



Entropy Stable Methods for the Euler Equations Revisited

High Order Central Differencing via Entropy Splitting & SBP
High Order Entropy Stable Split Schemes

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Outline



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- **Objective & Motivation**
- **High Order Entropy Stable Methods for the Euler Equations - Revisited**
 - **High Order Central Differencing on skew-symmetric splitting form of the inviscid flux derivative & SBP**
 - **Physical entropy for perfect gas & thermally perfect gas, including chemical reacting flows**
- **High Order Entropy Conserving Method for the Euler Equations**
 - **Under the frame work of Tadmor (2003) & high order central schemes**
 - **Employing Harten physical entropy (1983) resulting in high order entropy conservating method**
- **Results**
- **Summary**

Objectives



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Revisit & Show

- (I) **Skew-Symmetric Splitting of the Euler Flux Derivatives (perfect gas ...)** Harten 1983
 - Physical entropy of the Euler Equations
 - Homogeneous of degree one of the Euler Flux
 - Split the Euler flux into conservative & non-conservative portions
 - L^2 energy-norm estimate (integration-by-parts)
- (II) **High Order Central schemes (classical & DRP) with SBP operators**
Olsson & Olinger (1994), Gerritsen & Olsson (1996), and Yee et al. (2000)



Entropy Stable Split Schemes

Motivations

- **Improvement in Nonlinear Stability (reduce aliasing errors)**
 - > 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



Preliminary

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$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = 0$$

Entropy function: $E(\mathbf{U})$

Entropy variables: $\mathbf{W} = \nabla_{\mathbf{U}} E$ (require $E_{\mathbf{U},\mathbf{U}} > 0$)

Entropy flux: $f = f(\mathbf{U})$

Entropy conservation if

$$\mathbf{W}^T \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \nabla_{\mathbf{U}} f$$

Take conservation law & multiply by \mathbf{W} to give

$$\mathbf{W}^T \mathbf{U}_t + \mathbf{W}^T \mathbf{F}_x = 0 \quad \rightarrow \quad E_t + \mathbf{W}^T \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \mathbf{U}_x = 0 \quad \rightarrow \quad E_t + f_x = 0$$

Alternatively, if f is known, denote $\psi = \mathbf{W}^T \mathbf{F} - f$ and require

$$\psi_x = \mathbf{W}_x^T \mathbf{F}.$$

Entropy conservation shown by

$$\mathbf{W}^T \mathbf{F}_x = (\mathbf{W}^T \mathbf{F})_x - \mathbf{W}_x^T \mathbf{F} = (\mathbf{W}^T \mathbf{F})_x - (\mathbf{W}^T \mathbf{F} - f)_x = f_x$$

Entropy Conserving Discretization



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Numerical flux: $\mathbf{H}_{j+1/2}$

Entropy numerical flux: $\mathbf{h}_{j+1/2}$

Semi-discretized

$$\frac{d}{dt} \mathbf{U}_j + \frac{1}{\Delta x} (\mathbf{H}_{j+1/2} - \mathbf{H}_{j-1/2}) = \mathbf{0}$$

If

$$(\mathbf{W}_{j+1} - \mathbf{W}_j)^T \mathbf{H}_{j+1/2} = \psi_{j+1} - \psi_j$$

Then can derive discrete entropy conservation law

$$\frac{d}{dt} E_j + \frac{1}{\Delta x} (h_{j+1/2} - h_{j-1/2}) = 0$$

with

$$h_{j+1/2} = \frac{1}{2} (\mathbf{W}_{j+1} + \mathbf{W}_j)^T \mathbf{H}_{j+1/2} - \frac{1}{2} (\psi_{j+1} + \psi_j)$$

Local & Global Entropy Stability



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Local entropy conservation:

$$\frac{d}{dt} E_j + \frac{1}{\Delta x} (h_{j+1/2} - h_{j-1/2}) = 0$$

Local entropy stability:

$$\frac{d}{dt} E_j + \frac{1}{\Delta x} (h_{j+1/2} - h_{j-1/2}) \leq 0$$

Global entropy conservation:

$$\frac{d}{dt} \sum_j \Delta x E_j = 0$$

Global entropy stability:

$$\frac{d}{dt} \sum_j \Delta x E_j \leq 0$$

**Entropy Splitting of the Euler Flux Derivatives
Leads to Global Entropy Conservation (Stability) by the Energy Norm**

Entropy Split Schemes



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Entropies considered by Harten (1983)

$$E = -\rho(p\rho^{-\gamma})^{1/(\alpha+\gamma)}$$

Symmetrizable & Homogeneous property of the Euler Flux lead to

$$\mathbf{F}_w \mathbf{W} = \beta \mathbf{F} \quad (1)$$

for $\beta = \frac{\alpha+\gamma}{1-\gamma}$. Use the split form with $\beta \neq -1$

$$\mathbf{F}_x = \frac{\beta}{\beta+1} \mathbf{F}_x + \frac{1}{\beta+1} \mathbf{F}_w \mathbf{W}_x$$

in a semi-discrete approximation:

$$\frac{d}{dt} \mathbf{U}_j + \frac{\beta}{\beta+1} D \mathbf{F}_j + \frac{1}{\beta+1} (\mathbf{F}_w)_j D \mathbf{W}_j = 0$$

where D is a SBP difference operator.

Entropy Splitting Leads to Global Entropy Conservation & Stability



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Form the SBP scalar product by \mathbf{W}_j^T to obtain the entropy

$$\frac{d}{dt} \sum_j \omega_j \Delta x E_j + \frac{\beta}{\beta + 1} (\mathbf{W}, D\mathbf{F}) + \frac{1}{\beta + 1} (\mathbf{W}, \mathbf{F}_W D\mathbf{W}) = 0$$

(ω_j are SBP norm weights) where SBP and property (1) give

$$\begin{aligned} \beta(\mathbf{W}, D\mathbf{F}) &= -\beta(D\mathbf{W}, \mathbf{F}) - \beta\mathbf{W}_1^T \mathbf{F}_1 + \beta\mathbf{W}_N^T \mathbf{F}_N = \\ &= - (D\mathbf{W}, \mathbf{F}_W \mathbf{W}) - \beta\mathbf{W}_1^T \mathbf{F}_1 + \beta\mathbf{W}_N^T \mathbf{F}_N \end{aligned}$$

and symmetry of \mathbf{F}_W gives $(\mathbf{W}, \mathbf{F}_W D\mathbf{W}) = (\mathbf{F}_W \mathbf{W}, D\mathbf{W})$, so that

$$\frac{d}{dt} \sum_j \omega_j \Delta x E_j = \frac{\beta}{\beta + 1} (\mathbf{W}_1^T \mathbf{F}_1 - \mathbf{W}_N^T \mathbf{F}_N)$$

i.e., global entropy conservation with boundary contributions.

