W = -\frac{k_0 u_0}{2\pi}\left(\frac{x - x_{sp}}{x_{max} - x_{sp}}\right)(f - \langle f \rangle_{yz})$$

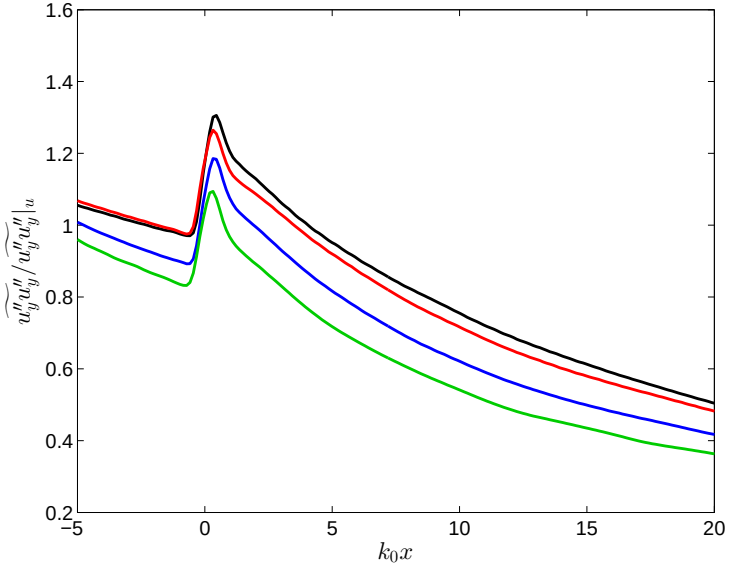
(Gently drive the flow towards a laminar state)

