Spurious Behavior of Shock-Capturing Methods

(Problems Containing Stiff Source Terms & Discontinuities)

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Goal

General Goal: Develop accurate & reliable high order methods for turbulence with shocks & stiff nonlinear source terms

(Employ nonlinear dynamics as a guide for scheme construction to improve the quantification of numerical uncertainties)

Specific Goal:

> *Illustrate spurious behavior of high order shock-capturing methods using pointwise evaluation of source terms & Roe's average state*

> *Relate numerical dissipation with the onset of wrong propagation speed of discontinuities*

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

Schemes to be considered:

TVD, WENO5, WENO7

WENO/SR – New scheme by Wang, Shu, Yee & Sjogreen

High order filter scheme by Yee & Sjogreen (SR counterpart)

Note: *Study based on coarse grid computations for obtaining the correct discontinuity locations (not accurate enough to resolve the detonation front)*

Spurious Solutions: *Not solutions of Gov. Eqns. But solutions of discretized counterparts*

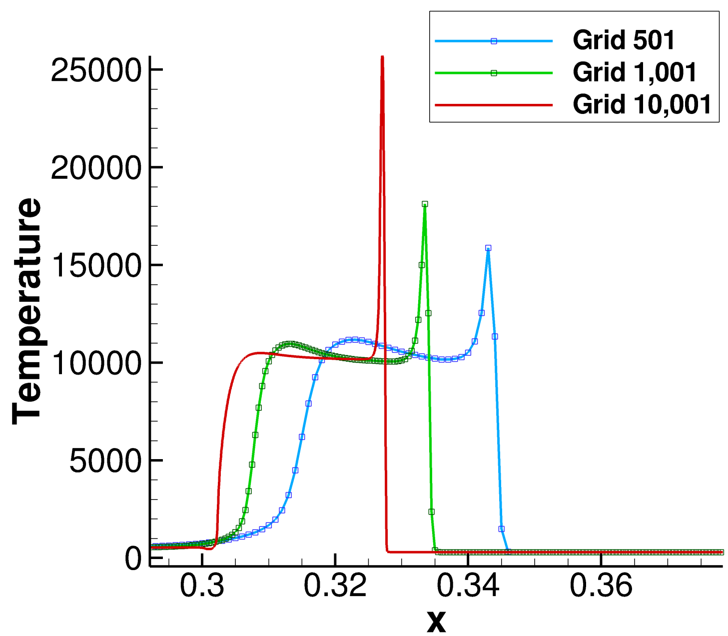
Outline

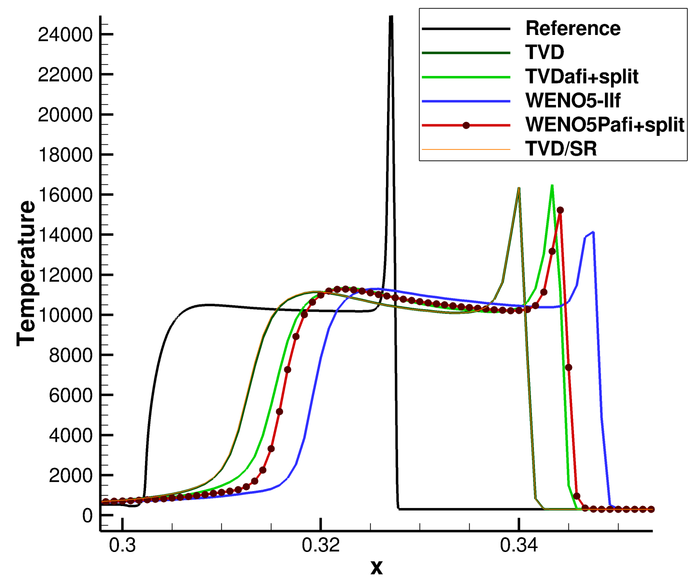
- **Motivation**
  - > *Quantification of numerical uncertainty for problems containing stiff source terms & discontinuities*
  - > *Wrong propagation speed of discontinuities by shock-capturing schemes*
- **Numerical Methods with Dissipation Control**
  - > *Turbulence with strong shocks & stiff source terms*
  - > *Can delay the onset of wrong speed for stiffer problems*
- **Three 1D & 2D Test Cases (2 & 13 species)**
- **Conclusions & Future Plan**

Motivation

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

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





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

Implication: *The danger in practical numerical simulation for this type of flow*
(Non-standard behavior of non-reacting flows)