Note, property (1) does not hold for $E = -\rho \log(\rho \rho^{-\gamma})$ commonly used in the literature

Entropy Splitting of Euler Flux Derivatives

(Oliger & Olsson, Olsson, Gerittsen & Olsson, Yee et al. (1994-1999))



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Entropy stable (generalized energy norm) with SBP for Central Schemes

Physical Entropy, Homogeneous of Degree One of Euler Flux Derivative f_x

$$\mathbf{F}_x = \frac{\beta}{\beta + 1} \mathbf{F}_x + \frac{1}{\beta + 1} \mathbf{F}_W W_x, \quad \beta \neq -1$$

$$\begin{aligned} W &= [w_1, w_2, w_3, w_3, w_5]^T \\ &= \frac{p^*}{p} \left[e + \frac{\alpha - 1}{\gamma - 1} p, -\rho u, -\rho v, \rho w, \rho \right]^T, \end{aligned}$$

where

$$p^* = -(p\rho^{-\gamma})^{\frac{1}{\alpha+\gamma}}$$

and

$$\beta = \frac{\alpha + \gamma}{1 - \gamma}, \quad \alpha > 0 \text{ or } \alpha < -\gamma.$$

Entropy Conserving (EC) Discretization Tadmor-type with Boundaries



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Entropy Split Schemes: Achieving global entropy conservation & stability automatically by standard SBP & energy norm estimate (periodic or non-periodic BC)

Entropy Conserving Schemes - Tadmor-type: Achieving global entropy conservation & stability require generalized SBP & dissipation

Domain $j = 1, 2, \dots$, with boundary at $j = 1$. Consider the scheme

$$\frac{d}{dt} \mathbf{U}_j + \frac{1}{\Delta x} (\mathbf{H}_{j+1/2}^{EC} - \mathbf{H}_{j-1/2}^{EC}) = \mathbf{0}$$

with the E.C. 2nd-order numerical flux $\mathbf{H}_{j+1/2}^{EC} = \mathbf{H}^{EC}(\mathbf{U}_j, \mathbf{U}_{j+1})$, defined at $j = 1, 2, \dots$,

Define $\mathbf{H}_{1/2}^{EC} = 2\mathbf{F}_1 - \mathbf{H}_{3/2}^{EC}$, then the local entropy conservation law

$$\frac{d}{dt} E_j + \frac{1}{\Delta x} (h_{j+1/2} - h_{j-1/2}) = 0$$

holds for $j = 1, 2, \dots$, with

$$h_{1/2} = \mathbf{W}_1^T \mathbf{F}_1 - \psi_1$$

and

$$h_{j+1/2} = \frac{1}{2} (\mathbf{W}_{j+1} + \mathbf{W}_j)^T \mathbf{H}_{j+1/2} - \frac{1}{2} (\psi_{j+1} + \psi_j)$$

for $j \geq 1$ (as previously).

Entropy Conserving (EC) Discretization of Tadmor-type with Boundaries (Cont.)



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The global entropy conservation with boundaries

$$\Delta x \frac{d}{dt} \left(\frac{1}{2} E_1 + \sum_{j=2} E_j \right) + \mathbf{W}_1^T \mathbf{F}_1 - \psi_1 = 0$$

follows, where $1/2$ is the SBP weight of the boundary entropy, and $f_1 = \mathbf{W}_1^T \mathbf{F}_1 - \psi_1$ is the boundary entropy flux.

For a construction that generalizes to higher order accuracy, see:

Parsani, Carpenter, Nielsen, J.Comput.Phys., 292(2015),pp. 88–113.

Advantage of Entropy Split Method over Standard Tadmor-Type Entropy Conserving Methods



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Tadmor-type entropy conserving method (logarithmic entropy or physical entropy)
requires 2 times CPU than entropy split method

+

Both Approaches Exhibit Similar Accuracy & Stability
(Same order of central discretization)

Dispersion Relation-Preserving (DRP) Schemes

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Three DRP schemes in CAA: DRP4S7 (Tam & Webb), DRP4S9, ST09 (Bogey & Bailly)

$$Du_j = \frac{1}{h} \sum_{k=1}^q a_k (u_{j+k} - u_{j-k}).$$

DRP4S7

Coefficients of DRP4S7, optimized over [0, 1.1].

k	a_k
1	0.77088238051822552
2	-0.16670590441458047
3	0.02084314277031176

DRP4S9

Coefficients of DRP4S9, optimized over $[\pi/16, \pi/2]$.

k	a_k
1	0.846863763009931
2	-0.251240526849904
3	0.063181723773749
4	-0.008481970157843

ST09

Coefficients of ST09, optimized over $[\pi/16, \pi/2]$, from [18].

k	a_k
1	0.841570216389881
2	-0.244678789340406
3	0.059463699920073
4	-0.007650934367322

Kennedy & Gruber Splitting (2008)



Split the derivative of triple products, kinetic energy preservation

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$$\frac{\partial}{\partial x}(abc) = \alpha \frac{\partial}{\partial x}(abc) + \beta \left[a \frac{\partial}{\partial x}(bc) + bc \frac{\partial}{\partial x}(a) \right] + \kappa \left[b \frac{\partial}{\partial x}(ac) + ac \frac{\partial}{\partial x}(b) \right] + \delta \left[c \frac{\partial}{\partial x}(ab) + ab \frac{\partial}{\partial x}(c) \right] + \epsilon \left[bc \frac{\partial}{\partial x}(a) + ac \frac{\partial}{\partial x}(b) + ab \frac{\partial}{\partial x}(c) \right],$$

where $\epsilon = 1 - \alpha - \beta - \kappa - \delta$.

Common parameter:

$$\alpha = \beta = \kappa = \delta = \frac{1}{4} \text{ and } \epsilon = 0,$$

$$(abc)_x = \frac{1}{4} (abc)_x + \frac{1}{4} (a_x (bc) + b_x (ac) + c_x (ab)) + \frac{1}{4} (a (bc)_x + b (ac)_x + c (ab)_x)$$

Numerical Example

Long Time Integration of Smooth Flows



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

2D Isentropic Vortex Convection

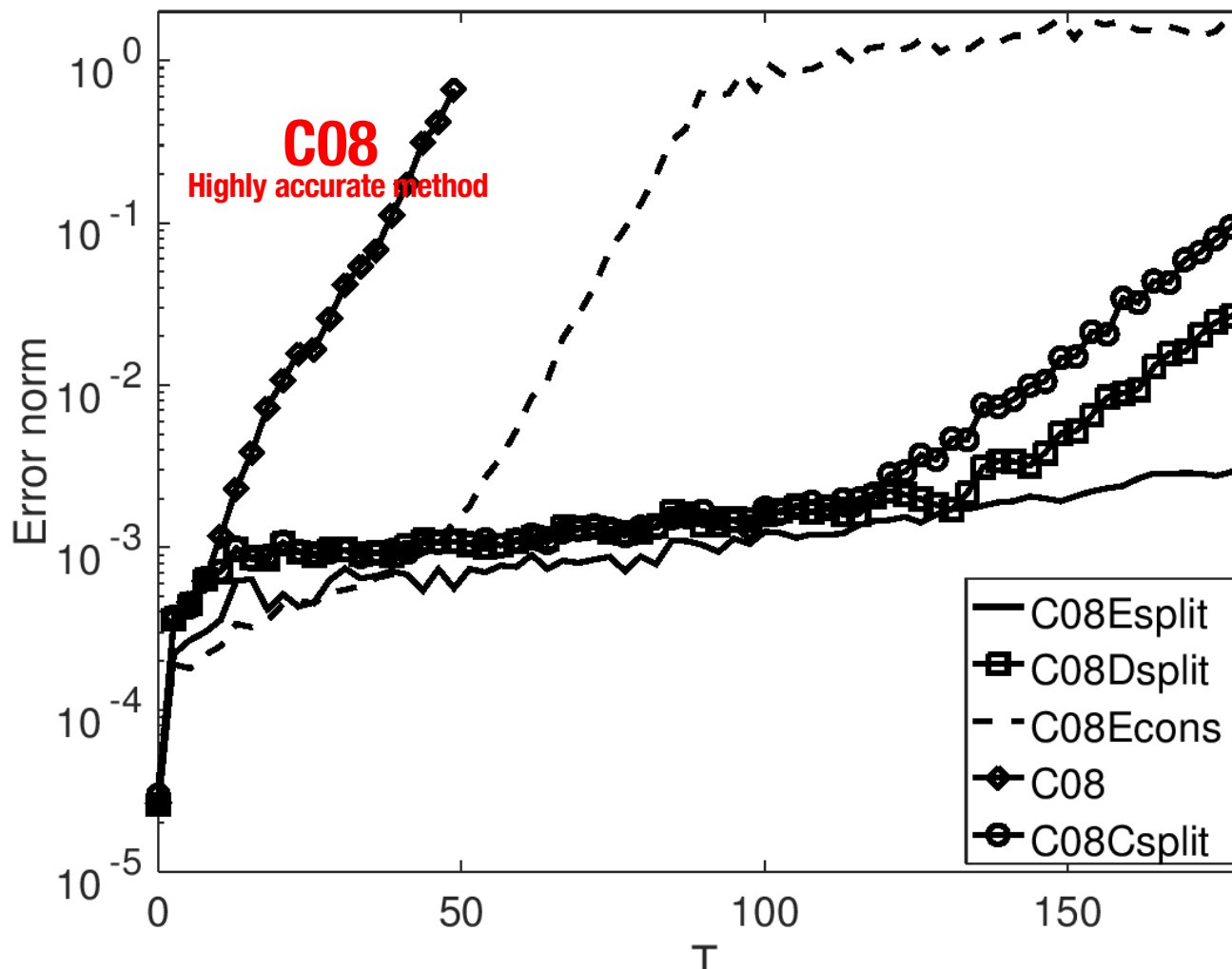
Exact Solution is Simple Translation



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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

