Behavior of Shock-Capturing Methods Below the CFL Limit

(Problems Containing Stiff Source Terms & Discontinuities)

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Outline

- **Motivation**

  (Wrong Propagation Speed of Discontinuities by Shock-Capturing Methods)

- **Numerical Methods with Dissipation Control**

  (Turbulence with Strong Shocks & Stiff Source Terms)

- **Three Test Cases: 1D, 2D detonation and 13 species nonequilibrium**

- **Conclusions**

Goal

Study the behavior of high order shock-capturing schemes for problems containing stiff source terms & discontinuities

The issue of "incorrect shock speed" is concerned with solving the conservative system with a conservative scheme

Schemes to be considered:

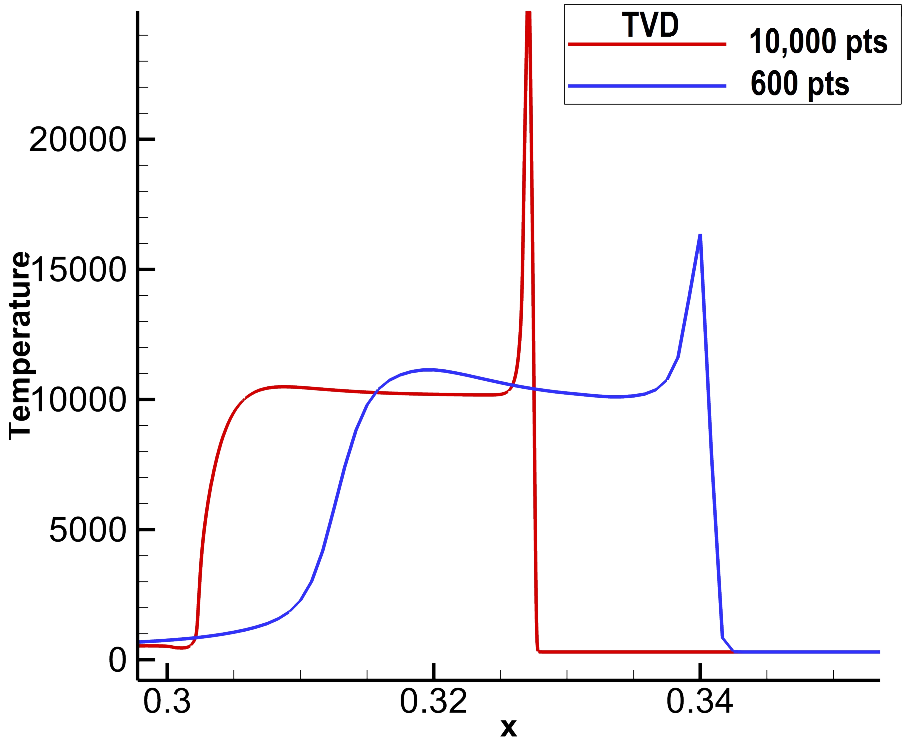
TVD, WENO
WENO/SR – New scheme by Wang, Shu, Yee & Sjögreen
High order filter scheme by Yee & Sjögreen
Note: ***Study based on coarse grid computations obtaining the correct discontinuity locations (not accurate enough to resolve the detonation front)***

Example:

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



Numerical Method Development Challenges

(Turbulence with Strong Shocks & Stiff Source Terms)

- **Conflicting requirements** *(for turbulence with strong shocks)*
  - turbulence cannot tolerate numerical dissipation but needs some for numerical stability
  - Proper amount of numerical dissipation is required in the vicinity of shock/contact
    (Recent development: Yee & Sjogreen, 2000-2009)

- **Non-linearity of the source terms**
  Incorrect numerical solution can be obtained for Δt below the CFL limit. (Allowable Δt consists of disjoint segments: *Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, 1990 – 2002)*

- **Stiffness of the source terms**
  Insufficient spatial/temporal resolution may lead to incorrect speed of propagation of discontinuities *(LeVeque & Yee, 1990, Collela et al., 1986 + large volume of research work the last two decades)*

Note: *(a) Standard shock-capturing methods have been developed for problems without source terms*
(b) Concern only source term of type S(U)

Wrong Propagation Speed of Discontinuities

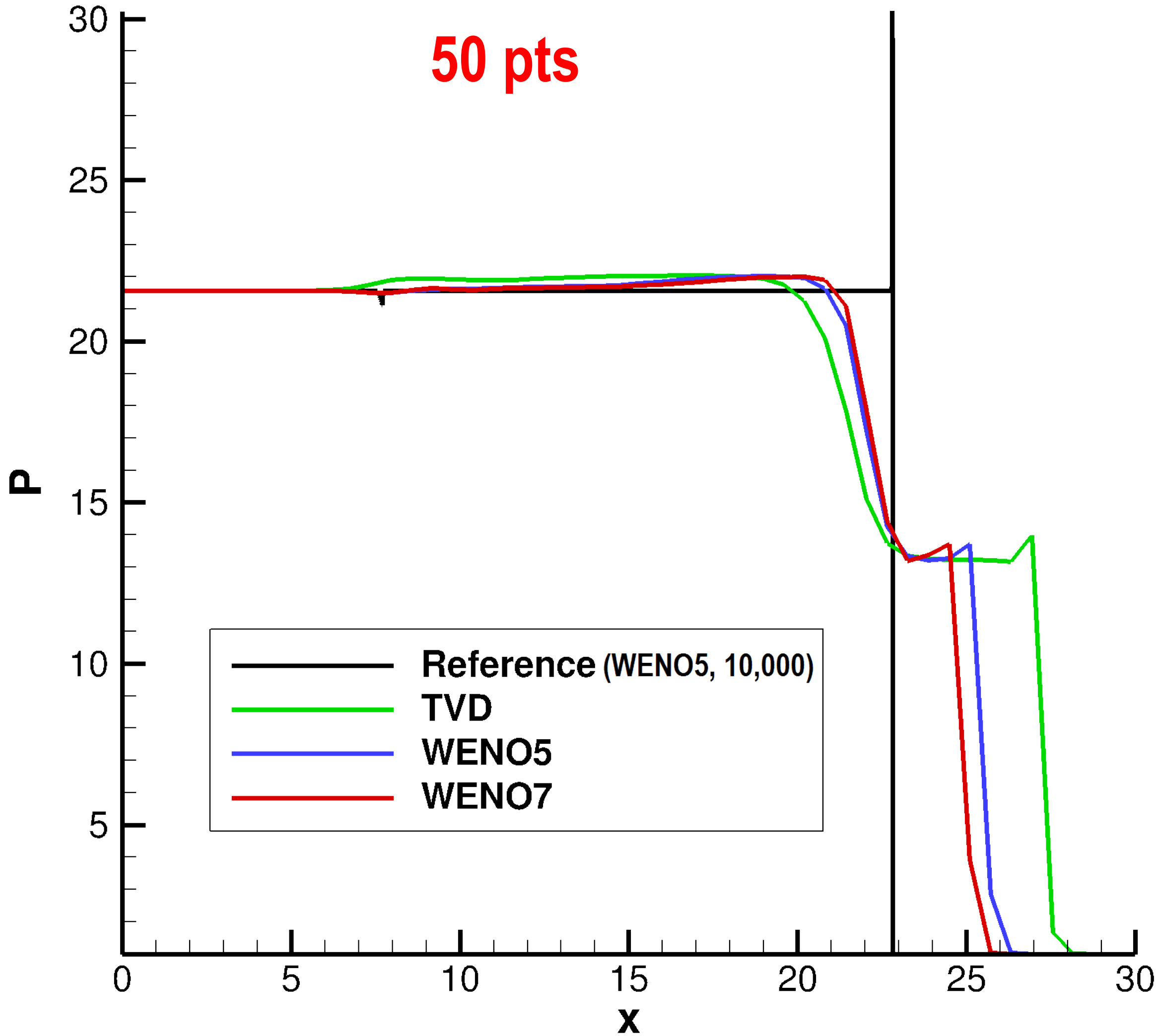
(Standard Shock-Capturing Schemes: TVD, WENO5, WENO7)

Chapman-Jouguet (C-J) 1D detonation wave,
Helzel et al. 1999

Arrhenius reaction rate:

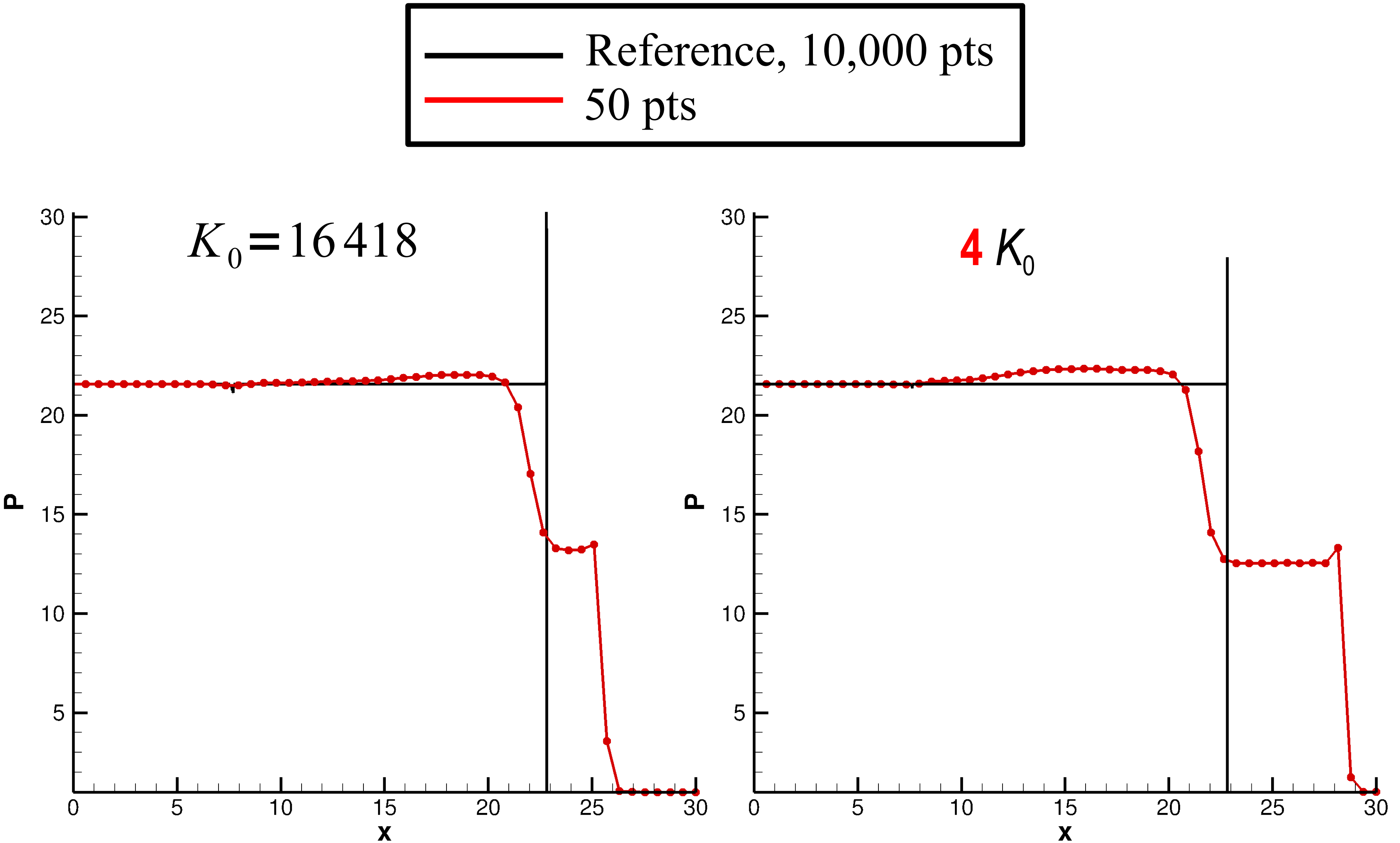
$$K(T) = K_0 \exp\left(\frac{-T_{ign}}{T}\right)$$