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

Streamwise Reynolds Stress



Streamwise Vorticity



Filtered DNS

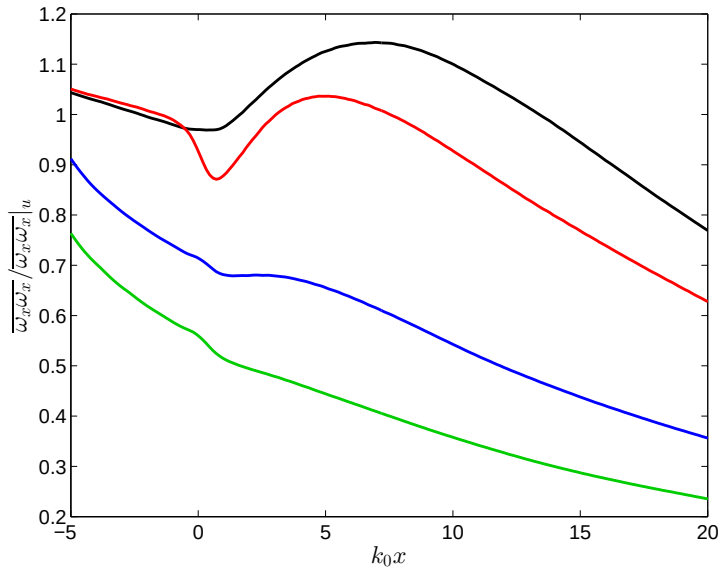
WENO7fi+split

WENO7

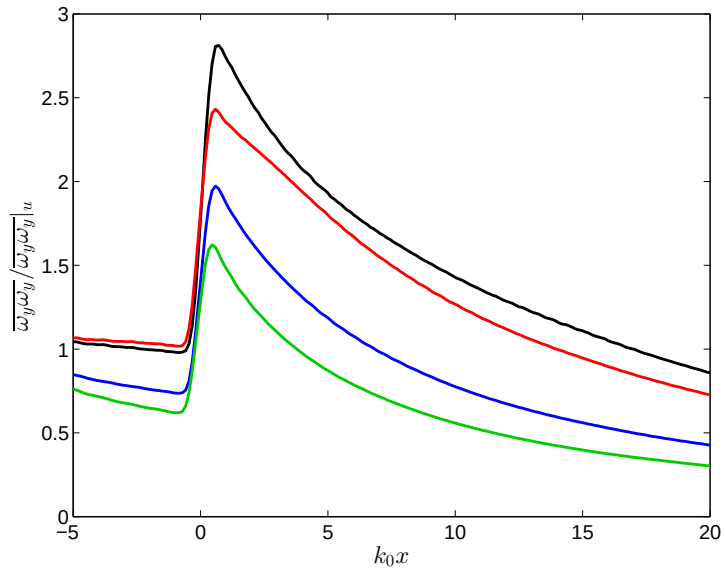
WENO5

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**

Astrophysical Applications: 2D Turbulence

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

Application: ***Energetics of the ISM in Galactic Disks***

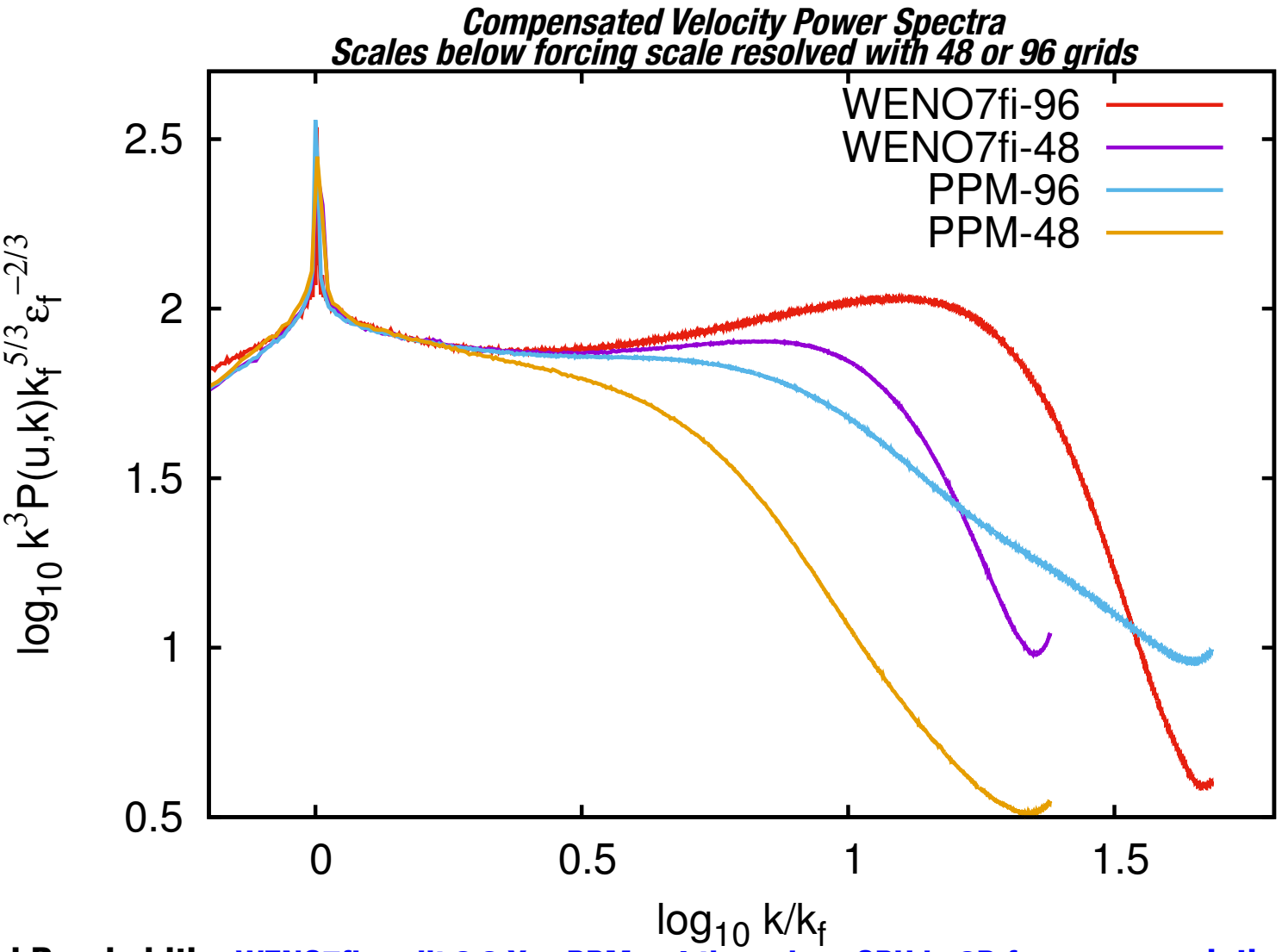
- ***Dual energy cascade study***
- ***Does the inverse energy cascade work in the compressible case?***
- ***What are the corresponding scaling relations?***