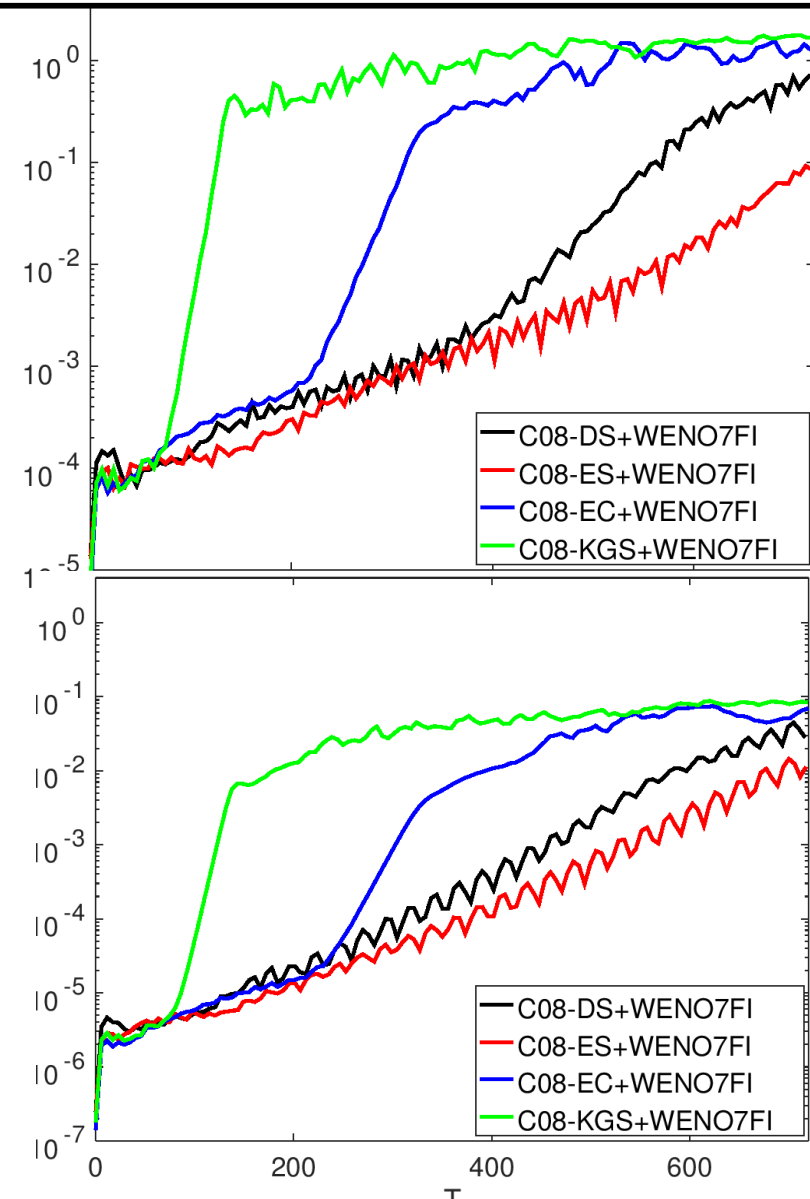
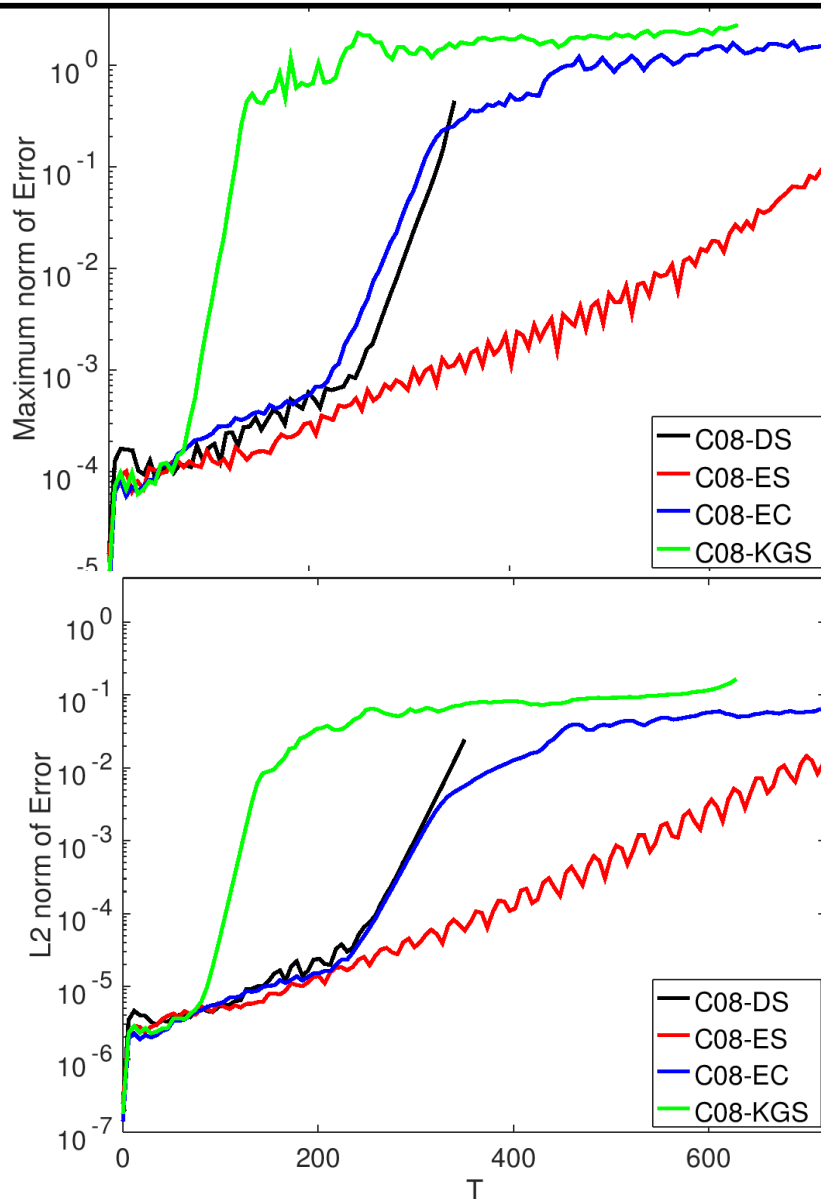
2D Isentropic Vortex Convection

Exact Solution is Simple Translation, **100x100 grid**



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Max Norm vs. L2 norm of errors: C08 on 3 different 8th-order skew-symmetric splittings



Treatment of Discontinuities for Entropy Split Schemes



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Yee et al. Nonlinear Filter Approach:

- High order entropy split schemes as the base scheme
- Local flow sensor to examine the regularity of the computed data after each full time step of the base scheme.
- Determine the location and amount of numerical dissipation needed
- Nonlinearly filter the computed data at these locations only