K_0 can be large (stiff coeff.)



Wrong Propagation Speed of Discontinuities

(WENO5, Two Stiff Coefficients, 50 pts)



2D Reactive Euler Equations

$$
\begin{aligned}
(\rho_1)_t + (\rho_1 u)_x + (\rho_1 v)_y &= K(T)\rho_2 \\
(\rho_2)_t + (\rho_2 u)_x + (\rho_2 v)_y &= -K(T)\rho_2 \\
(\rho u)_t + (\rho u^2 + p)_x + (\rho u v)_y &= 0 \\
(\rho v)_t + (\rho u v)_x + (\rho v^2 + p)_y &= 0 \\
E_t + (u(E+p))_x + (v(E+p))_y &= 0
\end{aligned}
$$

Unburned gas mass fraction: $z = \rho_2 / \rho \qquad \rho = \rho_1 + \rho_2$

Pressure: $p = (\gamma - 1)(E - \frac{1}{2}\rho(u^2 + v^2) - q_0 \rho_2)$

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

Stiff: **large** K_0

(b) $K(T) = \begin{cases} K_0 & T \geqslant T_{ign} \\ 0 & T < T_{ign} \end{cases}$

High Order Methods with Subcell Resolution

(Wang, Shu, Yee, & Sjögreen, JCP, 2012)

Procedure:

Split equations into convective and reactive operators
(Strang-splitting 1968)

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

$$U_t + F(U)_x + G(U)_y = 0 \qquad\qquad \frac{dU}{dt} = S(U)$$

Numerical solution: $$U^{n+1} = A\left(\frac{\Delta t}{2}\right) R(\Delta t)\, A\left(\frac{\Delta t}{2}\right) U^n$$

Convection operator   Reaction operator

Note: time accuracy after Strang splitting is at most 2nd order

Subcell Resolution (SR) Method
Basic Approach

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

  Test case: WENO5 with 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, 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

Well-Balanced High Order Filter Schemes for Reacting Flows *(Yee & Sjögreen, 1999-2010, Wang et al., 2009-2010)*

Preprocessing step

Condition (equivalent form) the governing equations by, e.g., Ducros et al. Splitting (2000) to improve numerical stability

High order base scheme step (Full time step)

e.g. the 6th order (or higher) central spatial scheme and 4th order RK

Nonlinear filter step

- Filter the base scheme step solution by a dissipative portion of high-order shock capturing scheme, e.g., WENO of 5th order
- Use Wavelet-based 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 exactly

Properties of the High-Order Filter Schemes

- High order (4th - 16th) Spatial Base Scheme conservative; no flux limiter or Riemann solver
- Physical viscosity is taken into account by the base scheme (reduce the amount of numerical dissipation to be used if physical viscosity is present)
- Efficiency: One Riemann solve per dimension per time step, independent of time discretizations
- Accuracy: Containment of numerical dissipation via a local wavelet flow sensor
- Well-balanced scheme: Able to exactly preserve certain nontrivial steady-state solutions of the governing equations *(Wang et al. 2011)*
- Parallel Algorithm: Suitable for most current supercomputer architectures

Three Test Cases
(Computed by ADPDIS3D code)

- **1D C-J Detonation Wave**
  (Helzel et al. 1999; Tosatto & Vigevano 2008)

- **2D Detonation Wave** *(Ozone decomposition)*
  (Bao & Jin, 2001)

- **2D EAST Problem (13 species nonequilibrium)**

All schemes employed in the study are included in *ADPDIS3D* solver *(Sjögreen, Yee & collaborators)*

1D C-J Detonation Wave

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

Left state (totally burned gas)

Right state (totally unburned gas)

$$\begin{pmatrix} \rho_b \\ u_b \\ p_b \end{pmatrix} = \begin{pmatrix} \rho_u \dfrac{[p_b(\gamma+1)-p_u]}{\gamma\, p_b} \\ S_{CJ}-(\gamma\, p_b/\rho_b)^{1/2} \\ -b+(b^2-c)^{1/2} \end{pmatrix} \qquad \begin{pmatrix} \rho_u \\ u_u \\ p_u \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