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

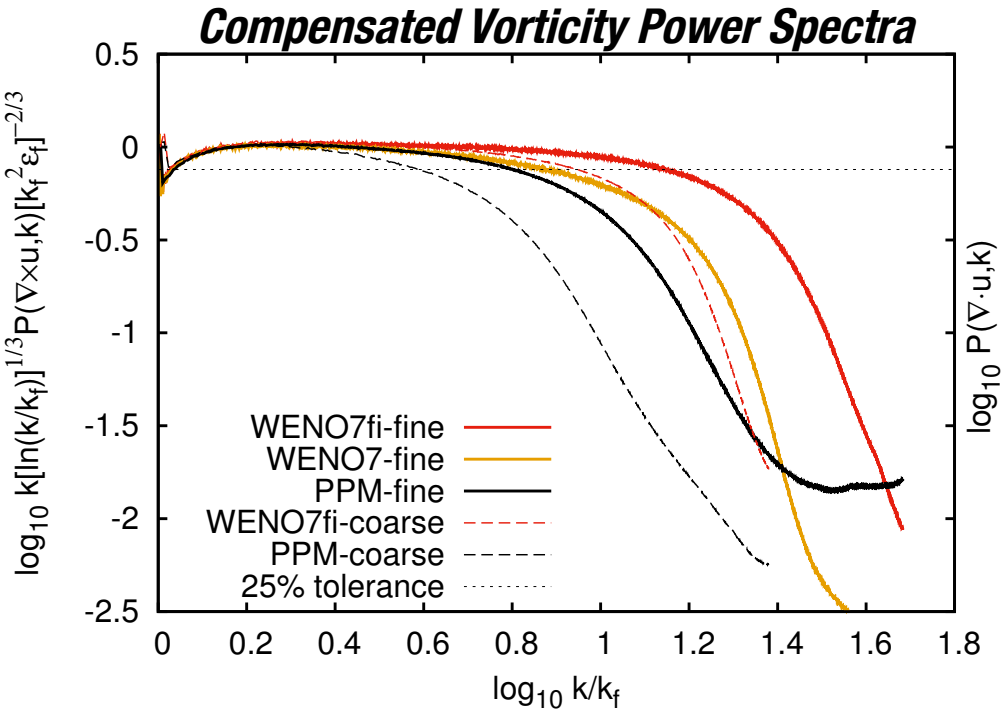


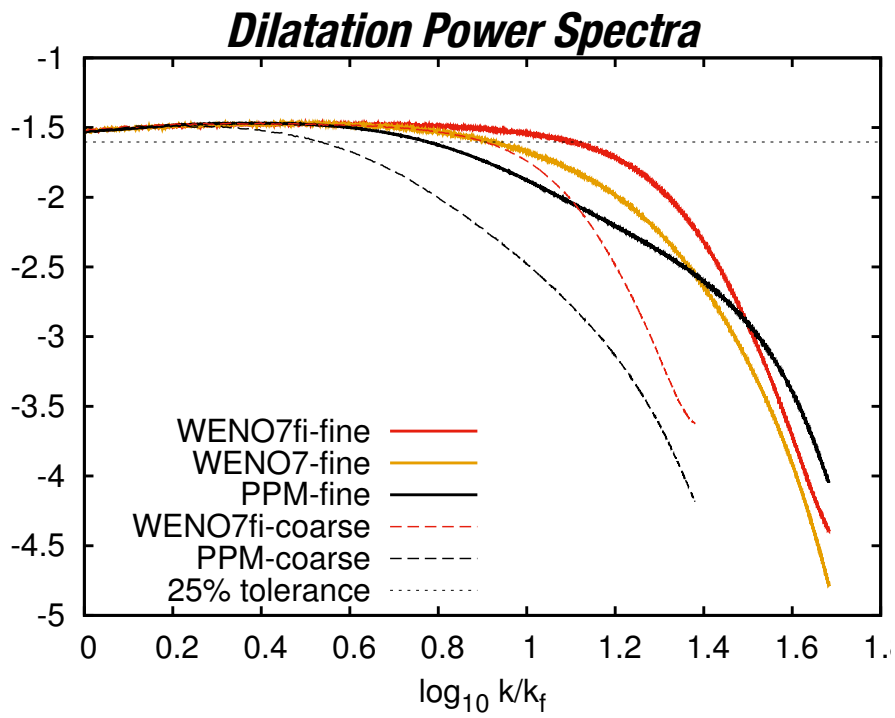
Spectral Bandwidth: **WENO7fi+split 2.2 X > PPM; ~4 times less CPU in 2D for same resolution** (assume 25%)
Note: If P(k) is a spectrum and P(k)~k^n, then the compensated spectrum is k^{-n}P(k)

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





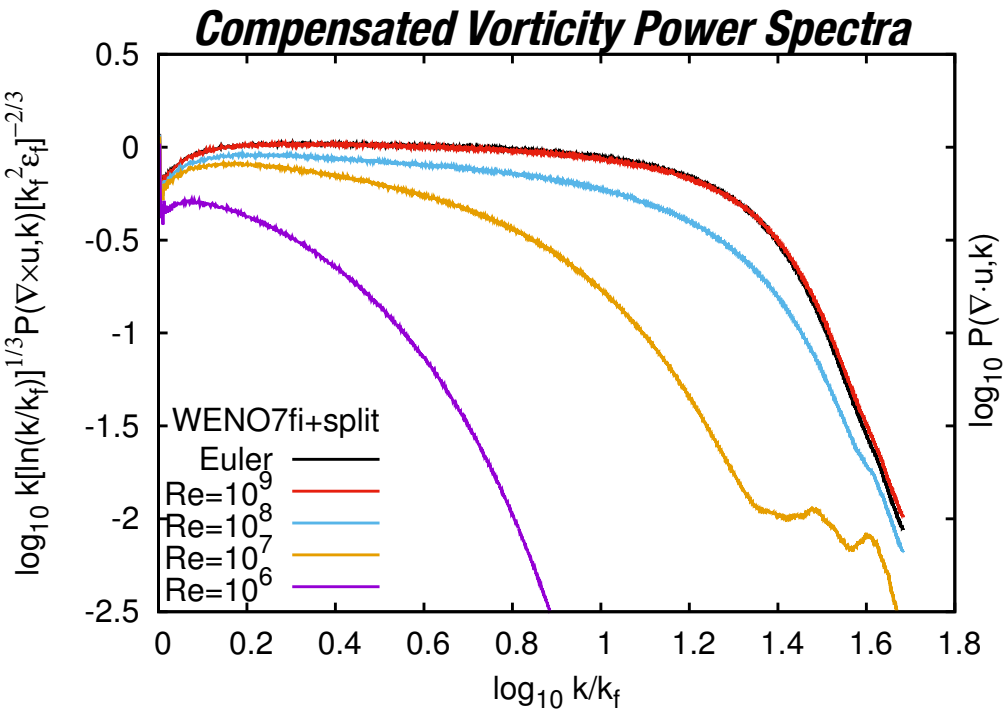
Conclusion:

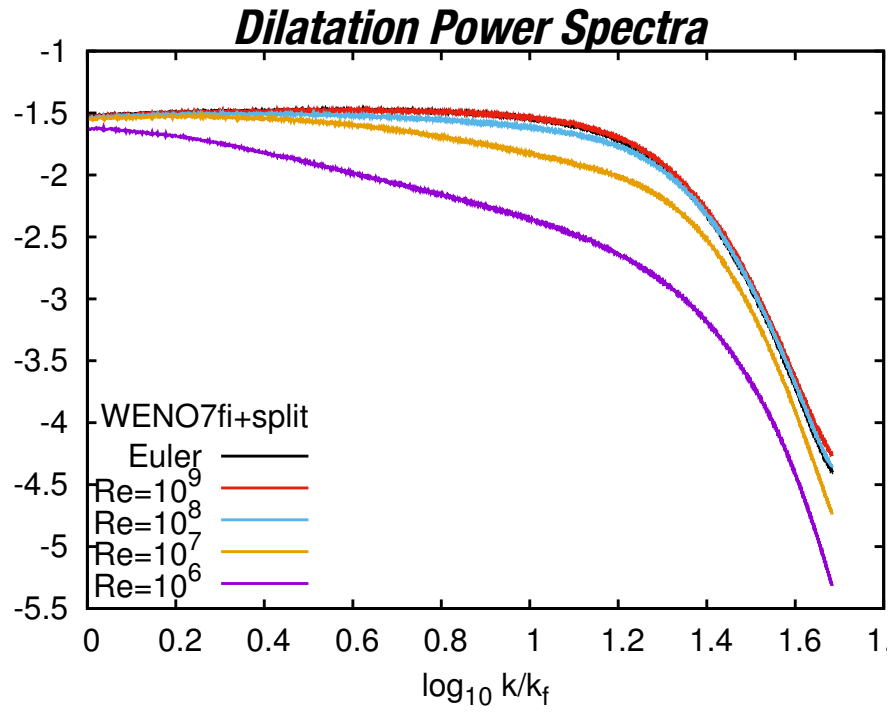
- **Vorticity bandwidth:** WENO7/PPM=1.2; WENO7fi/WENO7=1.8; WENO7fi/PPM=2.2
- **Dilatation bandwidth:** WENO7/PPM=1.5; WENO7fi/WENO7=1.5; WENO7fi/PPM=2.2
- **Absolute WENO7fi bandwidth:** for vorticity 68%; for dilatation 66%

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, $Re=10^6, 10^7, 10^8, 10^9$





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)*

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

I.C.

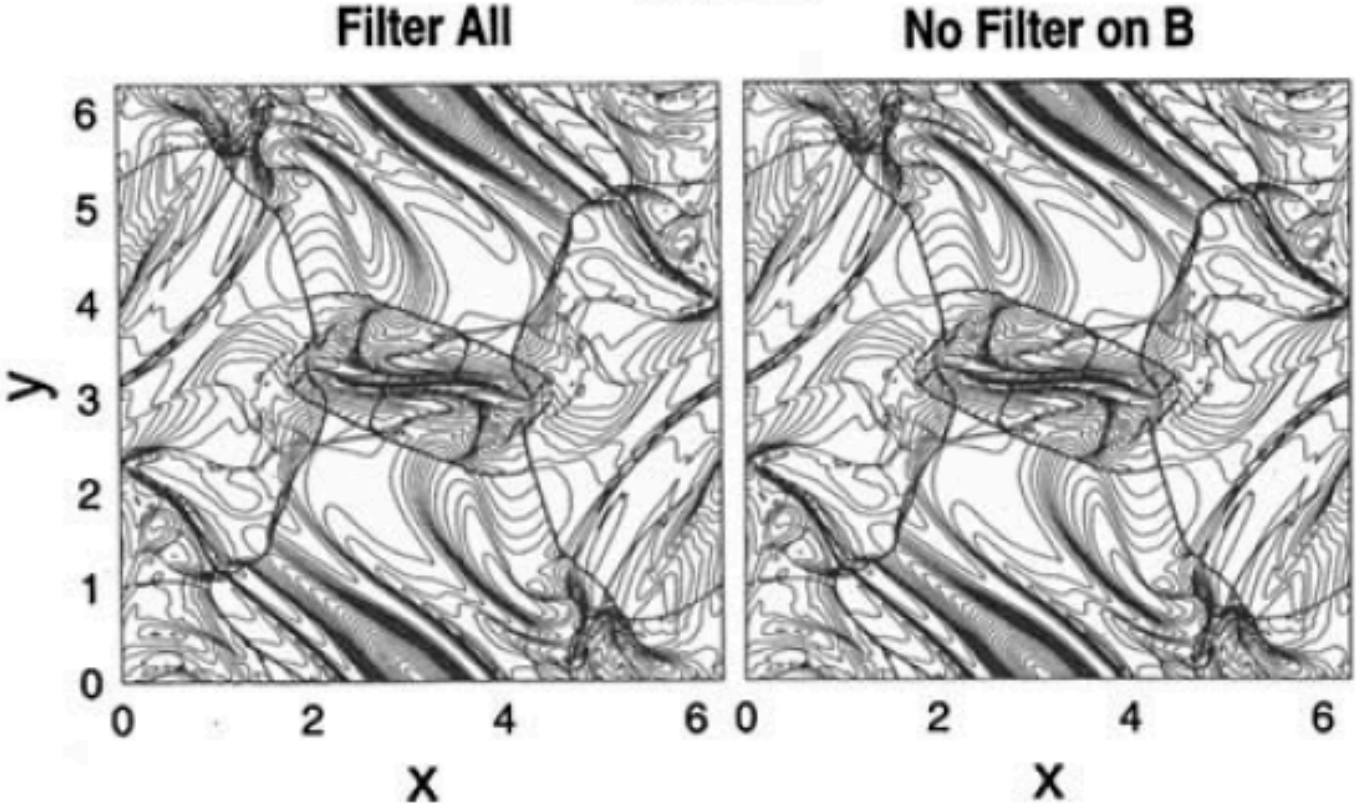
$$\begin{pmatrix} \rho \\ u \\ v \\ w \\ p \\ B_x \\ B_y \\ B_z \end{pmatrix} = \begin{pmatrix} 25/9 \\ -\sin y \\ \sin x \\ 0 \\ 5/3 \\ -\sin y \\ \sin 2x \\ 0 \end{pmatrix}$$