Well-Balanced High Order Nonlinear 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, Sjogreen & 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. 6th order central, 4th order RK)

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

- Solution by a nonlinear filter step

$$U_j^{n+1} = U_j^* - \frac{\Delta t}{\Delta x} [H_{j+1/2} - H_{j-1/2}]$$

$$H_{j+1/2} = R_{j+1/2} \bar{H}_{j+1/2}$$

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

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

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

$\phi_{j+1/2}^m$ - 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

$$\bar{h}_{j+1/2} = \frac{\kappa_{j+1/2}^m}{2} \left(s_{j+1/2}^m \right) \left(g_{j+1/2}^m - b_{j+1/2}^m \right)$$

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 & Sjögren, 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 & Sjögren, 2009*)

Numerical Examples



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

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- 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

$$\begin{aligned}\rho &= 1, \\ p &= 100 + ([\cos(2z) + 2][\cos(2x) + \cos(2y)] - 2)/16, \\ u_x &= \sin x \cos y \cos z \\ u_y &= -\cos x \sin y \cos z \\ u_z &= 0.\end{aligned}$$

Initial turbulent Mach number: $M_{t,0} = 0.042$

Final time: $t = 10$

Viscous case

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

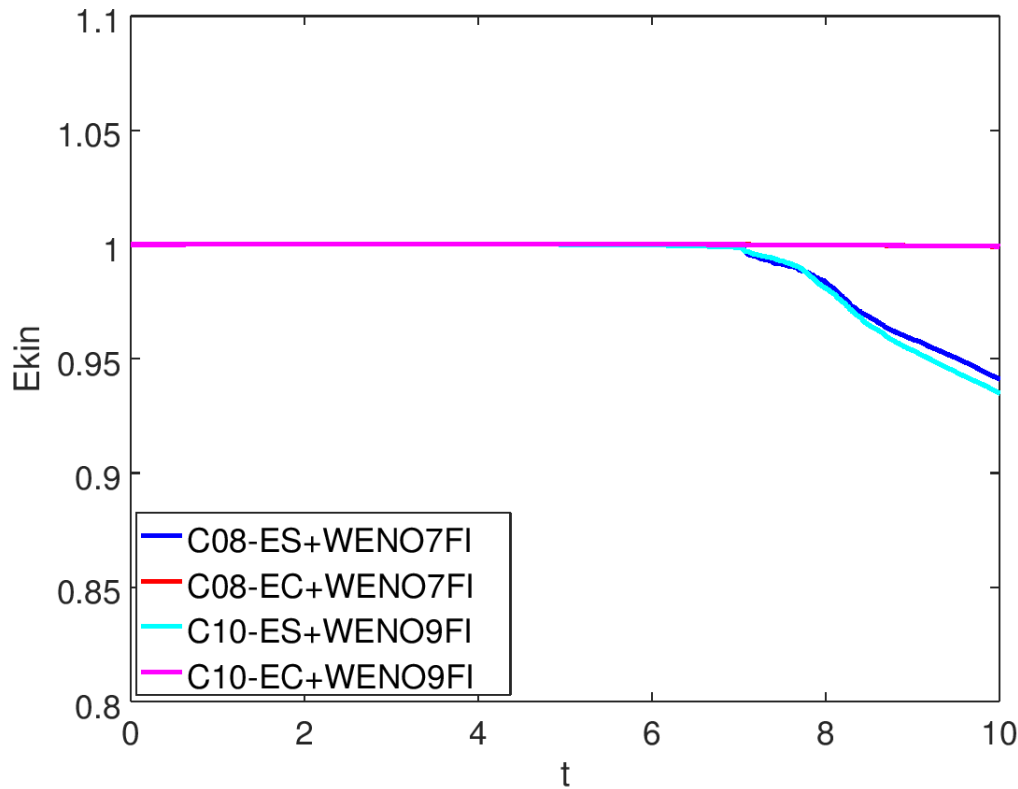
3D Taylor-Green Vortex (Shock-Free Turbulence)

(Comparison of 4 Methods, 64^3 grids)

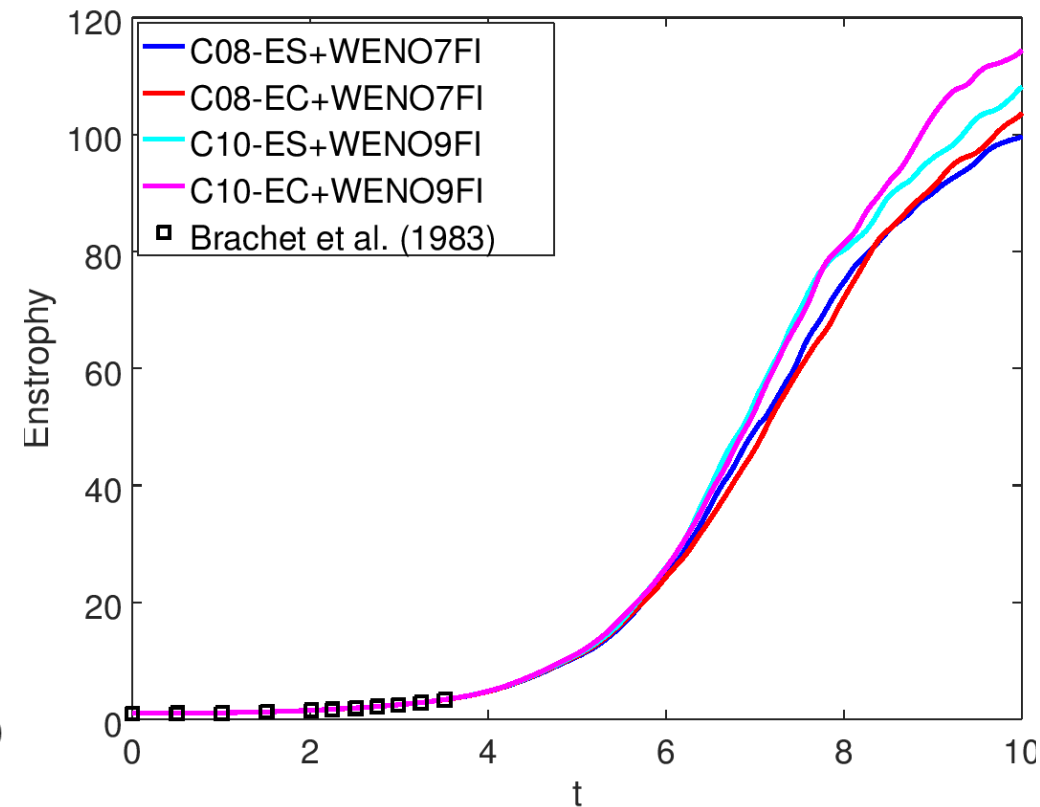


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Kinetic Energy



Enstrophy



C08-ES+WENO7fi: 8th-order central + Entropy split + WENO7fi
C08-ES+WENO7fi: 8th-order central + Entropy Cons. + WENO7fi
C010-ES+WENO7fi: 10th-order central + Entropy split + WENO9fi
C010-ES+WENO7fi: 10th-order central + Entropy Cons. + WENO9fi