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

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

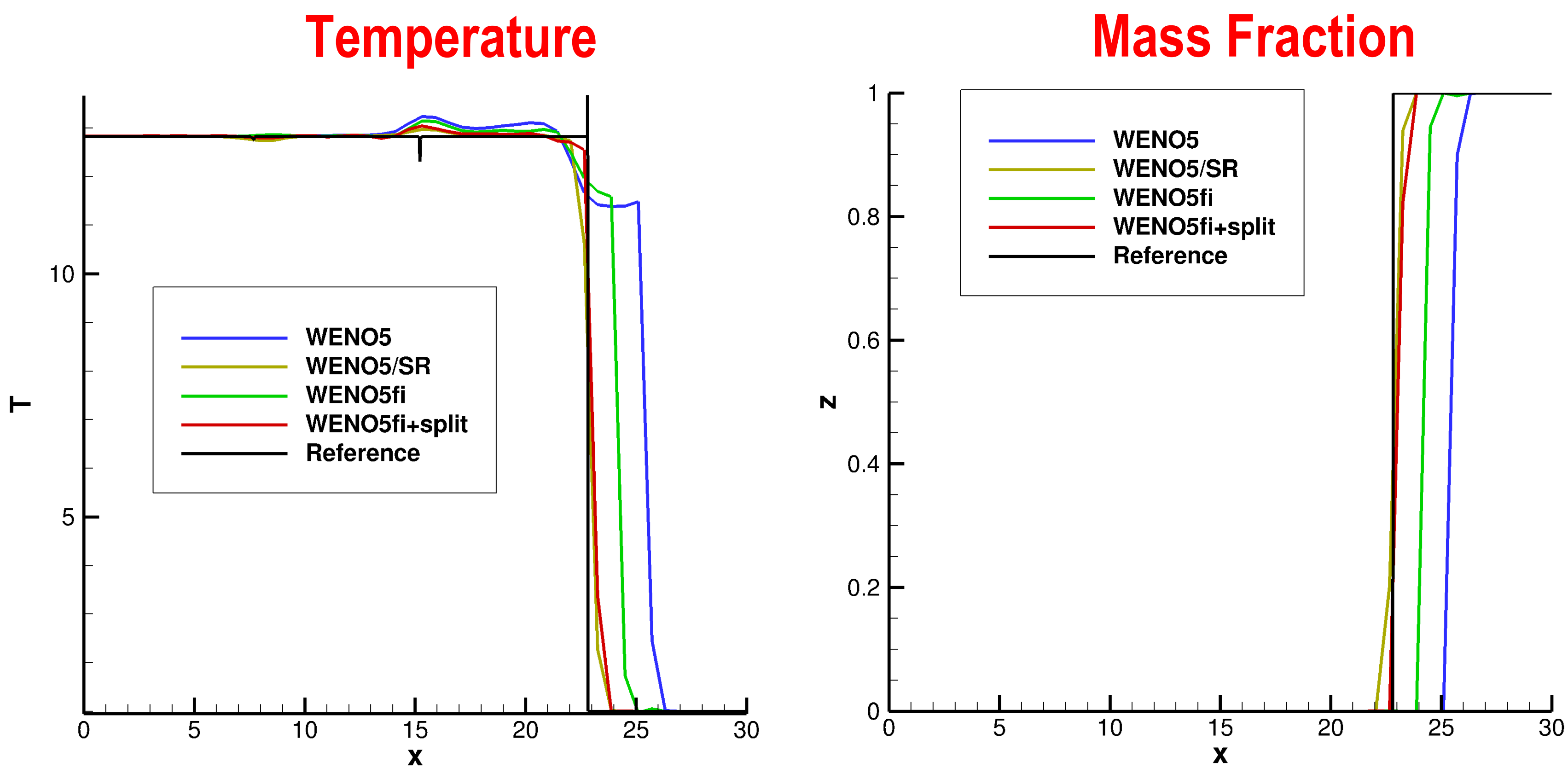
Ignition temperature $T_{ign}=25$

Heat release $q_0=25$

Rate parameter $K_0=16418$

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

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



WENO5: Standard 5th order WENO

WENO5/SR: WENO5 + subcell resolution

WENO5fi: Filter version of WENO5

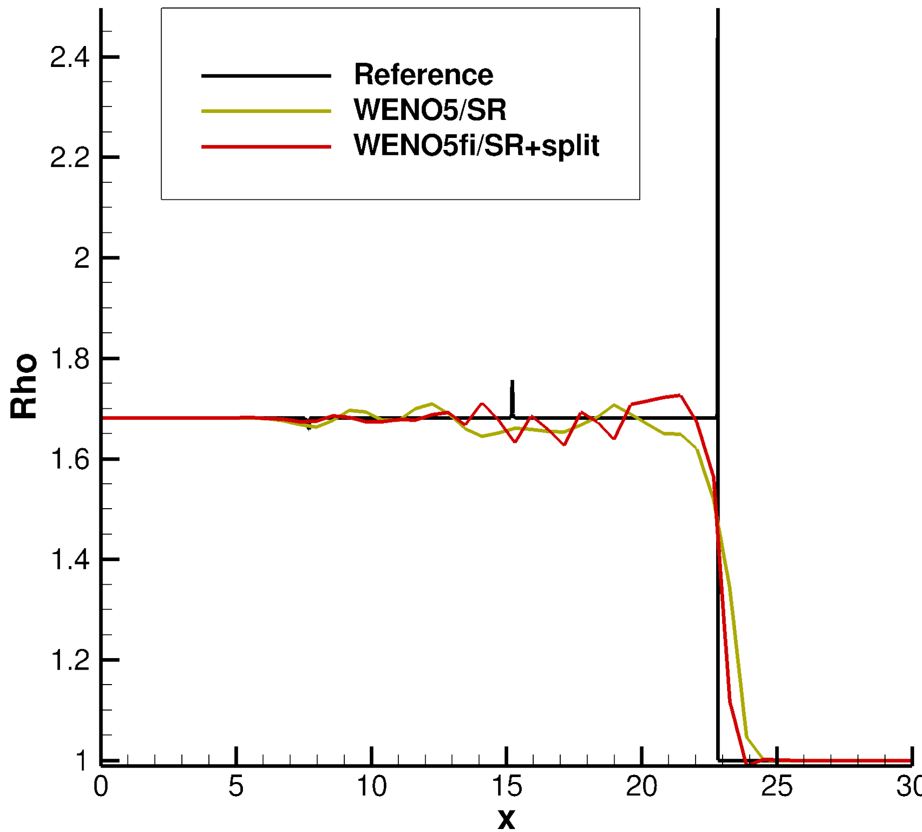
WENO5fi+split: WENO5fi + preprocessing (Ducros splitting)

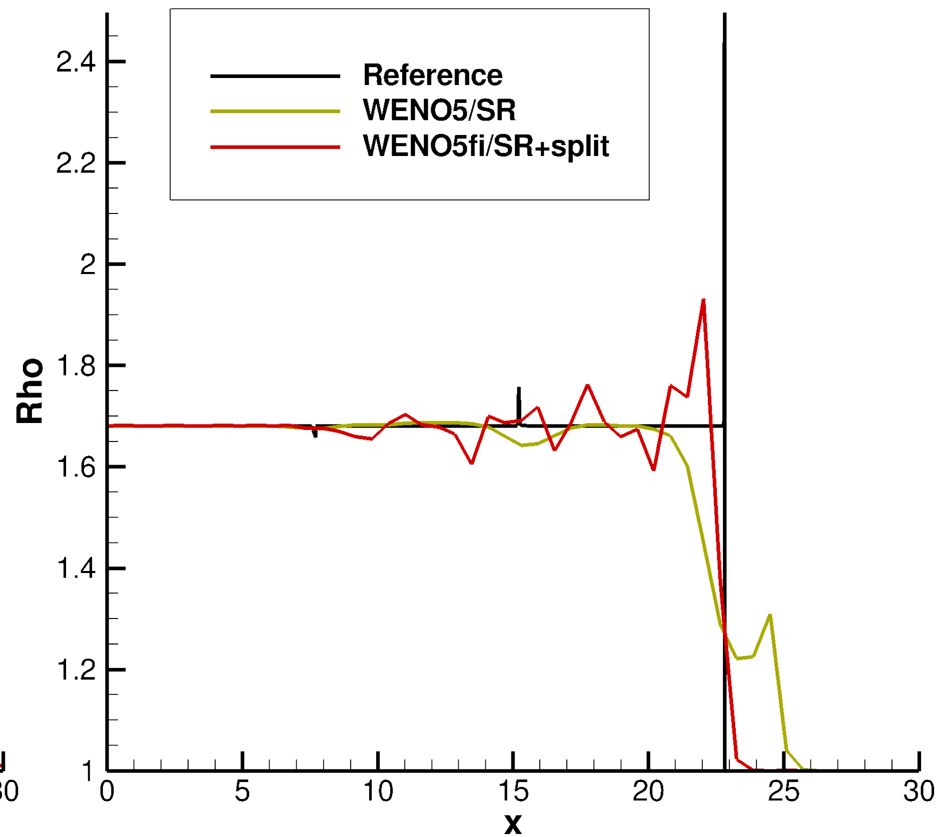
Reference: WENO5, 10,000 points

Filter Version of WENO5/SR: WENO5fi/SR

(50 pts, CFL = 0.025)