BC: Periodic

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

Density at T=3.14
WAV66+AD8

801 x 801



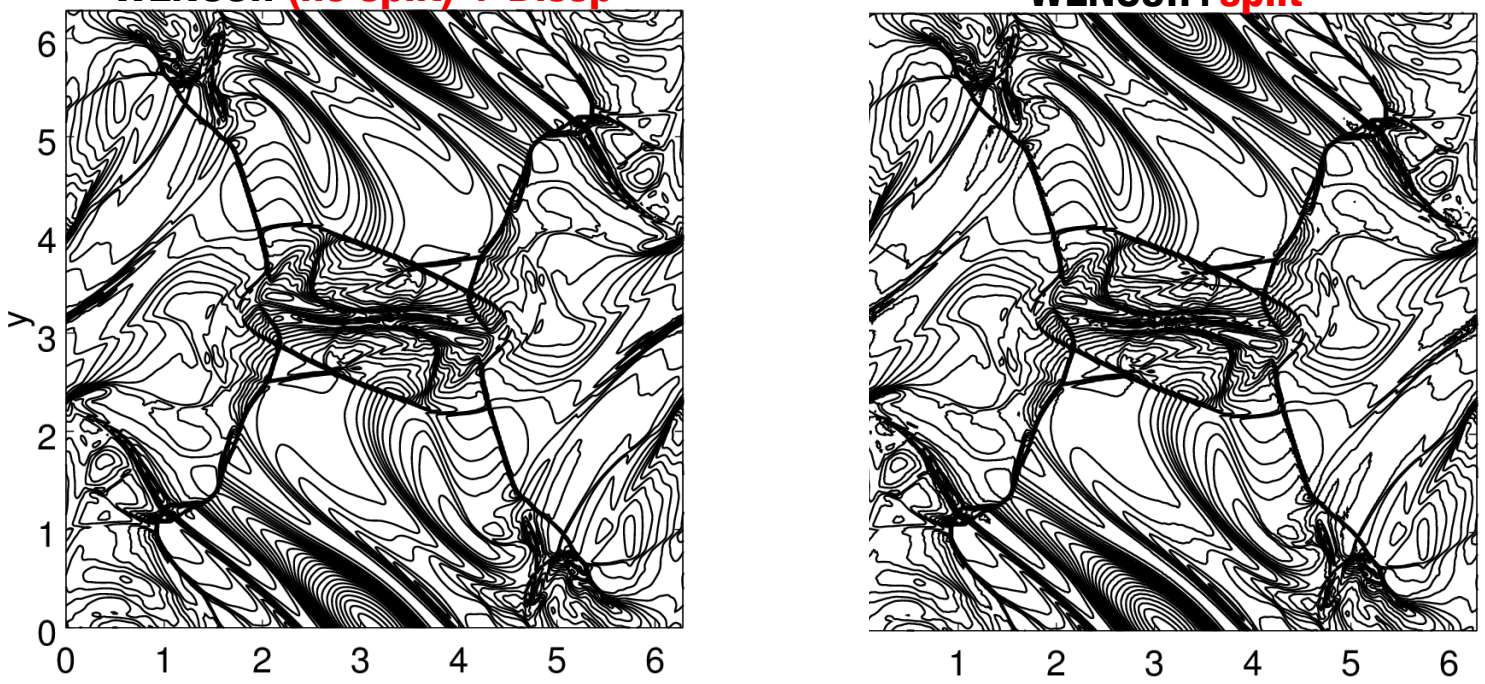
Ducros et al. Splitting - *Orszag-Tang Vortex Test case*

(Only on the Gas Dynamic Variables)