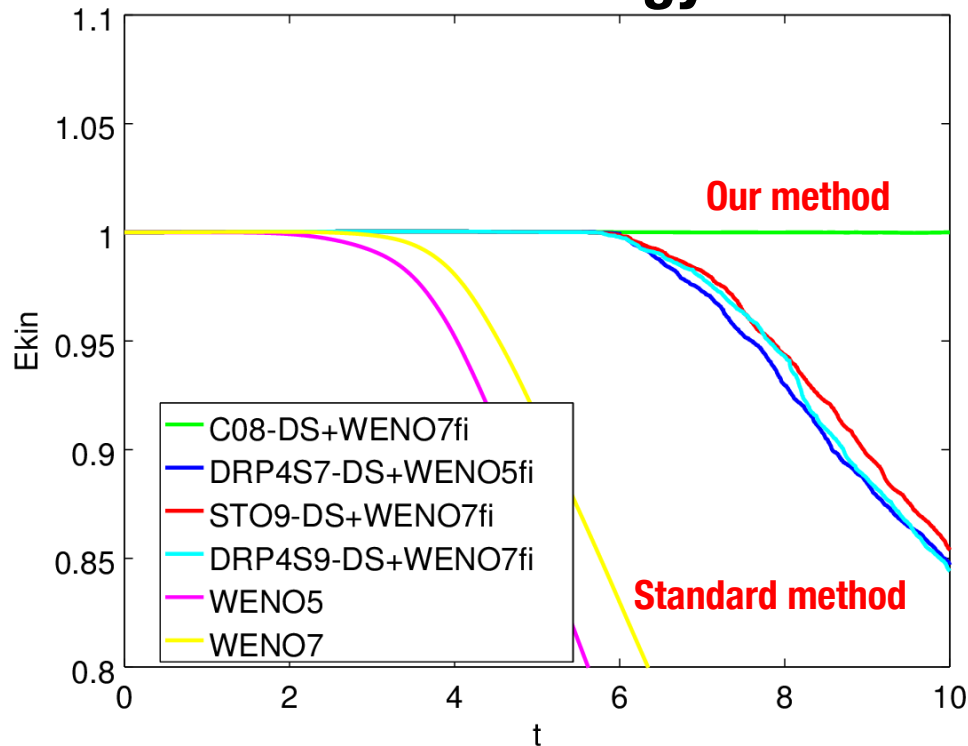
3D Taylor-Green Vortex (Shock-Free Turbulence)

(Comparison of 6 Methods, 64^3 grids)

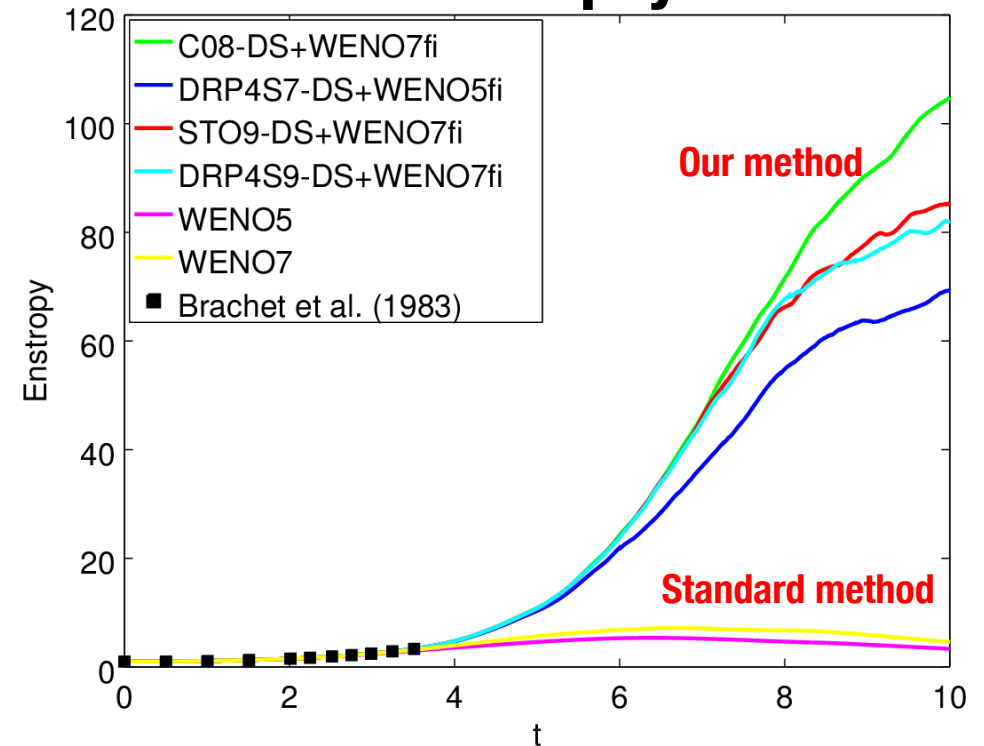


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Kinetic Energy



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
STO9-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

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

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

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

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

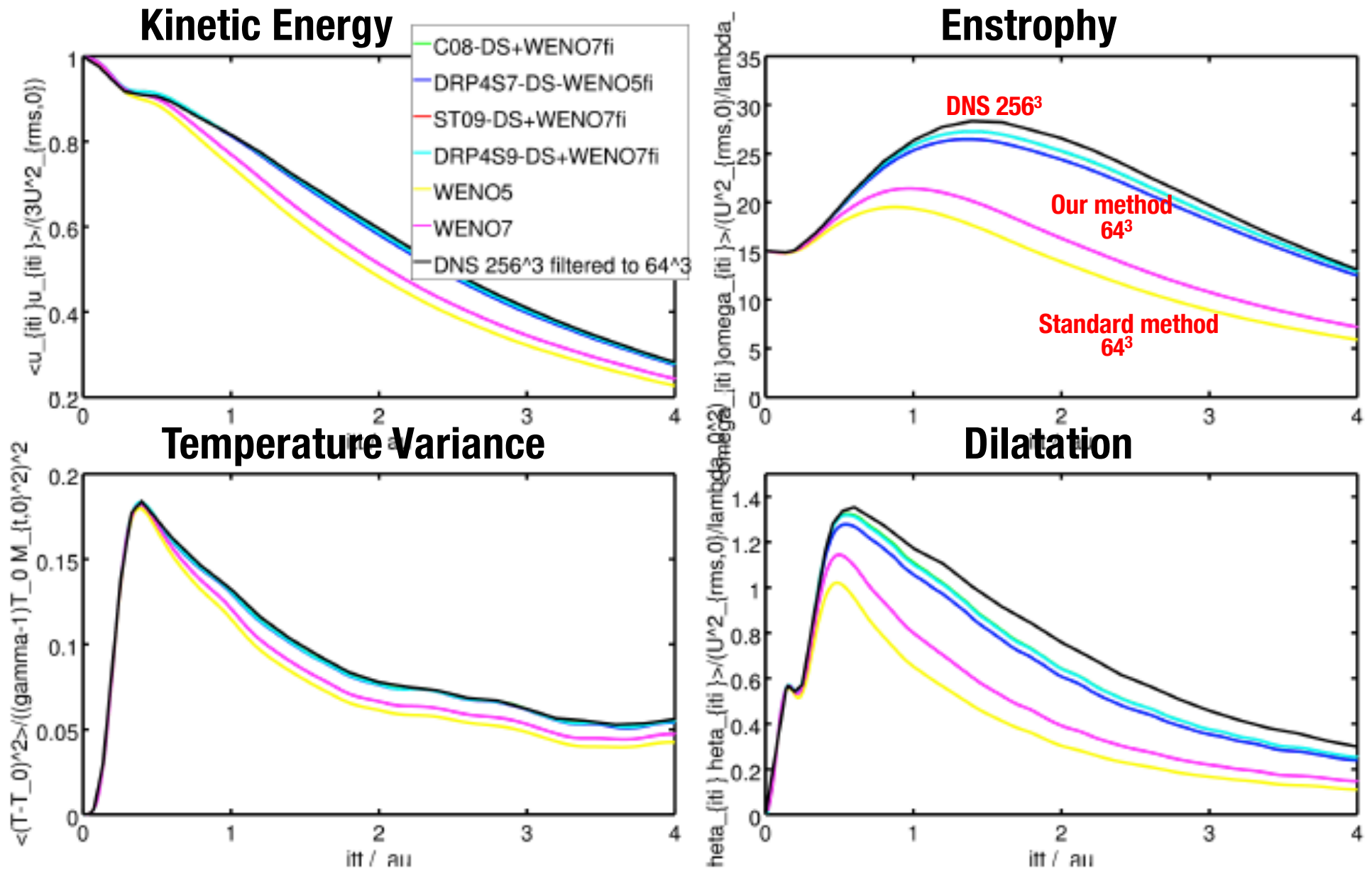
Final time: $t = 2$ or $t/\tau = 4$

3D Isotropic Turbulence with Shocklets

(Comparison of 6 Methods, 64^3 grids)