Stiffness 100 K_0 1000 K_0

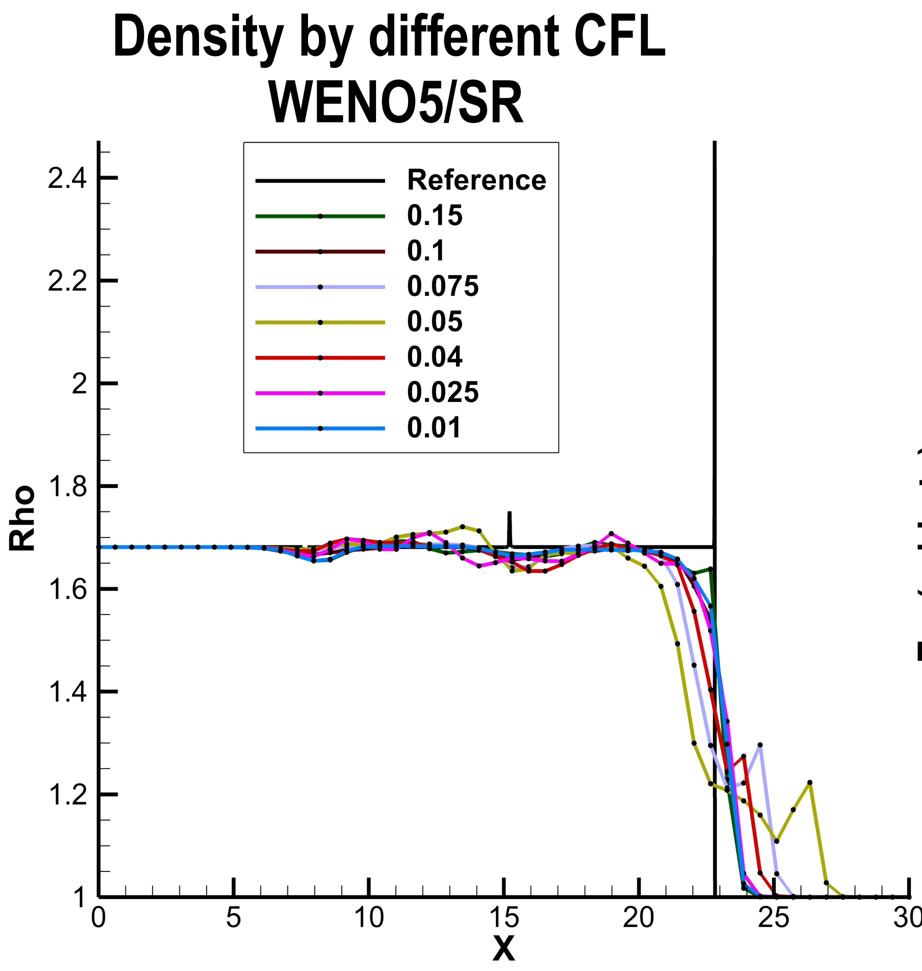


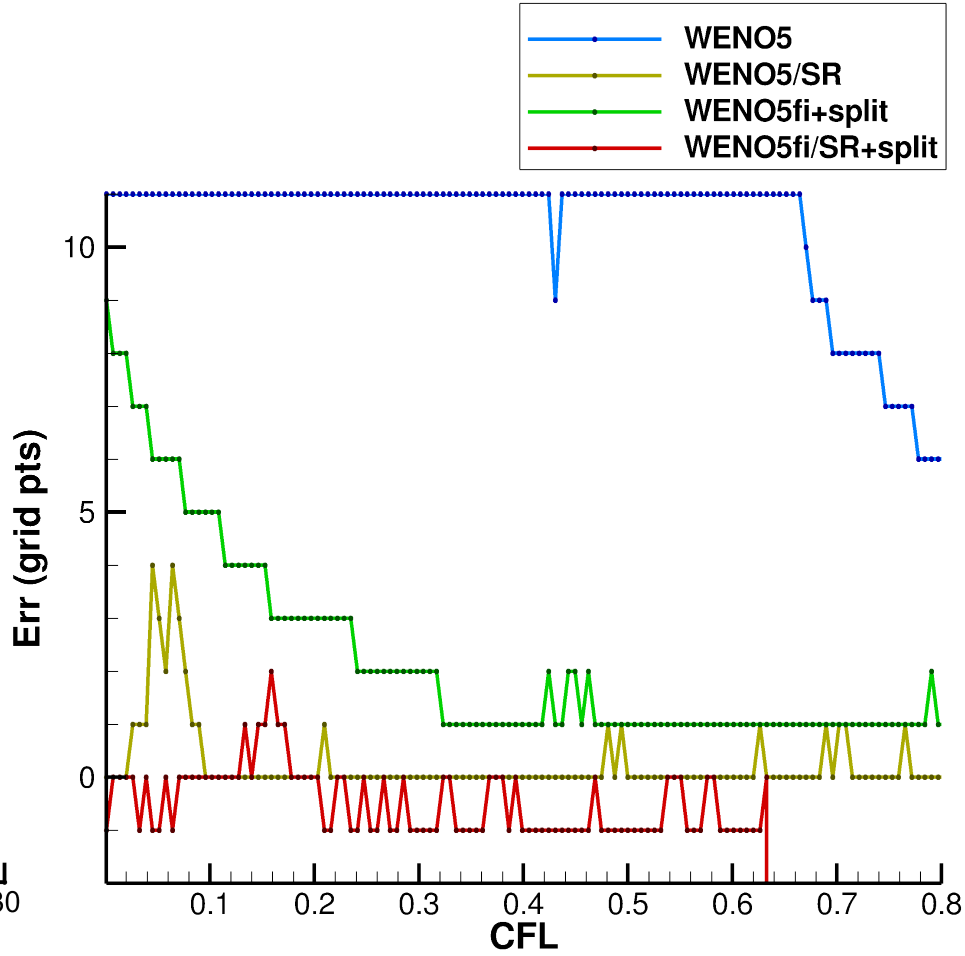


Behavior of the schemes below CFL limit

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

50 pts, Stiffness: 100 K_0





- *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)*

Behavior of the schemes below CFL limit

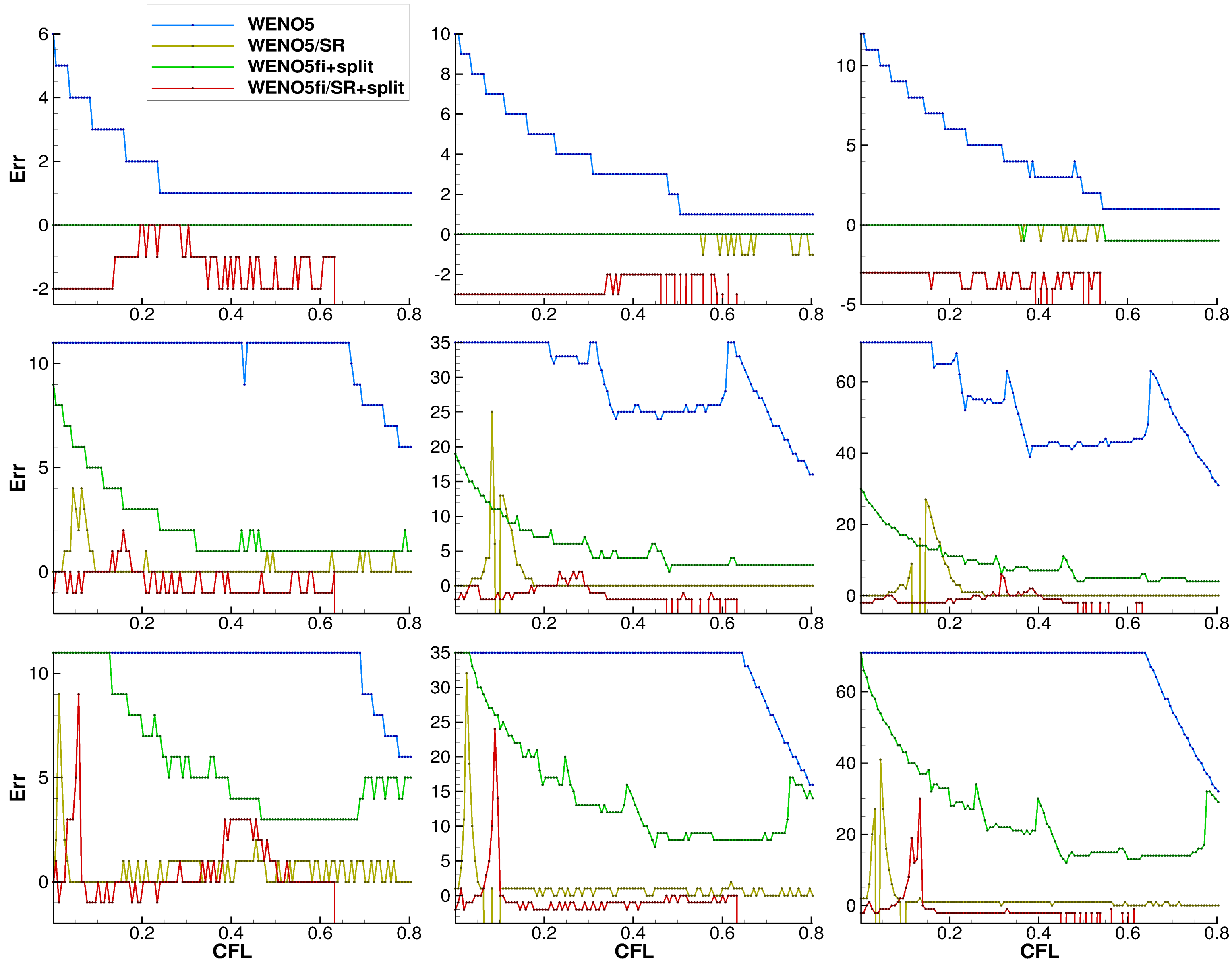
(Obtaining the Correct Shock Speed)

1D Detonation — **Grid 50** — **Grid 150** — **Grid 300**

Stiff. K_0

Stiff. 100 K_0

Stiff. 1000 K_0



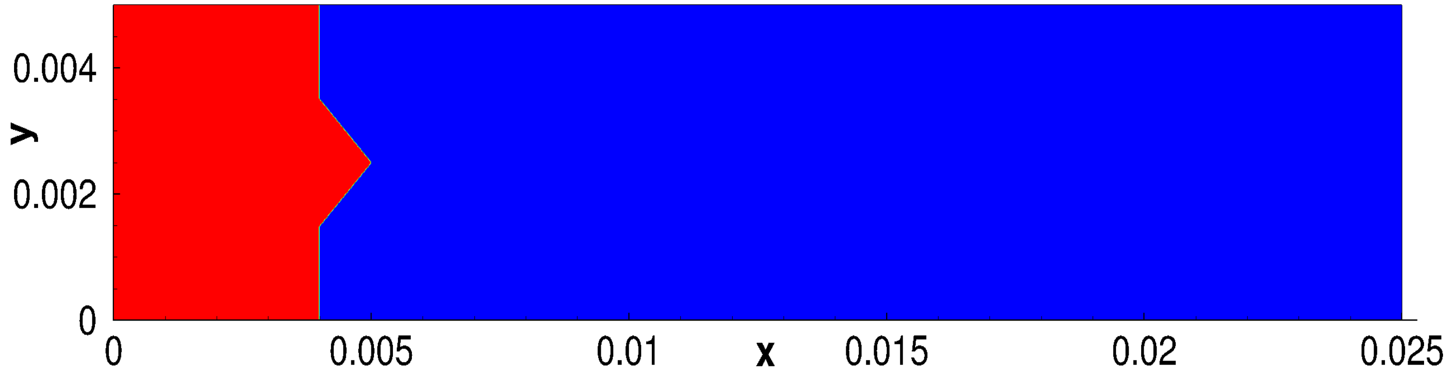
Note: CFL limit based on the convection part of PDEs

2D Detonation Wave *(Bao & Jin, 2001)*

Initial Condition

$$\begin{pmatrix}\rho\\u\\v\\p\\z\end{pmatrix}=\begin{pmatrix}\rho_b\\u_b\\0\\p_b\\0\end{pmatrix},\quad \text{if } x\leqslant\xi(y) \qquad \begin{pmatrix}\rho\\u\\v\\p\\z\end{pmatrix}=\begin{pmatrix}\rho_u\\u_u\\0\\p_u\\0\end{pmatrix},\quad \text{if } x>\xi(y)$$

$$\xi(y)=\begin{cases}0.004 & |y-0.0025|\geqslant 0.001\\ 0.005-|y-0.0025| & |y-0.0025|<0.001\end{cases}$$



2D Detonation Wave

Totally burned gas

$$\begin{pmatrix} \rho_b \\ u_b \\ p_b \end{pmatrix} = \begin{pmatrix} \rho_u \dfrac{[p_b(\gamma+1)-p_u]}{\gamma p_b} \\ 8.162\cdot 10^4 \\ -b+(b^2-c)^{1/2} \end{pmatrix}$$

Totally unburned gas

$$\begin{pmatrix} \rho_u \\ u_u \\ p_u \end{pmatrix} = \begin{pmatrix} 1.201\cdot 10^{-3} \\ 0 \\ 8.321\cdot 10^5 \end{pmatrix}$$

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

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

Ignition temperature $T_{ign} = 0.1155\cdot 10^{10}$

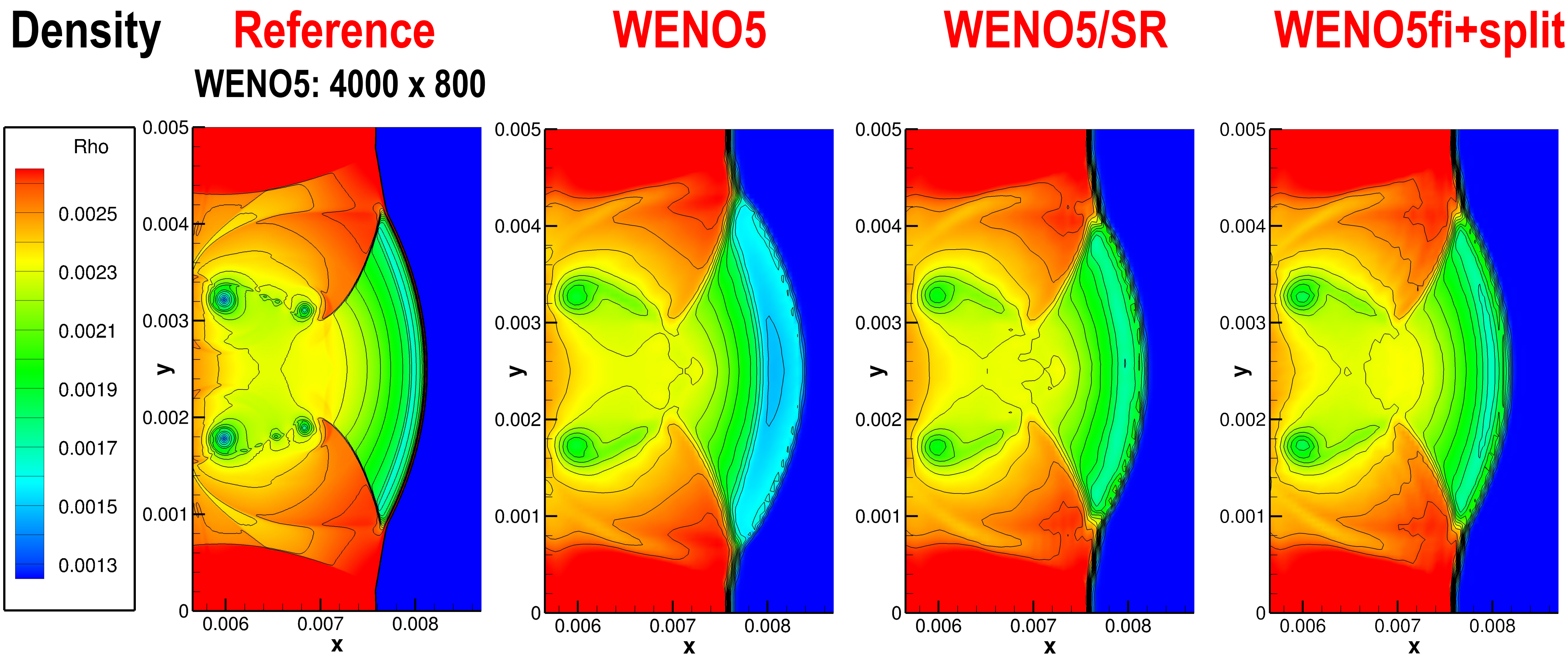
Heat release $q_0 = 0.5196\cdot 10^{10}$