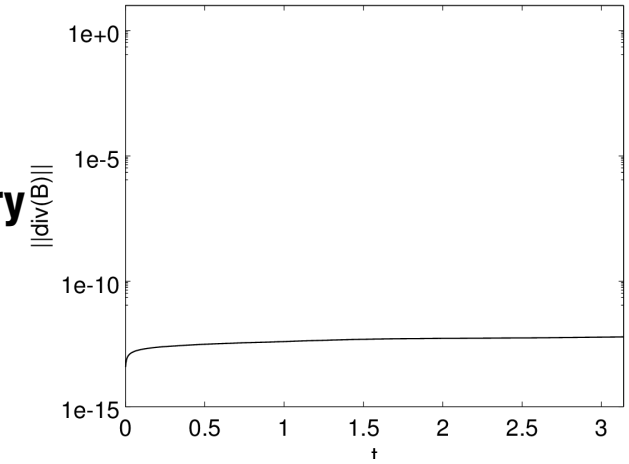
WENO5fi (no split) + Dissp

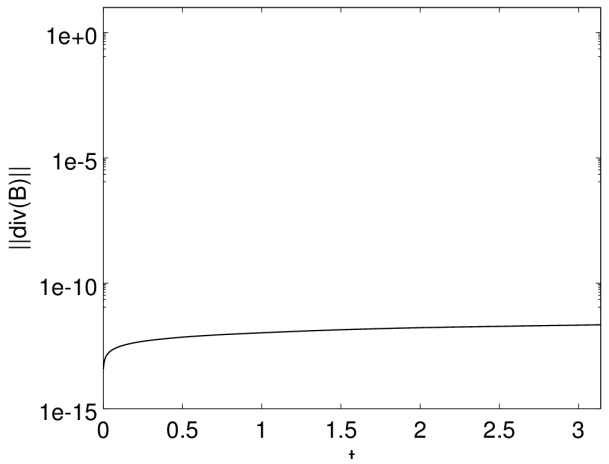
WENO5fi+split

Density



divB History





Integrated Approach for the Development of Numerical Tools for Compressible DNS & LES

High Order Nonlinear Filter Schemes
Adaptive Numerical Dissipation Control for Accurate Simulations of DNS & LES for Wide Range of Turbulent Flows
(Overset Grids for Complex Geometries)

Properties of Scheme & ADPDIS3D Unsteady Code

- Energy stable high order schemes with adaptive numerical dissipation control via local flow sensors to provide the correct amount of numerical dissipations where needed & leave the rest of the flow domain free of numerical dissipation contamination
- Low dissipation for a wide range of turbulence flow speeds & flow types
- High order positive schemes for stiff extreme flow problems
- Energy stable summation-by-parts (SBP) numerical boundary closure
- Conservative high order temporal & spatial metric for complex geometries

History of Development: (1998 – Present)

(I) Scheme Development & DNS Applications

1. Energy Stable SBP High Order Scheme with Dissipation Control (Yee et al., 1999-2002),
   Turbulence-shock interactions, mixing layer & DNS in curvilinear grids
   - > Yee et al., JCP (1999, 2000); Vinokur & Yee (2000) – Energy stable SBP high order scheme
   - > Yee & Sjogreen (2002) – Book Chapter
   - > Sandham et al., JCP (2002)– DNS of 3D channel flow

Integrated Approach for the Development of Numerical Tools for Compressible DNS & LES *(Cont.)*

2. Generalization of Energy Stable SBP High Order Schemes (Yee & Sjogreen, Kotov et al., 2002-2013),

   Smart flow sensors for a large class of numerical dissipation control by the dissipative portion of high order shock-capturing schemes

   > Yee & Sjogreen, JCP (2007) – Generalization of nonlinear filter schemes for a large class of schemes
   > Yee & Sjogreen, Shock Waves (2007) – Richtmyer –Meshkov instability (chaotic/turbulence flow studies)
   > ICOSAHOM (2009) – Generalized schemes using smart flow sensors
   > Sjogreen & Yee, TSFP-5 (2007) – SBP boundary closures for 10th-order scheme
   > Sjogreen & Yee, ENUMATH09, 2009 – Energy stable/entropy stable scheme development
   > Johnston et al., JCP (2010) – 3D DNS simulations (Taylor & Green, Isotropic Turbulence with Shocklets, etc.)
   > Kotov et al., CTR Tech. Brief, Stanford Univ. (2012- 2014) – 3D DNS simulations; Improve local flow sensors & positivity schemes to improve accuracy & stability of extreme flow types

3. Extension of Nonlinear Filter Schemes to Overset Grids with High Order Conservative Spatial & Temporal Metric Evaluations (Sjogreen & Yee, Lani et al., Sjogreen, Yee & Vinokur),

   Smart flow sensors for a large class of numerical dissipation control by the dissipative portion of high order shock-capturing schemes

   > Sjogreen & Yee, CiCP (2009) – 3D CEV coarse grid DNS simulations
   > Lani et al., CiCP (2013) – 3D CEV reacting flow coarse grid DNS simulations
   > Sjogreen, Yee & Vinokur, JCP (2014) – High Order Conservative Spatial & Temporal Metric Evaluations

(II) Scheme Development & LES Applications (2010 - Present)

> Yee et al., CiCP (2012) – 3D temporary mixing-layer by very high order filter schemes, comparison with DNS results
> Hadjadj et al. IJNMF (2012) – 3D temporary mixing-layer by an 8th-order filter scheme, comparison with experiments
> Kotov et al., ICCFD8 (2014), CTR Tech. Brief, Stanford Univ. (2014) – High order numerical methods for LES of Turbulent with shocks & modification of the Germano Dynamics Filter Procedure for Turbulence Flows containing shock waves

(III) ADPDIS3D – 3D Unsteady Highly Parallel Code: Major support from a 5 year multi-institute grant from DOE/SciDAC (10 years of code development for DNS & LES for turbulence with shocks)

> Ability to perform DNS and LES computations in non-trivial geometries through the use of overset curvilinear grids.
> Contain a large number of high fidelity high-order schemes and shock-capturing schemes
> These schemes can be used to perform accurate unsteady computations for flow speeds that range from nearly incompressible to hypersonic speeds
> Contain three choices of solvers: Standard compressible flow, combustion & chemical nonequilibrium hypersonic flows
> Contain many innovative low dissipative algorithms that adaptively use numerical dissipation from shock-capturing schemes as postprocessing filters on non-dissipative high-order centered schemes