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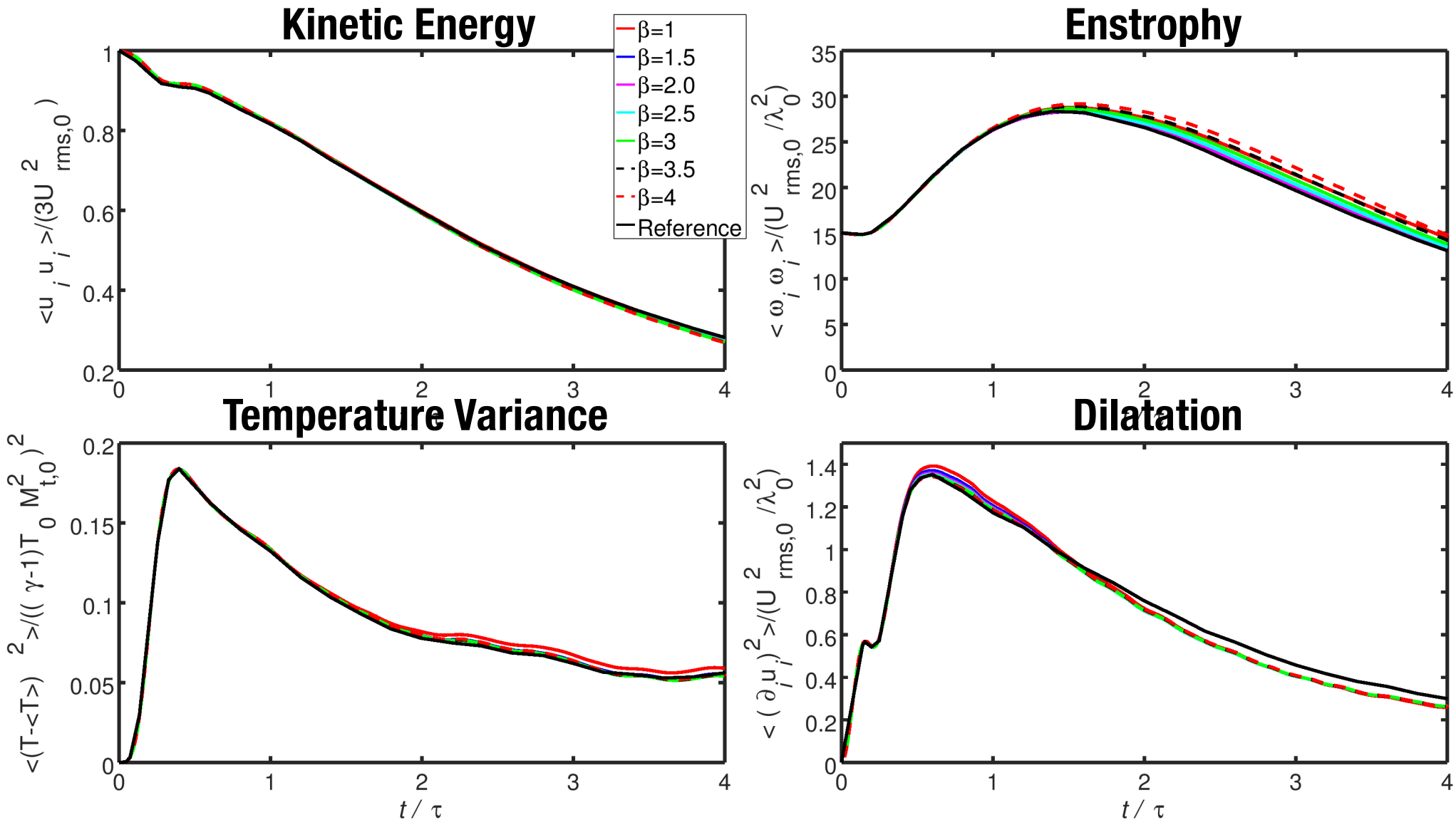


3D Isotropic Turbulence with Shocklets

(Entropy Split Scheme: Comparison of 7 Beta using WENO7fi, 64^3 grids)



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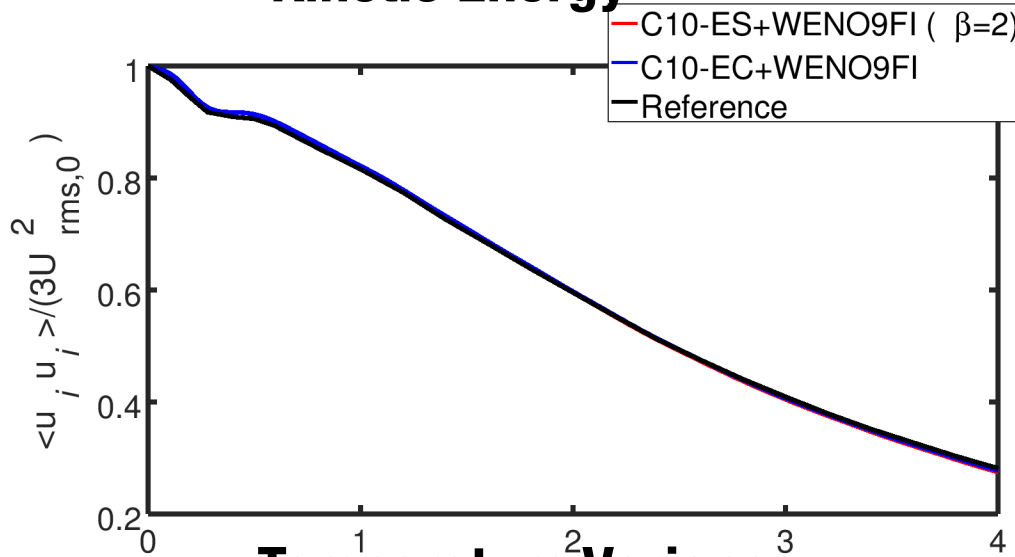
3D Isotropic Turbulence with Shocklets

(Comparison of Two 10th-order nonlinear filter Methods (ES vs. EC), 64³ grids)