Rate parameter $K_0 = 0.5825\cdot 10^{10}$

$$\boxed{K(T) = \begin{cases} K_0 & T \geqslant T_{ign} \\ 0 & T < T_{ign} \end{cases}}$$

2D Detonation, t=3e-8 s (500x100 pts)

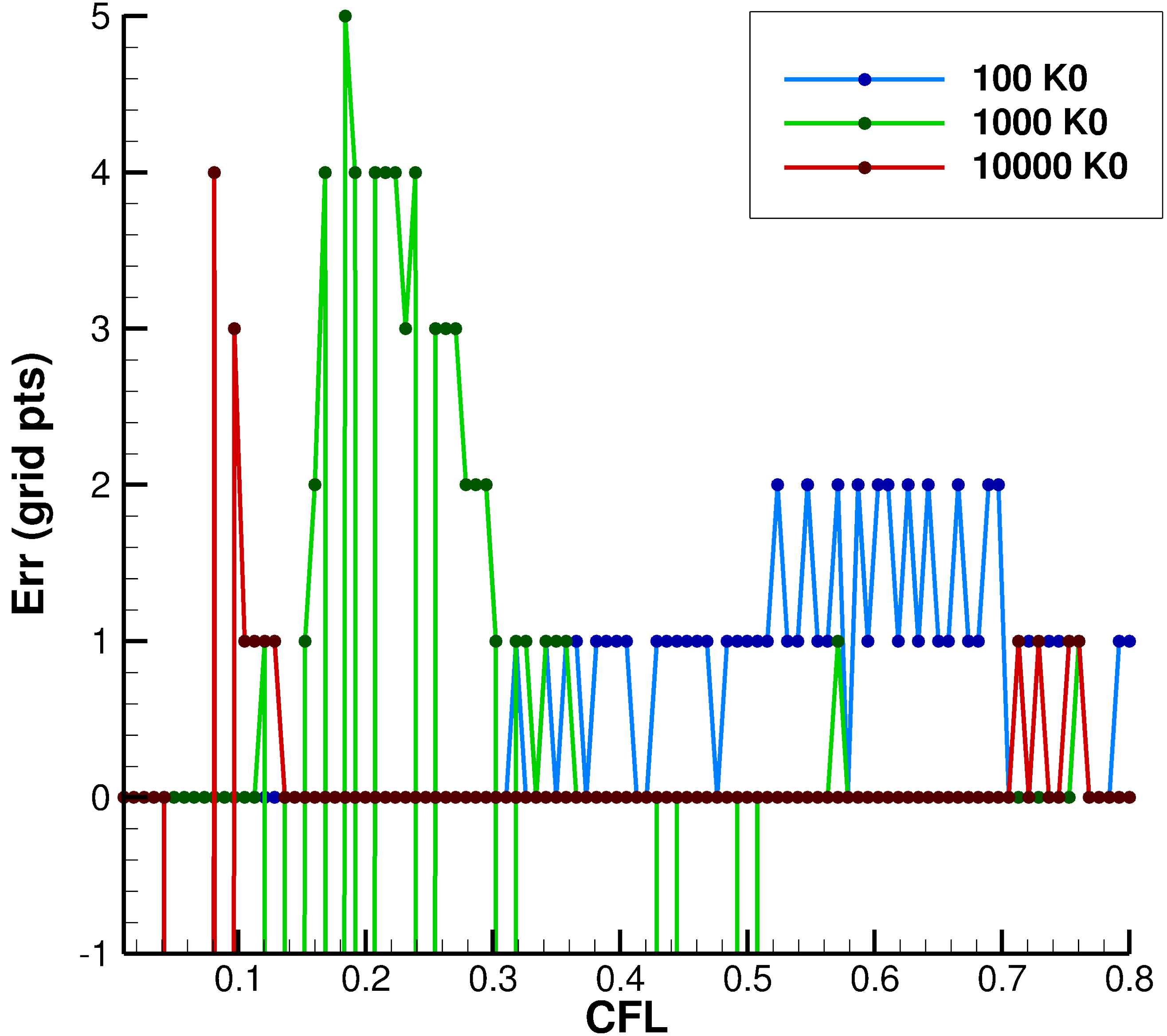
Comparison (WENO5,WENO5/SR,WENO5fi+split)



Behavior of the scheme below CFL limit

(Obtaining correct shock speed, 2D Detonation, 200x40 pts)

WENO5/SR, 3 stiff. coeff.



Note: CFL limit based on the convection part of PDEs

Behavior of the schemes below CFL limit

(Obtaining the Correct Shock Speed)

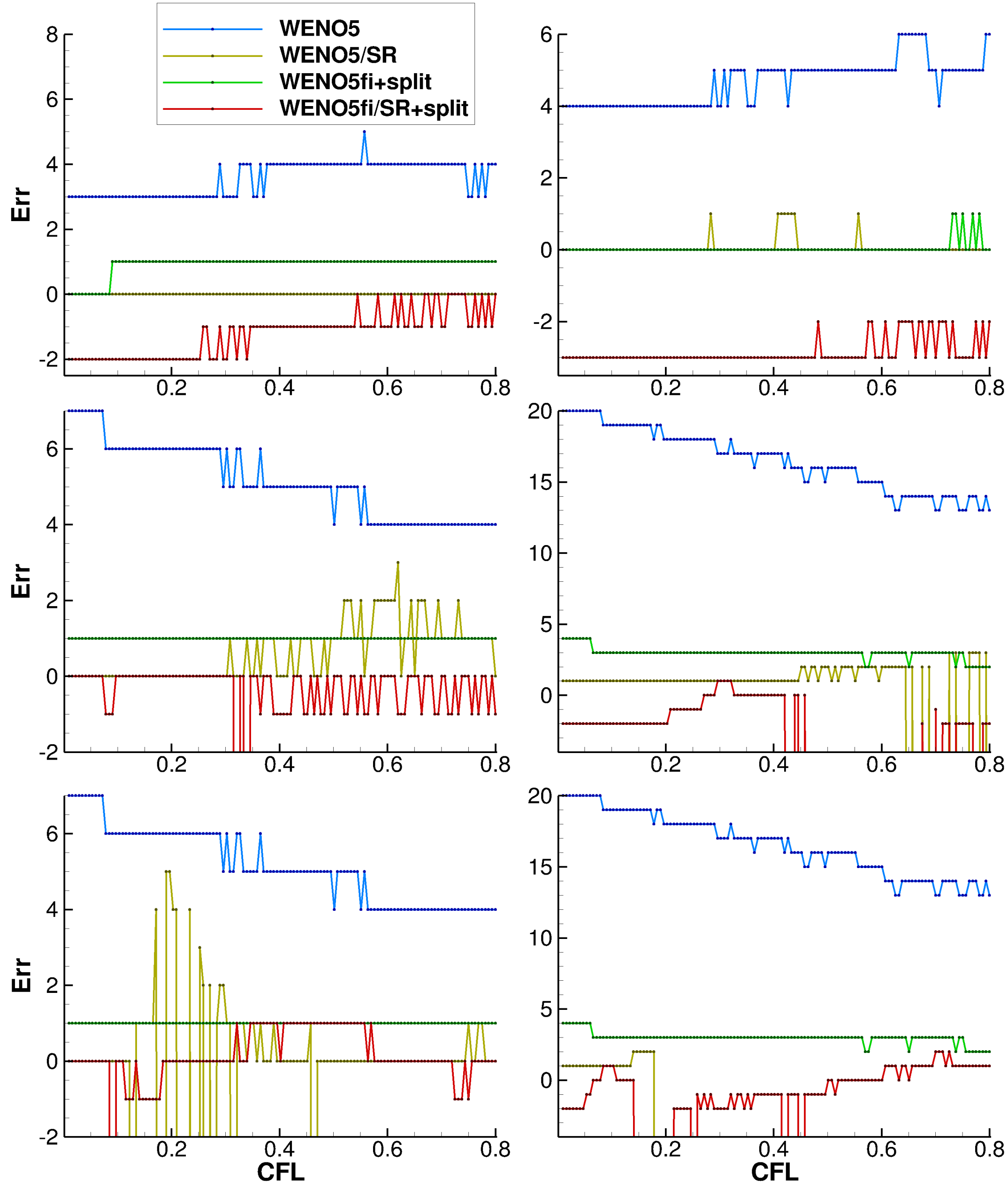
2D Detonation

Grid 200x40 **Grid 500x100**

Stiff. K_0

Stiff. 100 K_0

Stiff. 1000 K_0



Note: CFL limit based on the convection part of PDEs

Remark

<u>Spurious solutions</u> (below CFL limit):

(a) Wrong propagation speed of discontinuities

(b) Diverged solution

(c) Other wrong solution

These spurious solutions are solutions of the discretized counterparts but not the solutions of the governing equations

Scheme Performance (8 Procs.)