Wrong Propagation Speed of Discontinuities

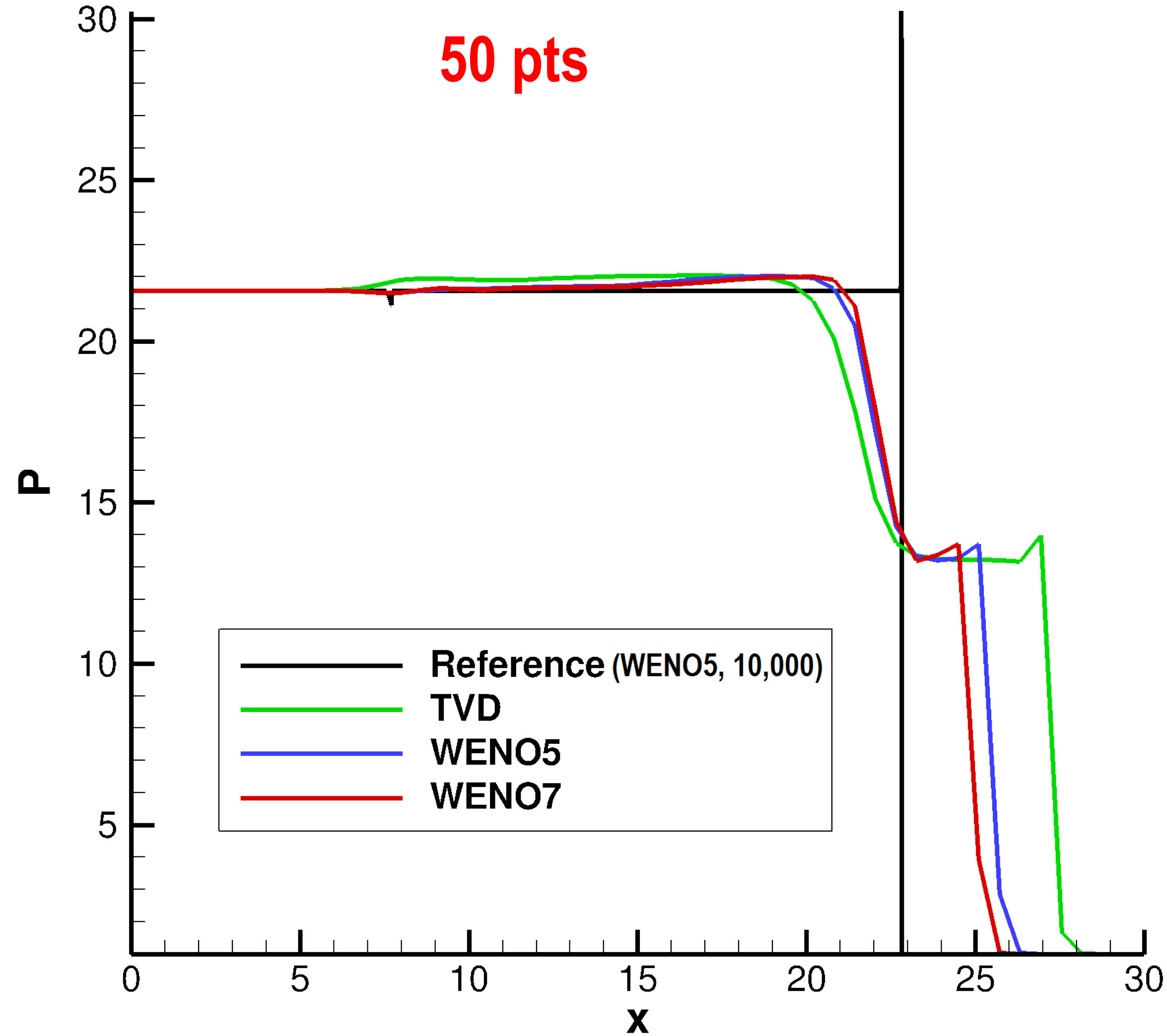
(Standard Shock-Capturing Schemes: TVD, WENO5, WENO7)

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

Arrhenius reaction rate:

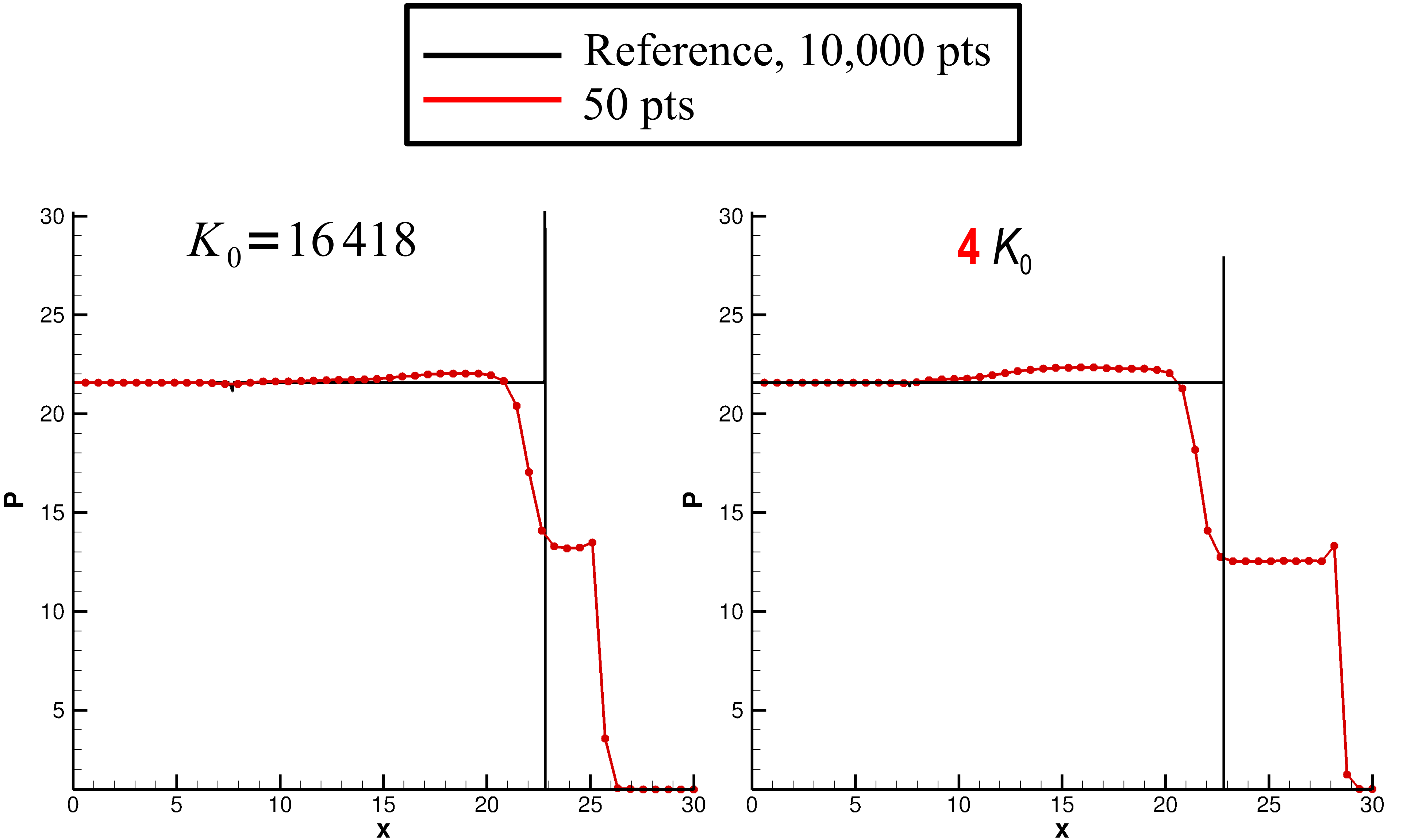
$$K(T) = K_0 \exp\left(\frac{-T_{ign}}{T}\right)$$

K_0 can be large (stiff coeff.)



Wrong Propagation Speed of Discontinuities

(WENO5, Two Stiff Coefficients, 50 pts)



Numerical Method Development Challenges

(Turbulence with Strong Shocks & Stiff Source Terms)

- **Conflicting Requirements** *(Turbulence with strong shocks):*
  - > *Turbulence cannot tolerate numerical dissipation*
  - > *Proper amount of numerical dissipation is required for stability & in the vicinity of shocks & contacts*
    (Recent development: Yee & Sjogreen, 2000-2009)

- **Nonlinearity of Source Terms:**
  - > *Incorrect numerical solution can be obtained for Δt below the CFL limit*
  - > *Time step, grid spacing, I.C. & B.C. dependence*

  (Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, 1990 – 2002)

- **Stiffness of Source Terms:**

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

Note: *(a) Standard methods have been developed for problems without source term*
(b) Investigate source terms of type $S(U)$ & $S(U_{j,k,l})$ – pointwise evaluation