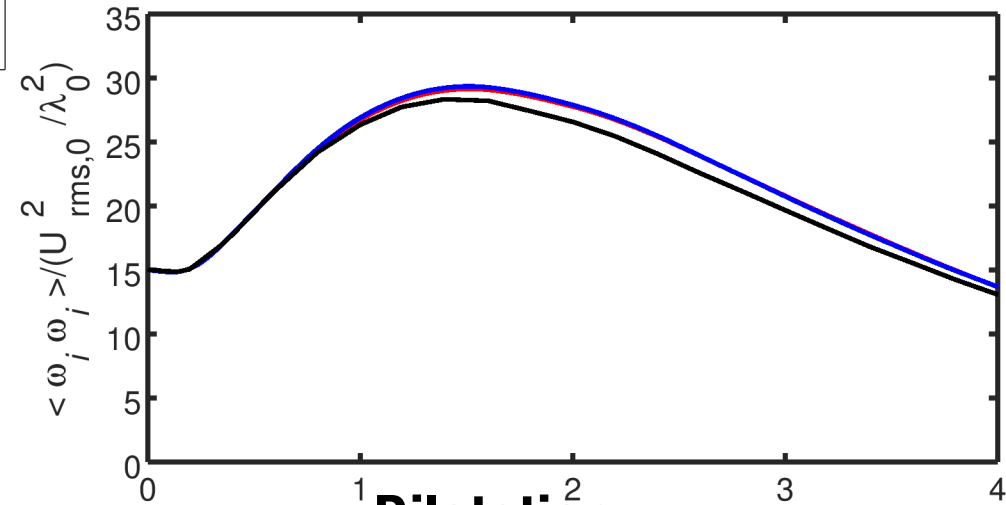


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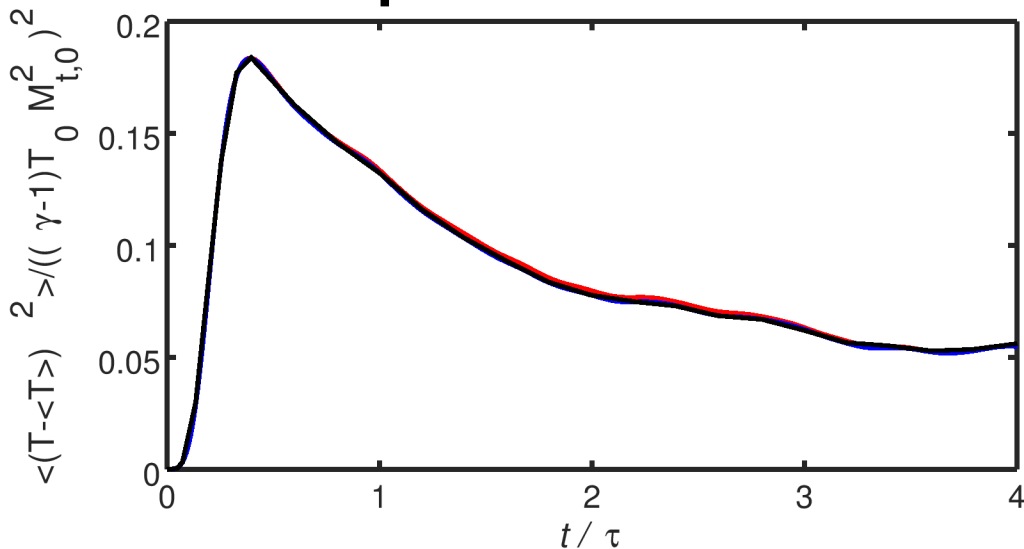
Kinetic Energy



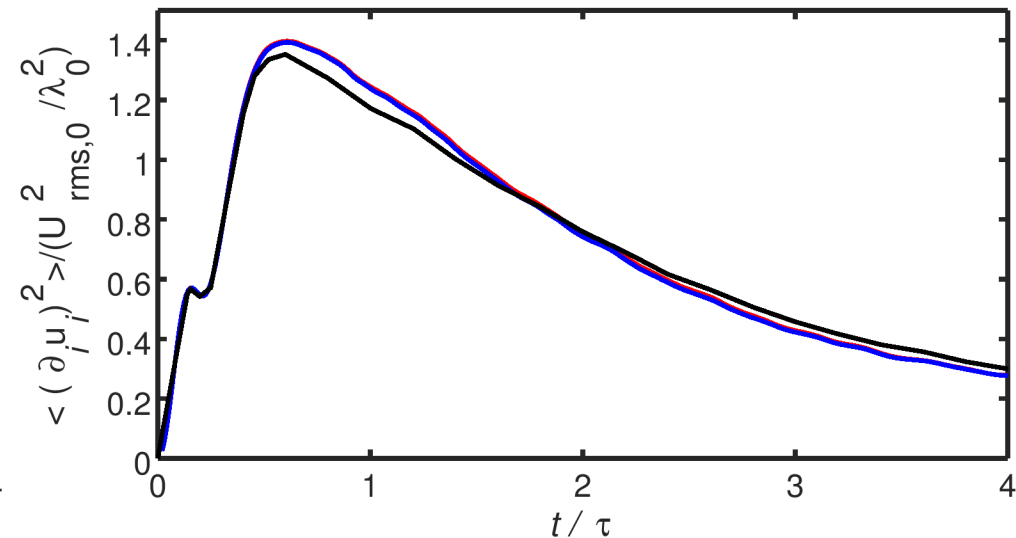
Enstrophy



Temperature Variance



Dilatation



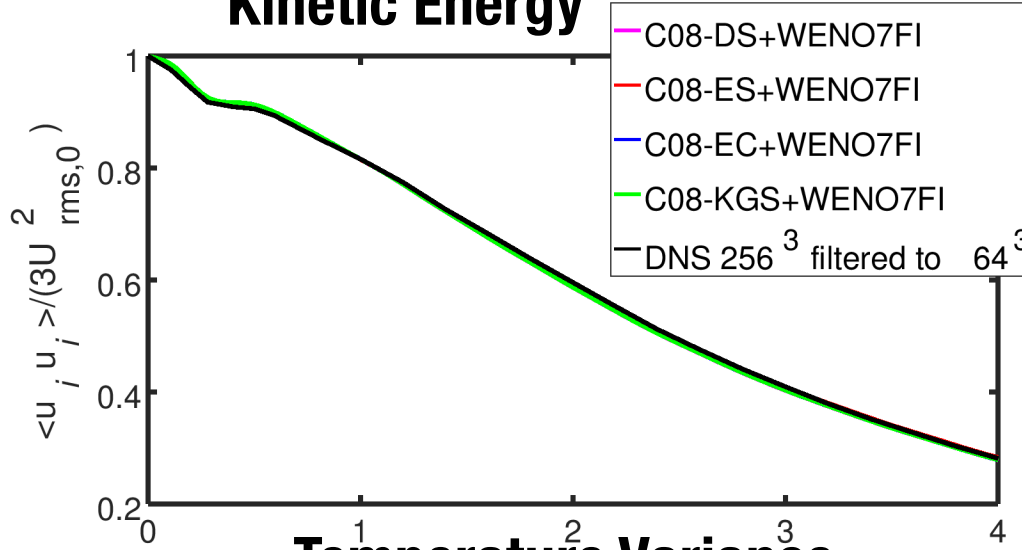
3D Isotropic Turbulence with Shocklets

(Comparison of 7th-order skew-symmetric splittings with EC method, 64³ grids)