1D Detonation Problem (Grid 300, CFL = 0.05, RK4)

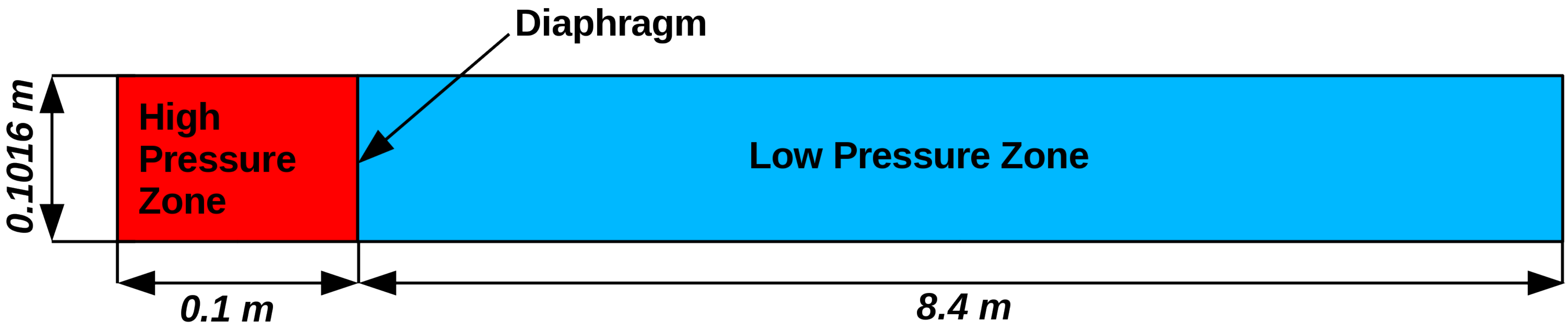
	WENO5	WENO5/SR	WENO5fi+split	WENO5fi/SR+split
CPU eff, iterations/sec	630	610	1720	1590
Discontinuity location error (grid points)	10	0	0	-3

2D Detonation Problem (Grid 500x100, CFL = 0.05, RK4)

	WENO5	WENO5/SR	WENO5fi+split	WENO5fi/SR+split
CPU eff, iterations/sec	4.0	3.6	9.5	5.7
Discontinuity location max error (grid points)	4	0	0	-3

2D EAST Problem (Viscous Nonequilibrium Flow)

NASA Electric Arc Shock Tube (EAST) – joint work with Panesi, Wray, Prabhu



13 Species mixture:

$$e^-, He, N, O, N_2, NO, O_2, N_2^+, NO^+, N^+, O_2^+, O^+, He^+$$

High Pressure Zone

ρ	$1.10546\, kg/m^3$
T	$6000\, K$
p	$12.7116\, MPa$
Y_{He}	0.9856
Y_{N_2}	0.0144

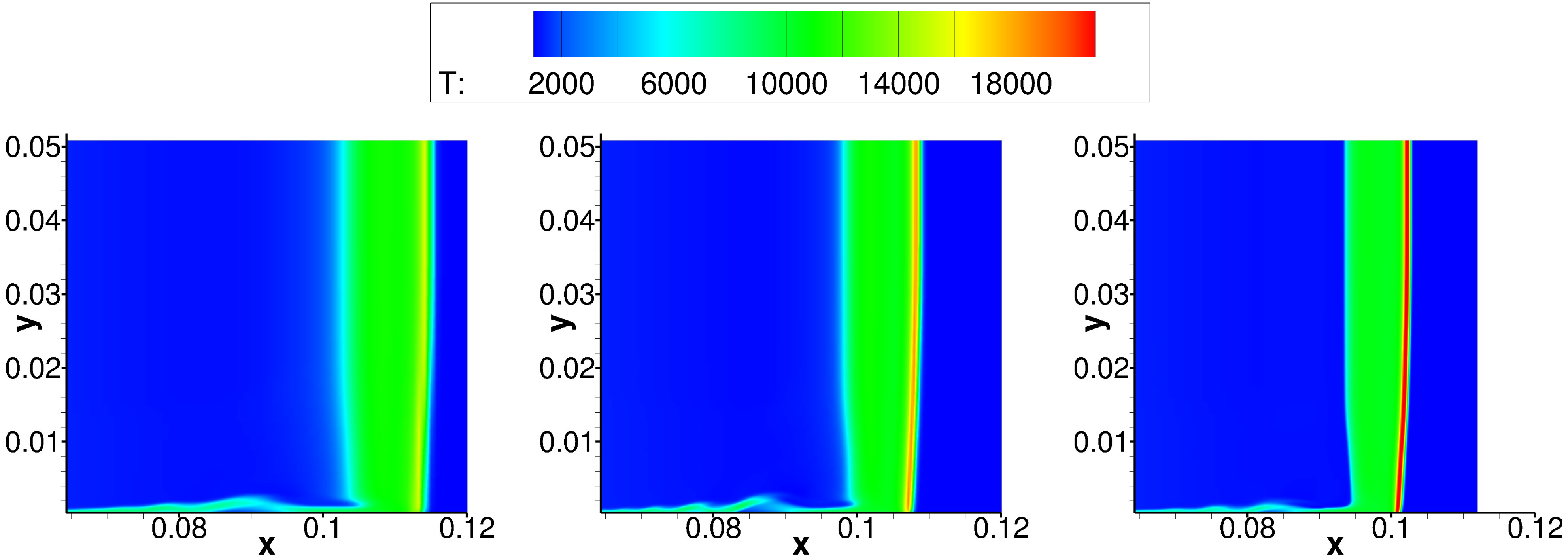
Low Pressure Zone

ρ	$3.0964\text{e}{-4}\, kg/m^3$
T	$300\, K$
p	$26.771\, Pa$
Y_{O_2}	0.21
Y_{N_2}	0.79

EAST: Temperature Computed at t = 1.e-5 s

Shock/Shear Locations Grid Dependance

TVD, CFL = 0.7



601x121	**1201x121**	**690x121**
Uniform	**Uniform**	**Cluster near shock**

Fine grid *h* = 0.05 *mm*
Grid points needed for x-dimension: 170,000

Concluding Remarks & Future Plans

- High order methods performance:
  - WENO5/SR performs slightly better then WENO5fi+split *(For Considered Test Cases)*
  - For Turbulence & Combustion WENO5fi+split is more accurate then WENO5/SR *(Work in progress)*
- Containment of numerical dissipation on existing shock-capturing schemes can delay the onset of wrong propagation speed of discontinuities

Future Work:

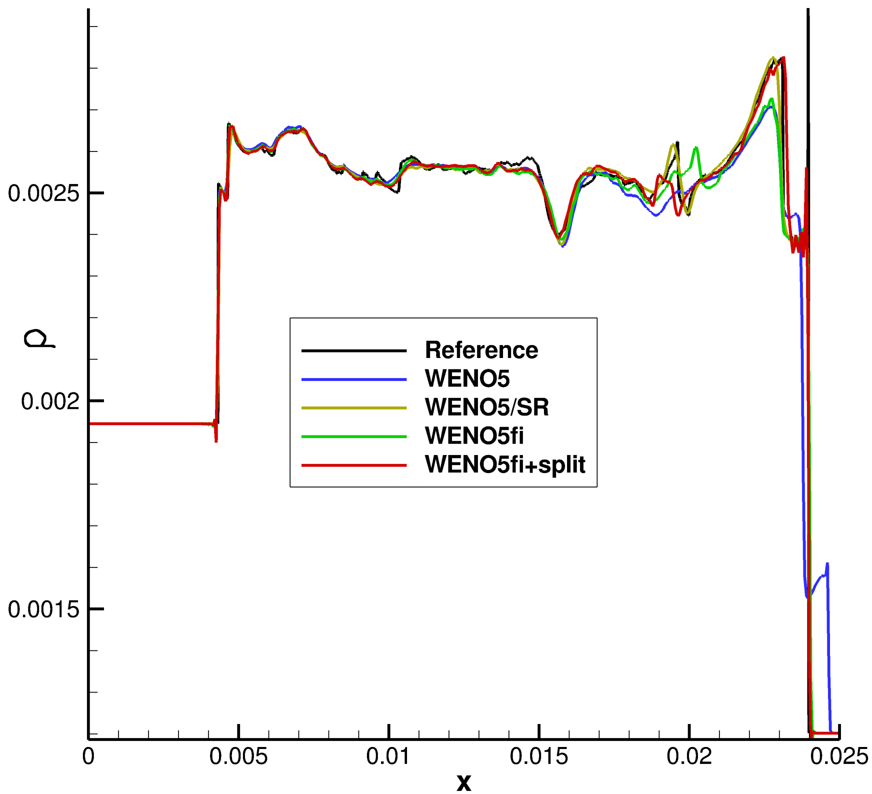
- Method extension for multispecies case
- Test cases that include Turbulence & Combustion

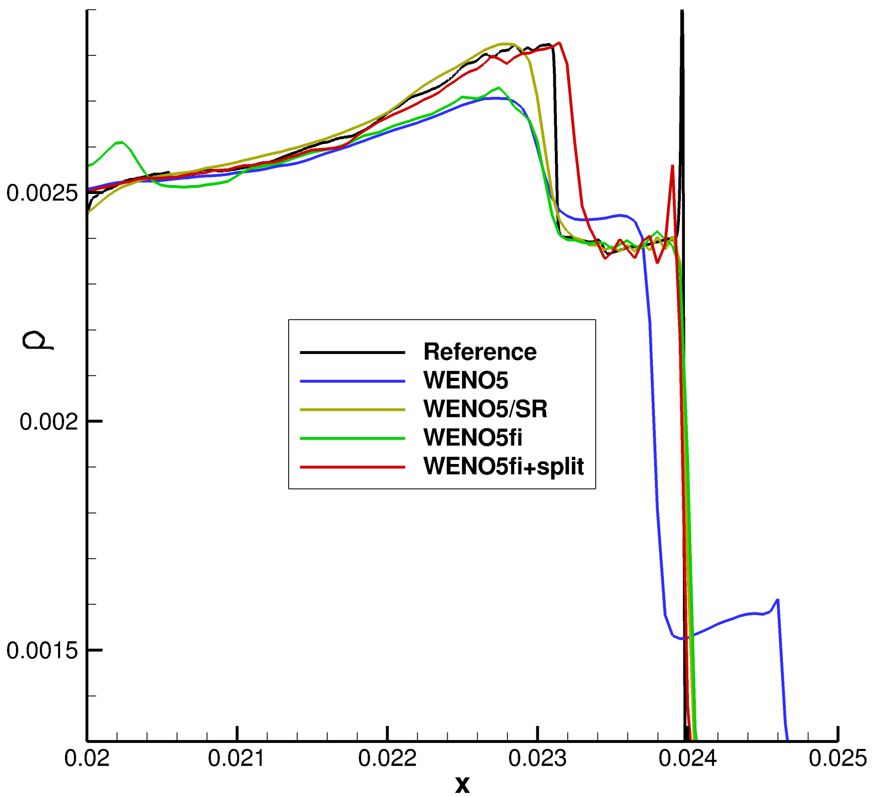
Thank you!