Spurious Numerics Due to Source Terms

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

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

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

Stiff Source Terms:

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

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

> *A New Sub-Cell Resolution Method has been developed for stiff systems on coarse mesh*

Nonlinear Source Terms:

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

Stiff Nonlinear Source Terms with Discontinuities:

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

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

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

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

Stiff: large K_0

High Order Methods with Subcell Resolution

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

Procedure:

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

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

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

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 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

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)**

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

Well-Balanced High Order Filter Schemes for Reacting Flows *(Any number of species & reactions)*

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)

- **6th-order (or higher) central spatial scheme & 3th or 4th-order RK**
- **SBP numerical boundary closure, matching order conservative metric eval.**

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

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**

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

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

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

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

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

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

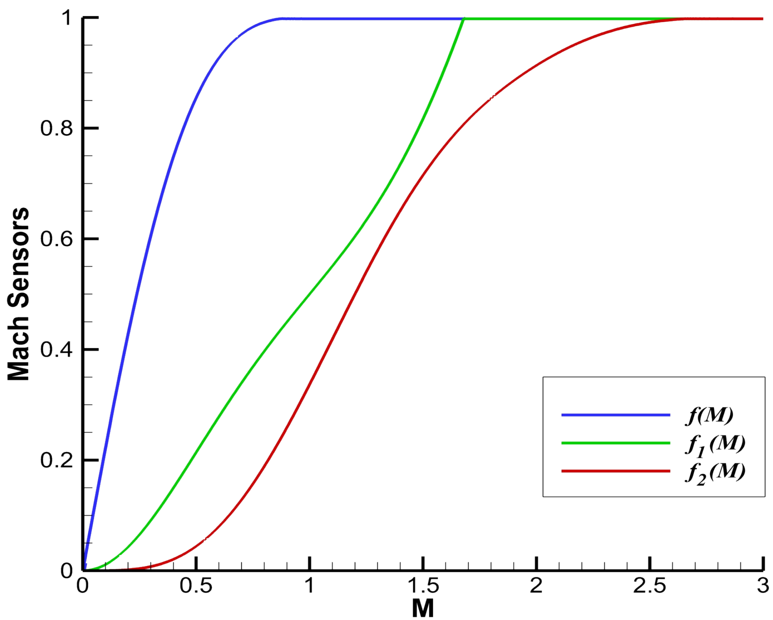
I. Mach # < 0.4

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

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

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

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



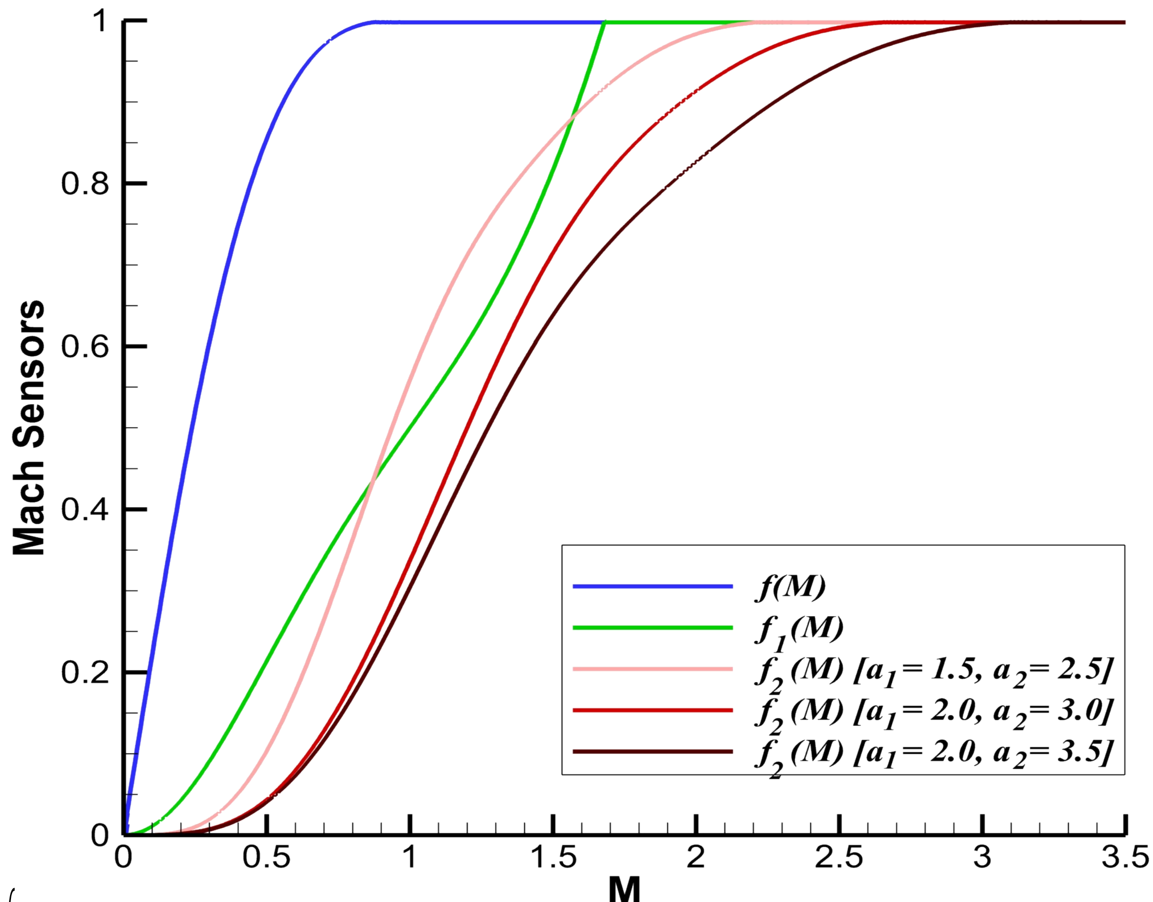
II. Mach # > 0.4

- 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)

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



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

Properties of the High-Order Filter Schemes

(Any number of species & reactions)

- 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)*

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 governing equations

Inaccurate solution: not part of spurious solution

1D C-J Detonation Wave

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

Left state (totally burned gas)	Right state (totally unburned gas)