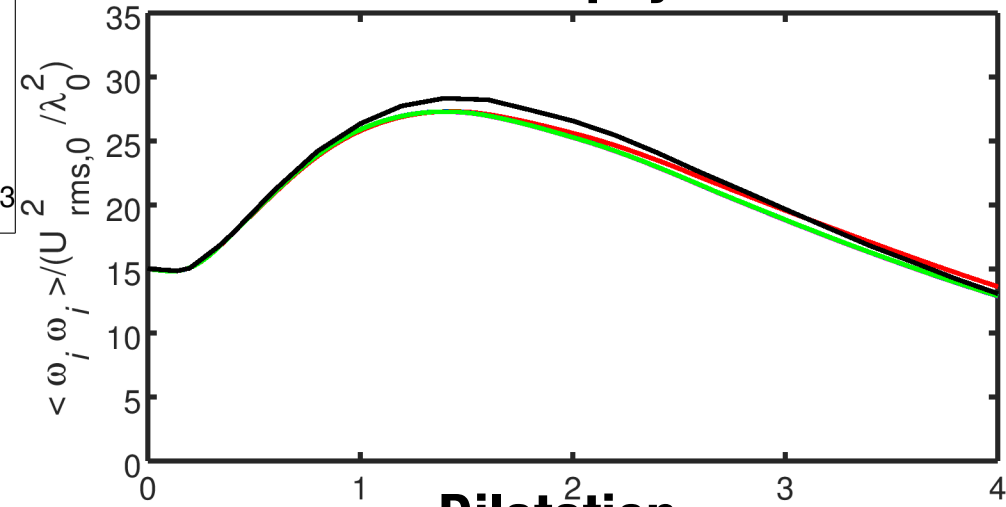


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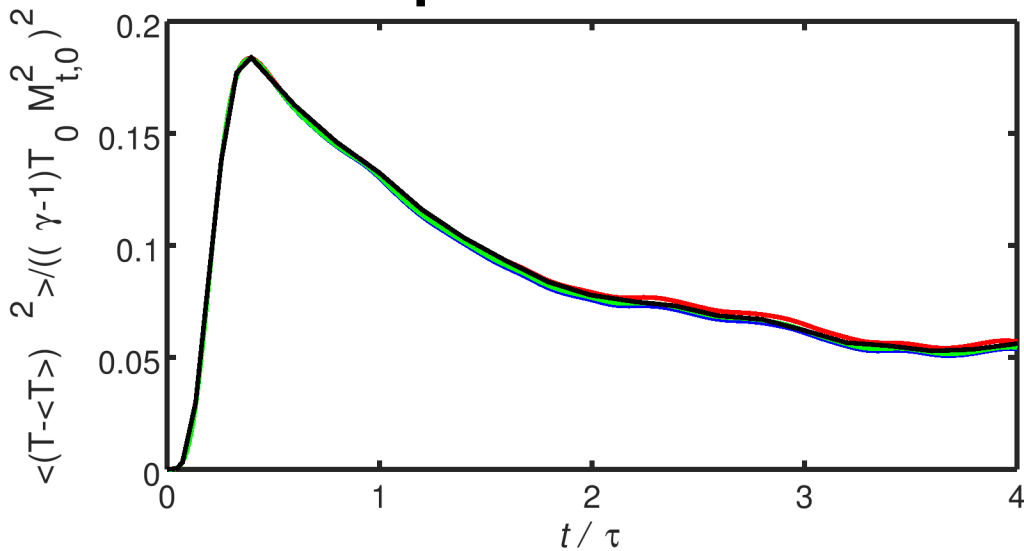
Kinetic Energy



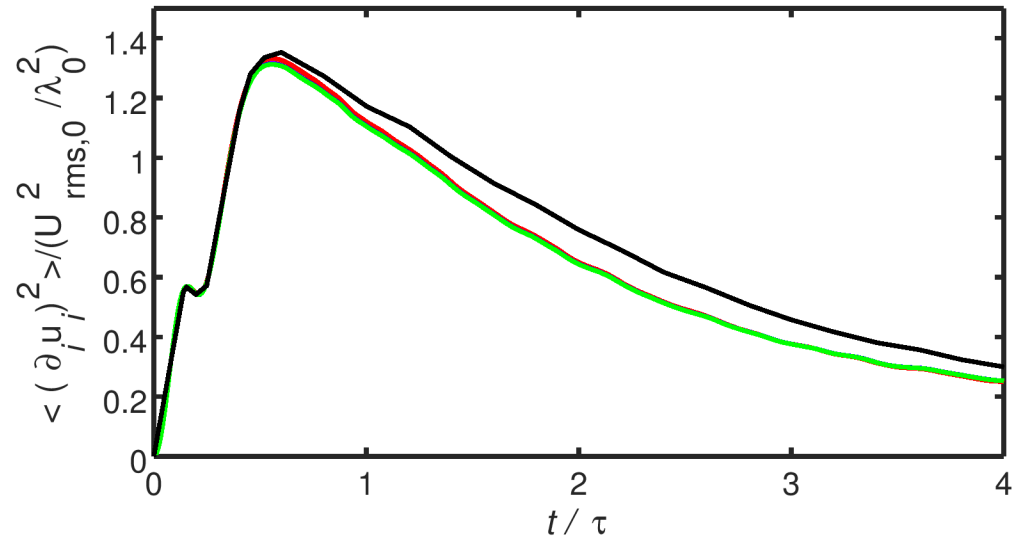
Enstrophy



Temperature Variance



Dilatation



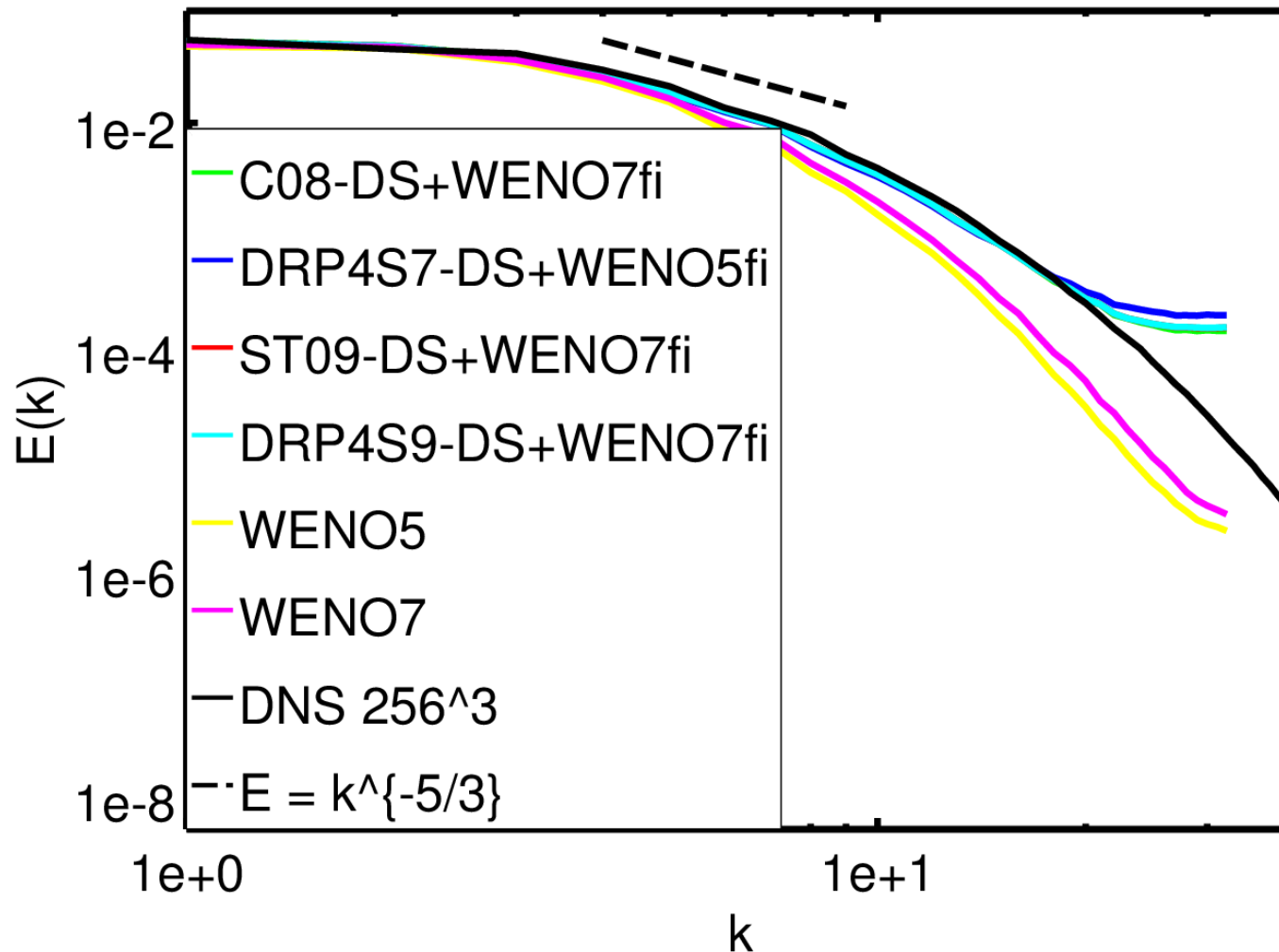
3D Isotropic Turbulence with Shocklets (Compressible & Inviscid)



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Comparison of 6 Methods, 64^3 grids

Energy Spectra



Advantage of Entropy Split Method over Standard Tadmor-Type Entropy Conserving Methods



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Tadmor-type entropy conserving method (logarithmic entropy or physical entropy)
requires 2 times CPU than entropy split method

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Both Approaches Exhibit Similar Accuracy & Stability
(Same order of central discretization)