2D Detonation, 500x100 pts

WENO5,WENO5/SR,WENO5fi,WENO5fi+split

1D Cross-Section of Density at t = 1.7E-7





Zoom

Note: Wrong shock speed by WENO5fi using 200x40 pts

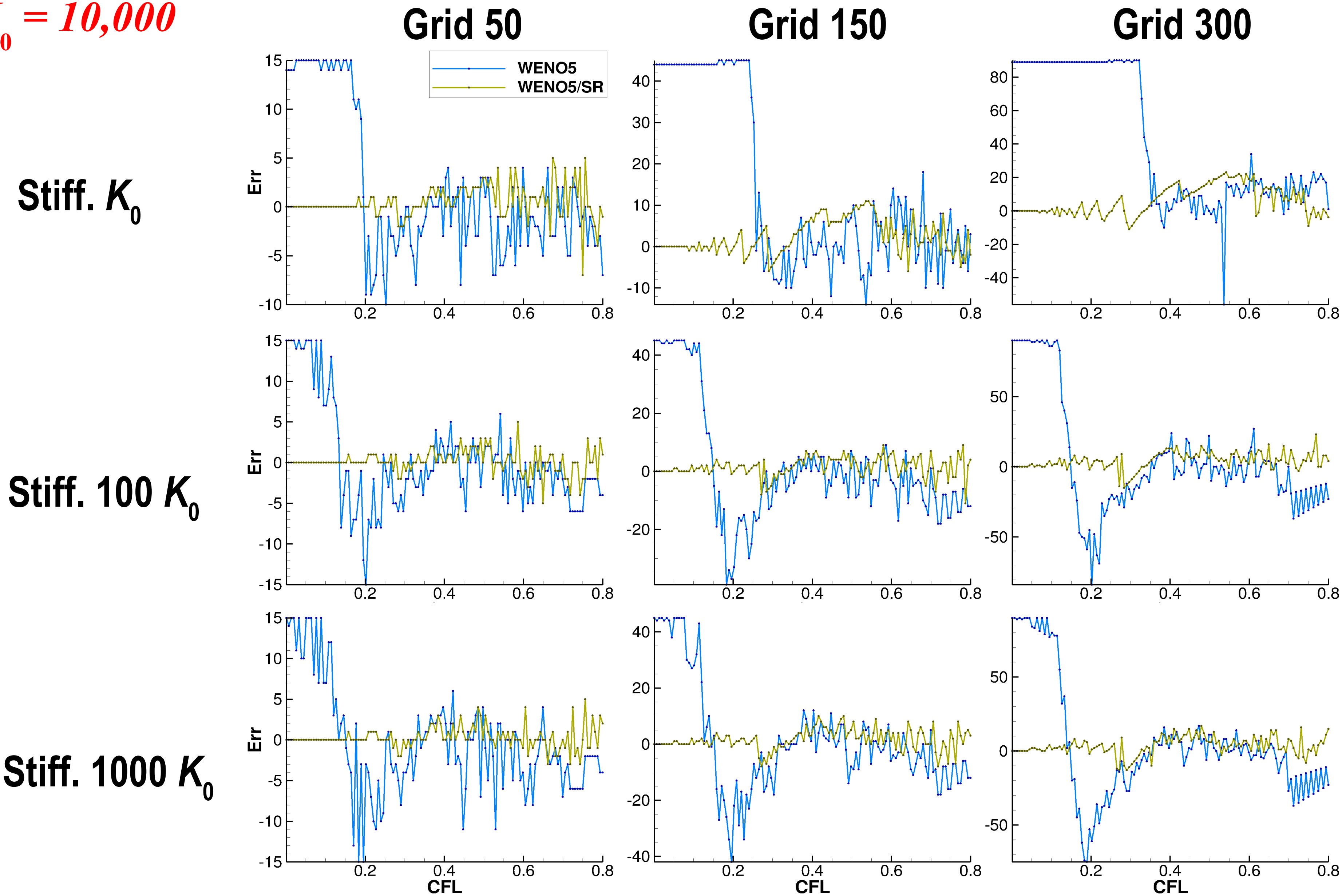
Scalar Case Behavior of WENO5 & WENO5/SR below CFL limit

Source term:

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

$K_0 = 10{,}000$

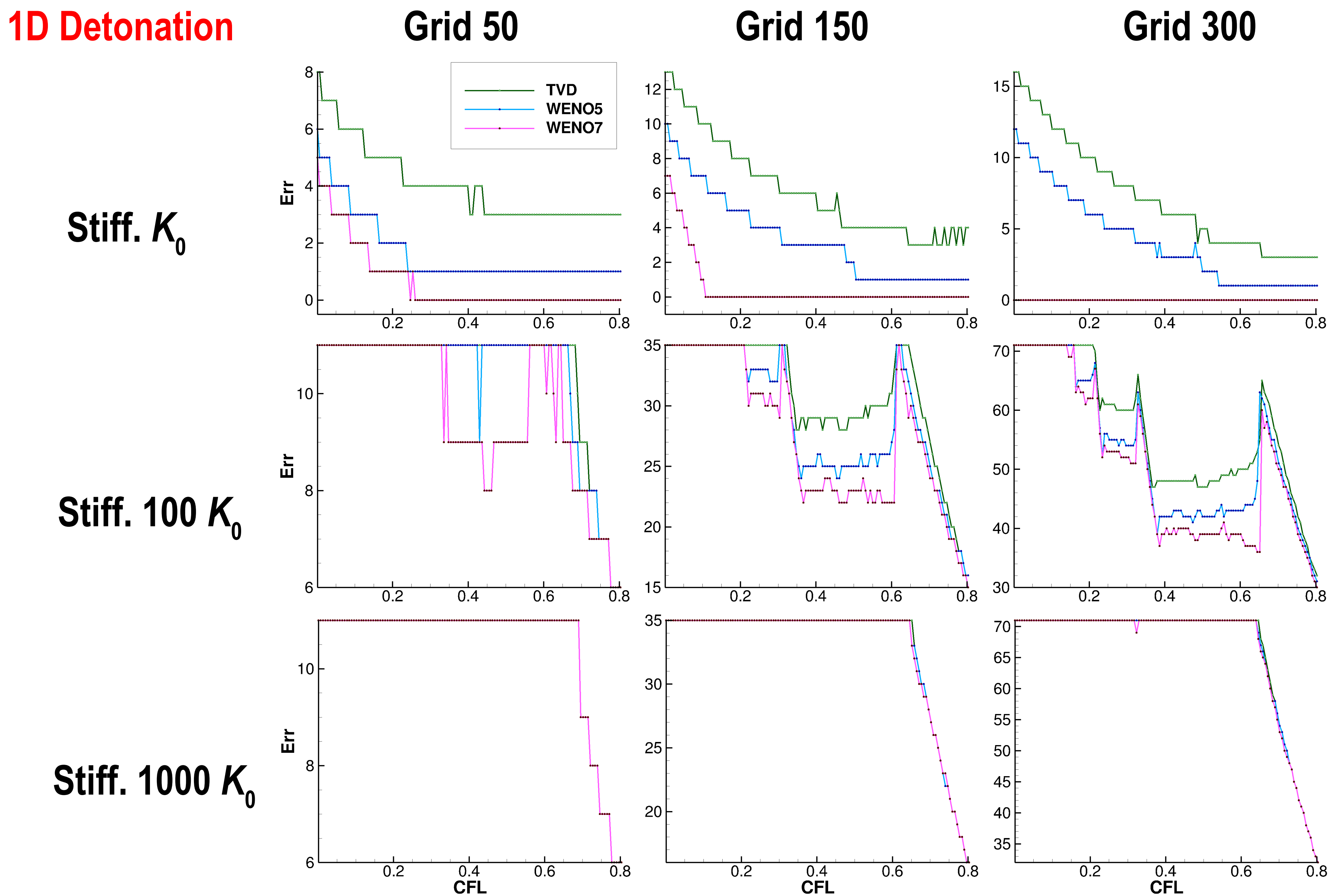
(Obtaining the Correct Discontinuity Speed)



Note: CFL limit based on the convection part of PDE

Behavior of standard schemes below CFL limit

(Obtaining the Correct Shock Speed)



Note: CFL limit based on the convection part of PDEs

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EAST Problem. Governing equations

NS equations for 2D (i=1,2) or 3D (i=1,2,3) chemically non-equilibrium flow:

$$\frac{\partial \rho_s}{\partial t}+\frac{\partial}{\partial x_j}(\rho_s u_j+\rho_s d_{sj}) = \Omega_s$$