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

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

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

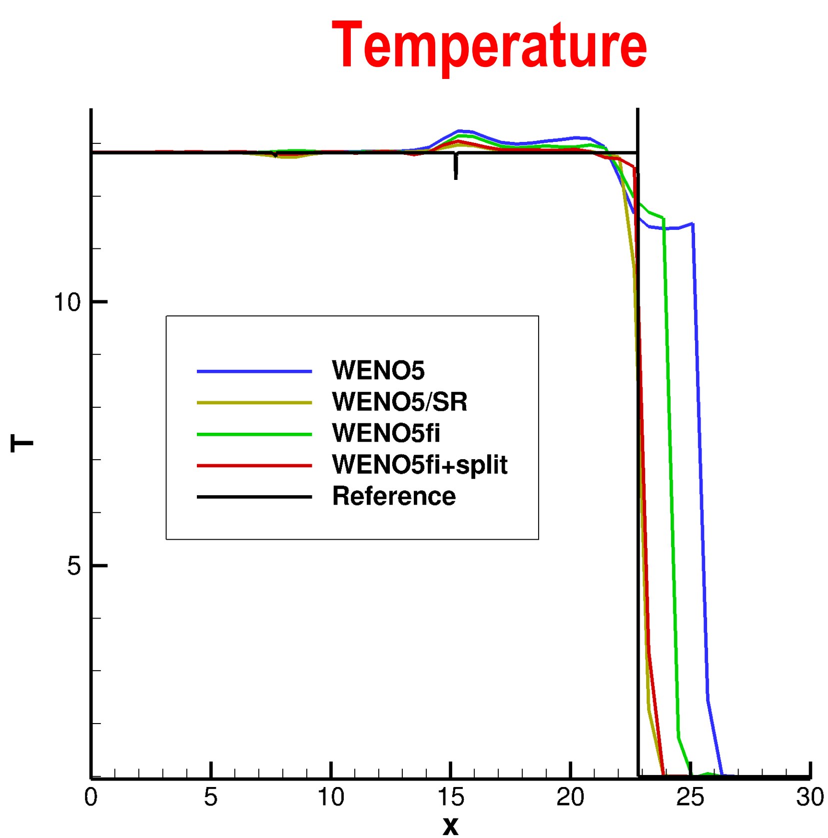
Ignition temperature $T_{ign}=25$

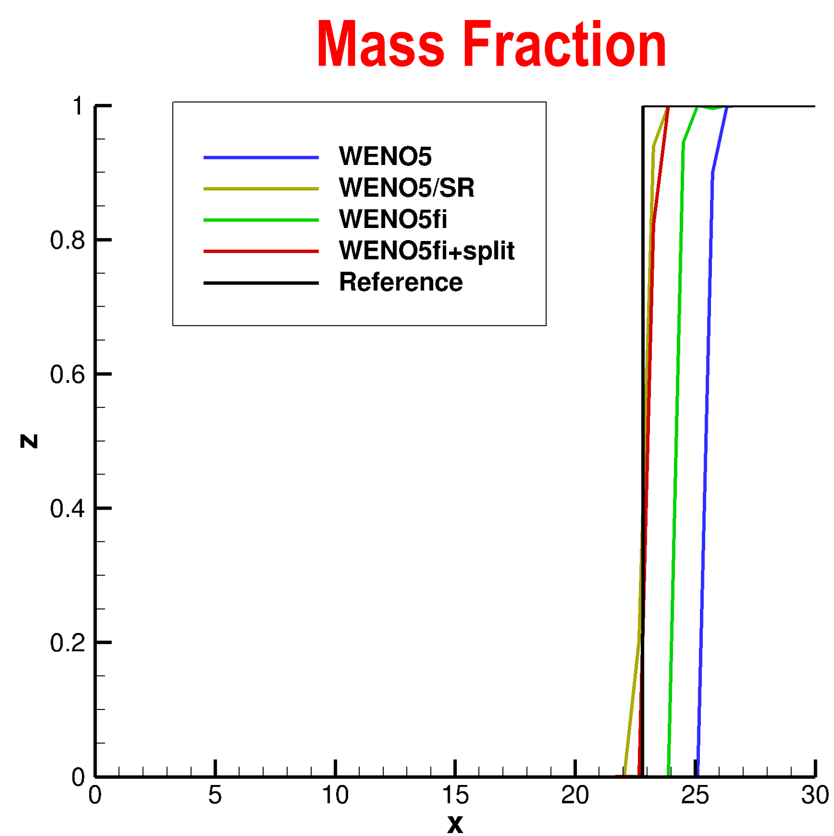
Heat release $q_0=25$

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)