Current Research (2016 – Present)

- **Develop high order low dispersion and low dissipative schemes to further improve numerical accuracy of compressible turbulent flows (wide range of flow speeds)**
  - Sjogreen & Yee, 2017
- **Develop high order entropy conservative numerical fluxes for MHD application**
  - Low Order: Janhunen (2000), Winters & Gassner (2016), Chandrasekar-Klingenberg (2015)
  - High Order: Sjogreen & Yee (2009-present) - Central, Fjordholm, Mishra & Tadmor (2012) - ENO, etc.

Integrated Approach for Stability, Accuracy & *Reliable Simulations*

(Construction of High Order Low Dissipative Numerical Methods)

Yee et al. (1999-2003), Yee & Sjogreen (2004-2009), Kotov et al. (2013-2016)

➔ **Stability & Accuracy:**

- > *Interior Scheme & Num. Boundary Scheme (non-periodic BC)*
  Summation-by-parts (SBP) boundary closures (Strand 1994, Olsson 1996)
- > *Short Time Integration vs. Long Time Integration (DNS & LES)*
- > *High Order GCL (Geometric Conservation Law) metric evaluation (Sjogreen et al. 2014)*

Skew-symmetric Splitting of Inviscid Flux Derivatives:

Further improvement of Stability & Minimize Num. Dissipation

- > *Yee et al. Entropy Splitting (2000)*
- > *Ducros et al. Splitting (2000) & generalization*
- > *High Order Extension of Tadmor Entropy Conservative Numerical Fluxes (Sjogreen & Yee 2009)*

Discrete Conservation Methods: *FV vs. FD & DG, etc.*

- > *Entropy stable conservative high order numerical fluxes (Sjogreen & Yee 2009)*
- > *Momentum conservation, Kinetic energy preservation, etc.*

➔ **Numerical Dissipation Control:** *Yee et al., Yee & Sjogreen, and Kotov et al. (1999-2016)*

- > *Turbulence cannot tolerate num. dissipation*
  Proper amount is needed in the vicinity of high shear, shocks & contacts
- > *Different requirements in the minimization of num. dissipation for different flow types*
- > *Adaptive flow sensor to control the amount of num. dissipation*

➔ **Reacting Flow/Combustion:** *Yee et al., Wang et al., Yee & Sweby, LeVeque & Yee (1990 – 2015)*

- > *Stiff source terms with shock - May lead to incorrect shock speed*
- > *Preserve certain physical steady states exactly – Well-balanced scheme*

Gas Dynamics vs. MHD scheme constructions

Some Gas Dynamics development can carry over to MHD (Items with an arrow)

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

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 2pth-order split form in conservation form:

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

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

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

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

2pth-order Central Ducros et al. Splitting Numerical Flux for 3D Gas Dynamics

3D Inviscid Flux Derivative in x-Direction:

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

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

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

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

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 (6^{th}-order & 8^{th}-order)*

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

Among studied test cases
Classical central schemes provide slightly more improvement than DRP

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

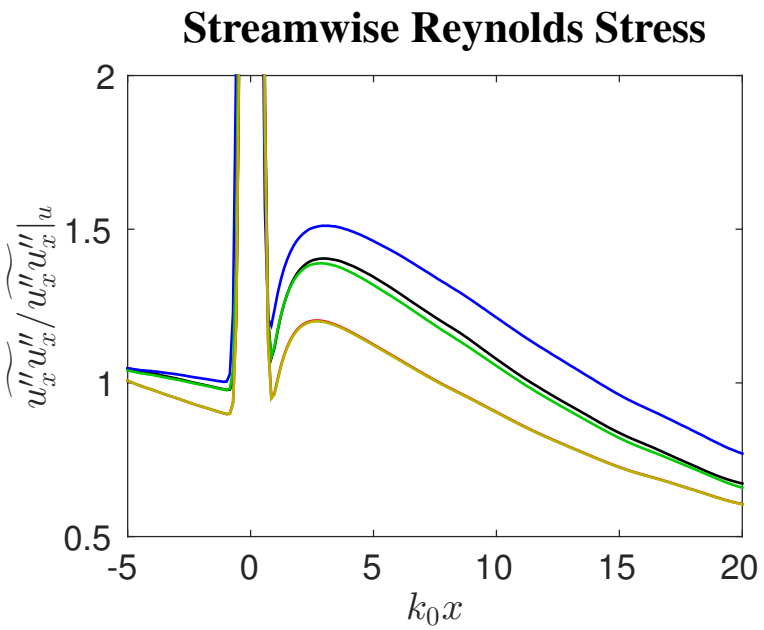
- **Entropy splitting:** Semi-conservative splitting for shock-free turbulence
  (Olsson & Oliger 1994, Yee et al. 1999-2007, Sandham et al. 2002-present)
- **Natural Splitting:** Linearized Euler & Non-conservative Systems
- **Splitting to Preserve Discrete Momentum and/or Energy Conservation:**
  (Arakawa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