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j+p\delta_{ij}-\tau_{ij}) = 0$$

$$\frac{\partial}{\partial t}(\rho E)+\frac{\partial}{\partial x_j}\left(u_j(E+p)+q_j+\sum_s \rho_s d_{sj} h_s-u_i\tau_{ij}\right) = 0$$

$$\rho=\sum_s \rho_s \qquad p=RT\sum_{s=1}^{N_s}\frac{\rho_s}{M_s} \qquad \rho E=\sum_{s=1}^{N_s}\rho_s\left(e_s(T)+h_s^0\right)+\frac{1}{2}\rho v^2$$

$$\tau_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\mu\frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \qquad d_{sj}=-D_s\frac{\partial X_s}{\partial x_j} \qquad q_j=-\lambda\frac{\partial T}{\partial x_j}$$

$$\Omega_s=M_s\sum_{r=1}^{N_r}\left(b_{s,r}-a_{s,r}\right)\left[k_{f,r}\prod_{m=1}^{N_s}\left(\frac{\rho_m}{M_m}\right)^{a_{m,r}}-k_{b,r}\prod_{m=1}^{N_s}\left(\frac{\rho_m}{M_m}\right)^{b_{m,r}}\right]$$

Reaction Operator

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

- Identify shock location, e.g. using Harten's indicator for z_{ij} – x-mass fraction of unburned gas:

$$s_{ij}^{x} = minmod\left(z_{i+1,j} - z_{ij},\, z_{ij} - z_{i-1,j}\right)$$

Shock present in the cell I_{ij} if

$$\left|s_{i,j}^{x}\right| > \left|s_{i-1,j}^{x}\right| \quad \text{and} \quad \left|s_{i,j}^{x}\right| > \left|s_{i+1,j}^{x}\right|$$

y-direction, similarly:

$$s_{ij}^{y} = minmod\left(z_{i,j+1} - z_{ij},\, z_{ij} - z_{i,j+1}\right)$$

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

$$\left|s_{ij}^{x}\right| \quad \text{or} \quad \left|s_{ij}^{y}\right|$$

Reaction Operator *(Cont.)*

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

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

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

where Θ is determined by the conservation of energy E:

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

- **Advance time by modified values for the Reaction operator (use, e.g., explicit Euler)**

$$(\rho z)_{ij}^{n+1} = (\rho z)_{ij}^{n} + \Delta t\, S(\tilde{z}_{ij}, \tilde{T}_{ij}, \tilde{\rho}_{ij})$$

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

- **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**

$$\boxed{\begin{array}{c} U_j^{n+1} = U_j^* - \dfrac{\Delta t}{\Delta x}\left[H_{j+1/2} - H_{j-1/2}\right] \\ H_{j+1/2} = R_{j+1/2}\overline{H}_{j+1/2} \end{array}}$$

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

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

$$\boxed{\bar{h}_{j+1/2}^m = \frac{\kappa_{j+1/2}^m}{2}\left(s_{j+1/2}^m\right)\left(\phi_{j+1/2}^m\right) \qquad m = 1 \ldots 3 + N_S - 1}$$

$\phi_{j+1/2}^m$ **- Dissipative portion of a shock-capturing scheme**

$s_{j+1/2}^m$ **- Wavelet sensor (indicate location where dissipation needed)**

$\kappa_{j+1/2}^m$ **- Control the amount of** $\phi_{j+1/2}^m$

Improved High Order Filter Method

Form of nonlinear filter:

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

Wavelet sensor

Shock capturing numerical flux (e.g. WENO5)

High-order central numerical flux (e.g. 6th 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)

Control the Amount of $\phi^m_{j+1/2}$

($\phi^m_{j+1/2}$ - Dissipative portion of a shock-capturing scheme)

$$\boxed{\kappa = f(M)\cdot\kappa_0}$$

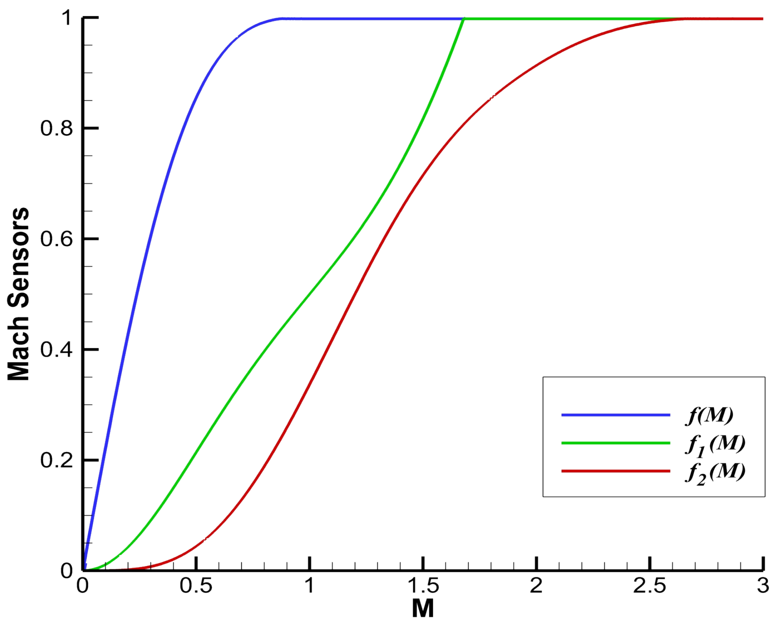
I. Mach # < 0.4

$$f_1(M) = \min\left(\frac{M^2}{2}\frac{\sqrt{(4+(1-M^2)^2)}}{1+M^2}, 1\right)$$

$$f_2(M) = (Q(M,2)+Q(M,3))/2$$

$$Q(M,a) = \begin{cases} P(M/a) & M < a \\ 1 & M \geqslant a \end{cases}$$

$$P(x) = x^4(35 - 84x + 70x^2 - 20x^3)$$



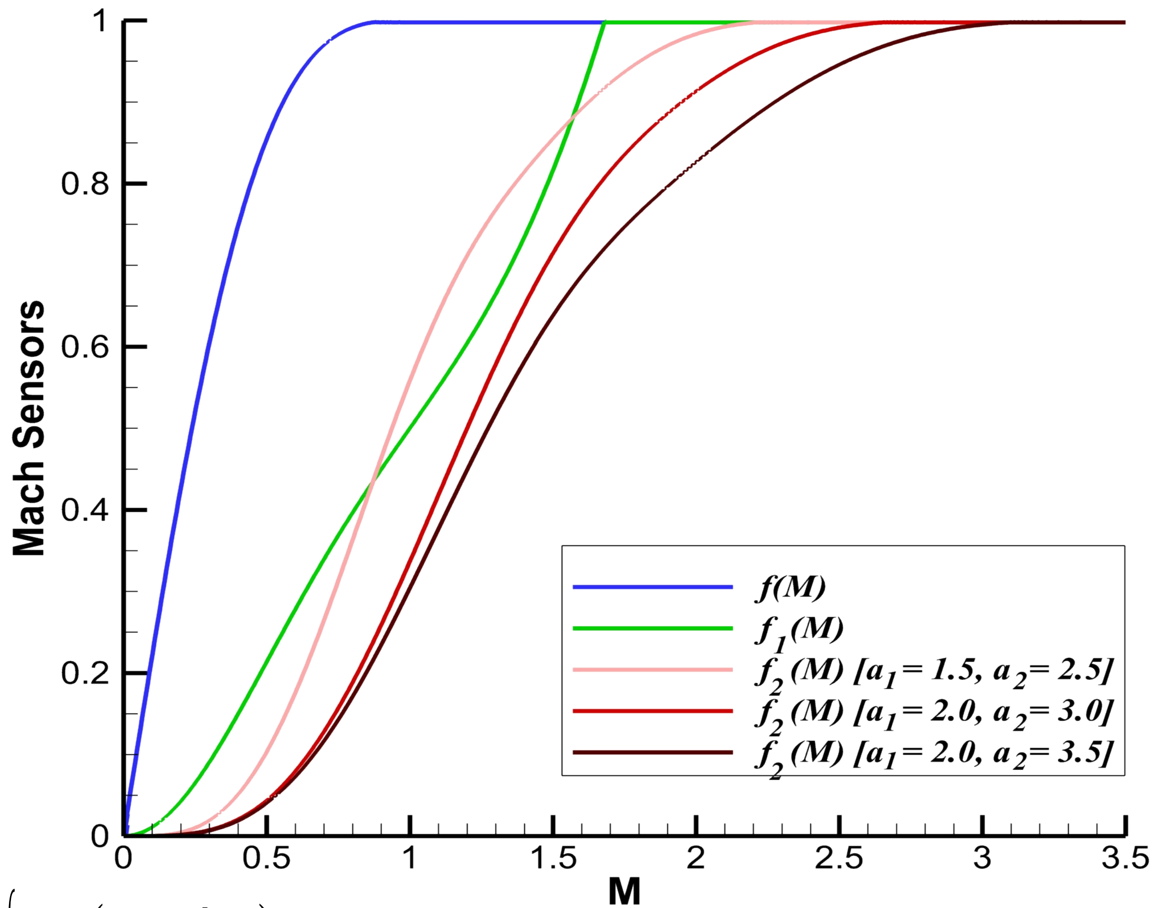
II. Mach # > 0.4

- Shock strength indicator (e.g. numerical Schlieren)
- Dominating shock jump variable
- Turbulent fluctuation region
  - Wavelets with high order vanishing moments
  - Wavelet based Coherent Vortex Extraction (CVE), Farge et. al (1999, 2001)

Control the Amount of $\phi^{m}_{j+1/2}$

($\phi^{m}_{j+1/2}$ - Dissipative portion of a shock-capturing scheme)

$$\kappa = f(M)\cdot\kappa_0 \qquad f_2(M) = (Q(M,a_1) + Q(M,a_2))/2$$



$$Q(M,a) = \begin{cases} P(M/a) & M < a \\ 1 & M \geqslant a \end{cases} \qquad P(x) = x^4(35 - 84x + 70x^2 - 20x^3)$$

High Order Methods with Subcell Resolution

Wang, Shu, Yee, & Sjögreen, 2012, JCP

- **Procedure: splitting equations into convective and reactive operators**

Using Strang-splitting (Strang, 1968)

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

$$U_t + F(U)_x + G(U)_y = 0 \qquad\qquad \frac{dU}{dt} = S(U)$$

A – Convection operator

R – Reaction operator

Numerical solution: $U^{n+1} = A\left(\frac{\Delta t}{2}\right) R(\Delta t)\, A\left(\frac{\Delta t}{2}\right) U^n$

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