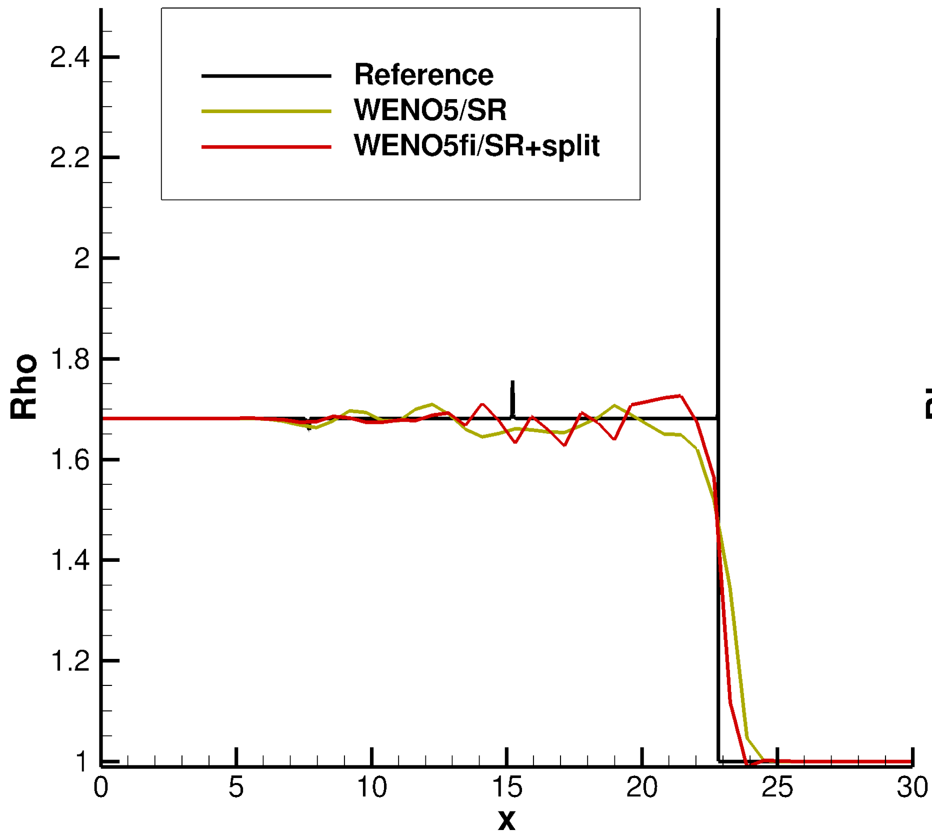


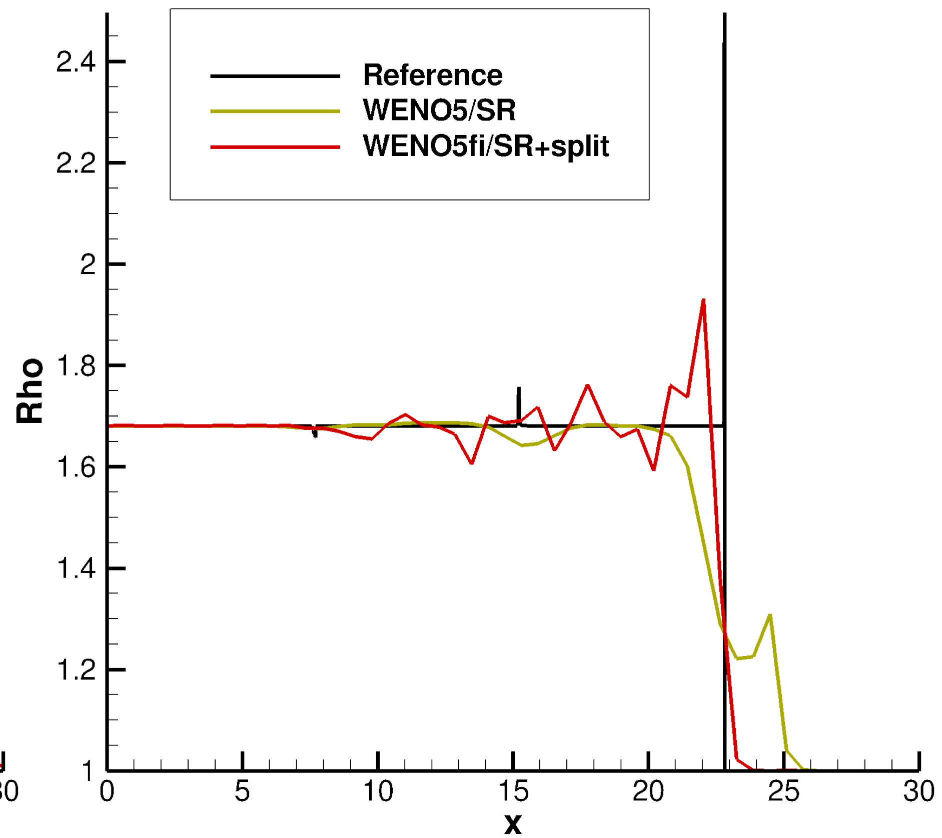
WENO5: Standard 5th order WENO
WENO5/SR: WENO5 + subcell resolution
WENO5fi: Filter version of WENO5
WENO5fi+split: WENO5fi + preprocessing (Ducros splitting)
Reference: WENO5, 10,000 points

Filter Version of WENO5/SR: WENO5fi/SR

(50 pts, CFL = 0.025)