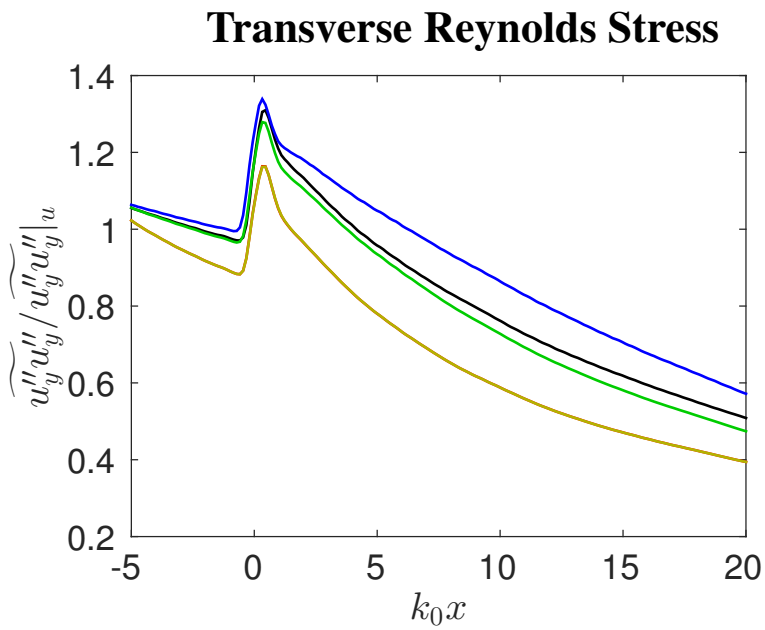
➡ **This talk concentrates only on Ducros et al. type conservative splitting**

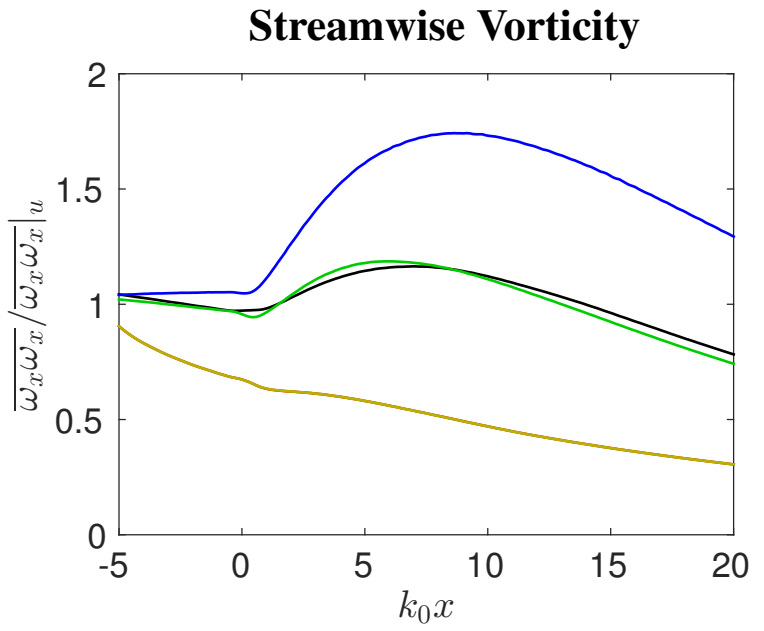
Significance

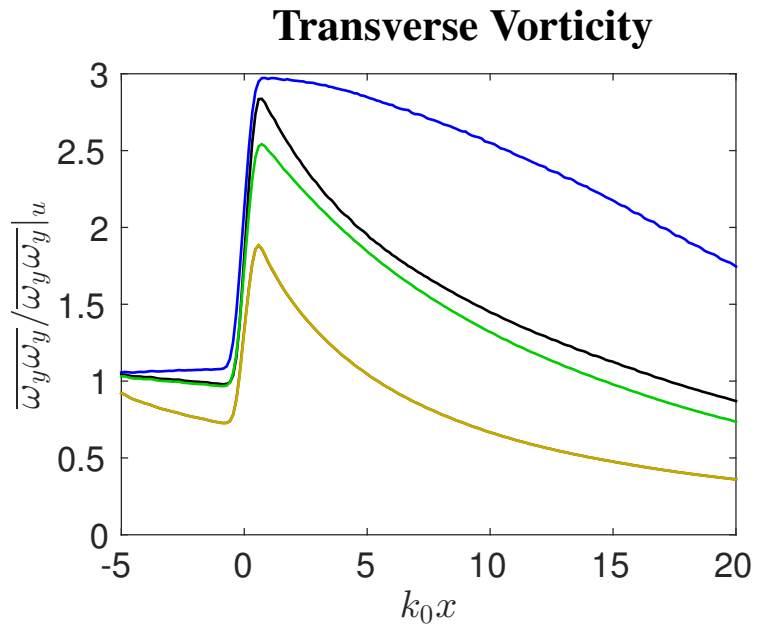
- The key advantage of the adaptive flow sensor is that no a priori knowledge of the flow structure of the entire evolution is needed, even for compressible shock-free turbulence & low speed turbulence with shocklets.
- The proposed developments provide an improved predictability & reliability of CFD 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.

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









WENO7:

- Filtered DNS
  WENO7fi+split
- No-LES
  WENO7fi+split
- LES
  WENO7fi+split
- LES + fix:
  $C_s = 0$ at
  shock
  WENO7
- LES + fix:
  One-sided
  filter at shock
  WENO7