Stiffness   **100 K_0**   **1000 K_0**

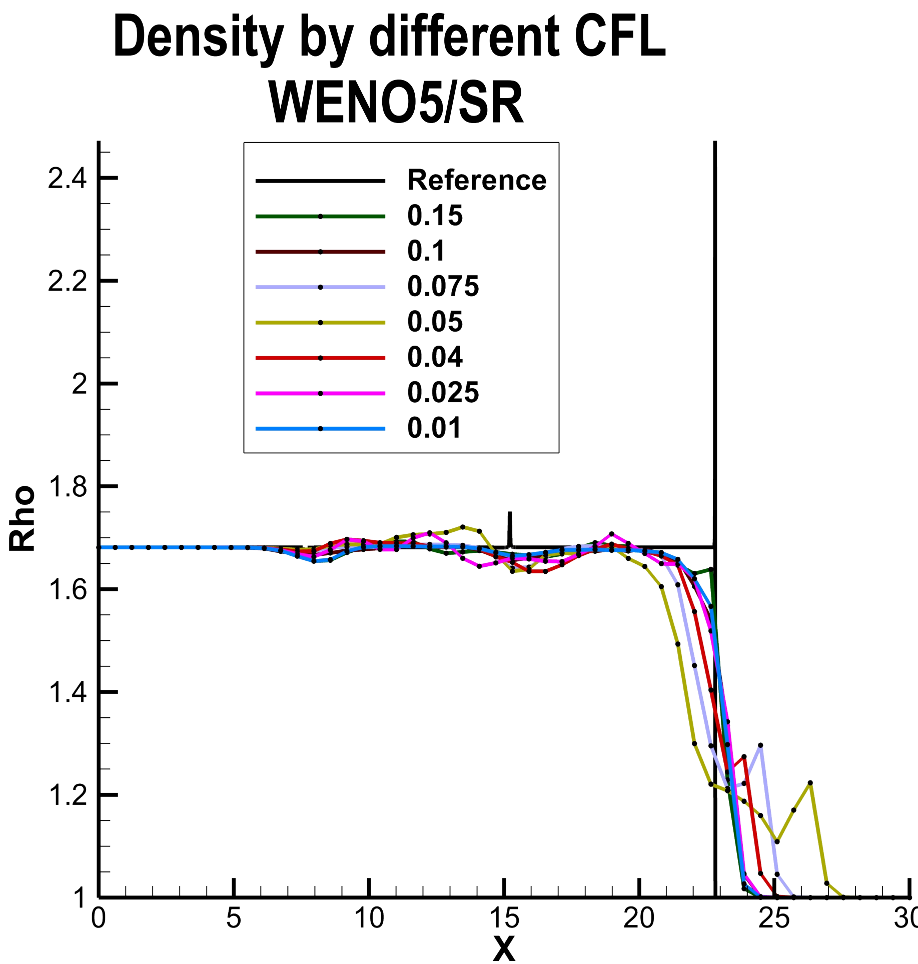


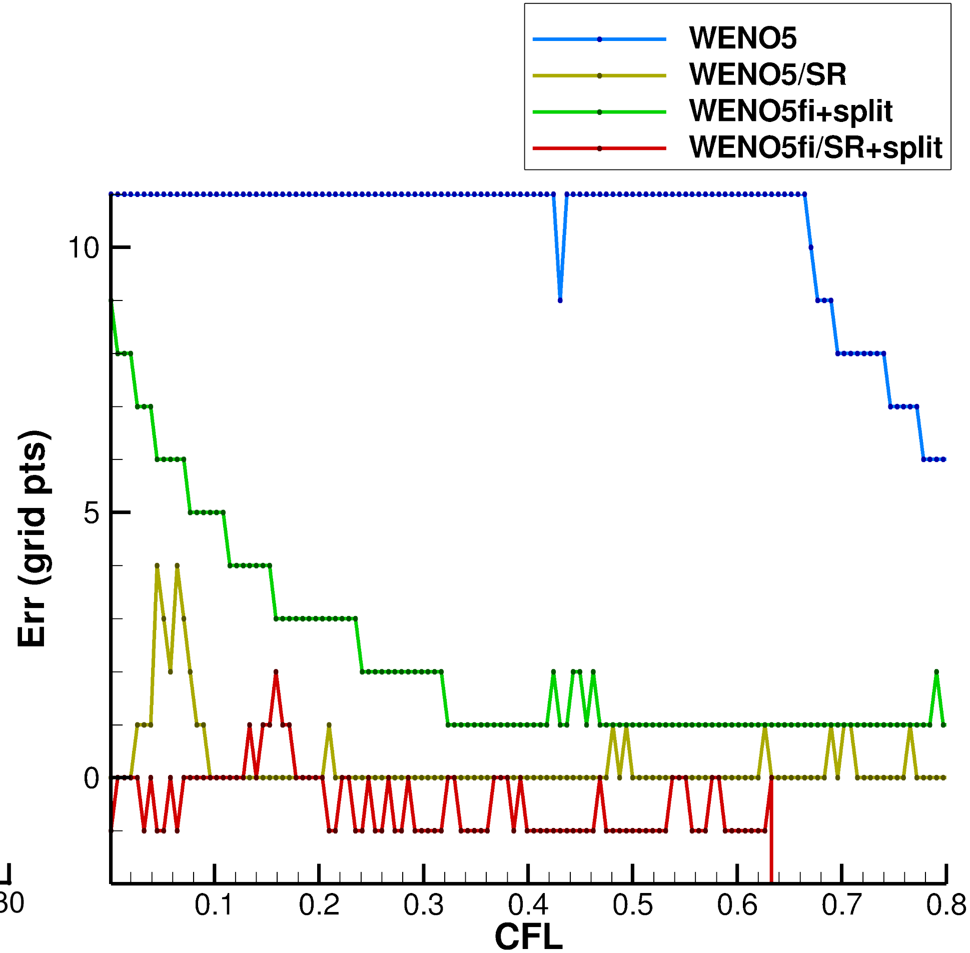


Behavior of the schemes below CFL limit

(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 standard schemes below CFL limit

(Obtaining the Correct Shock Speed)

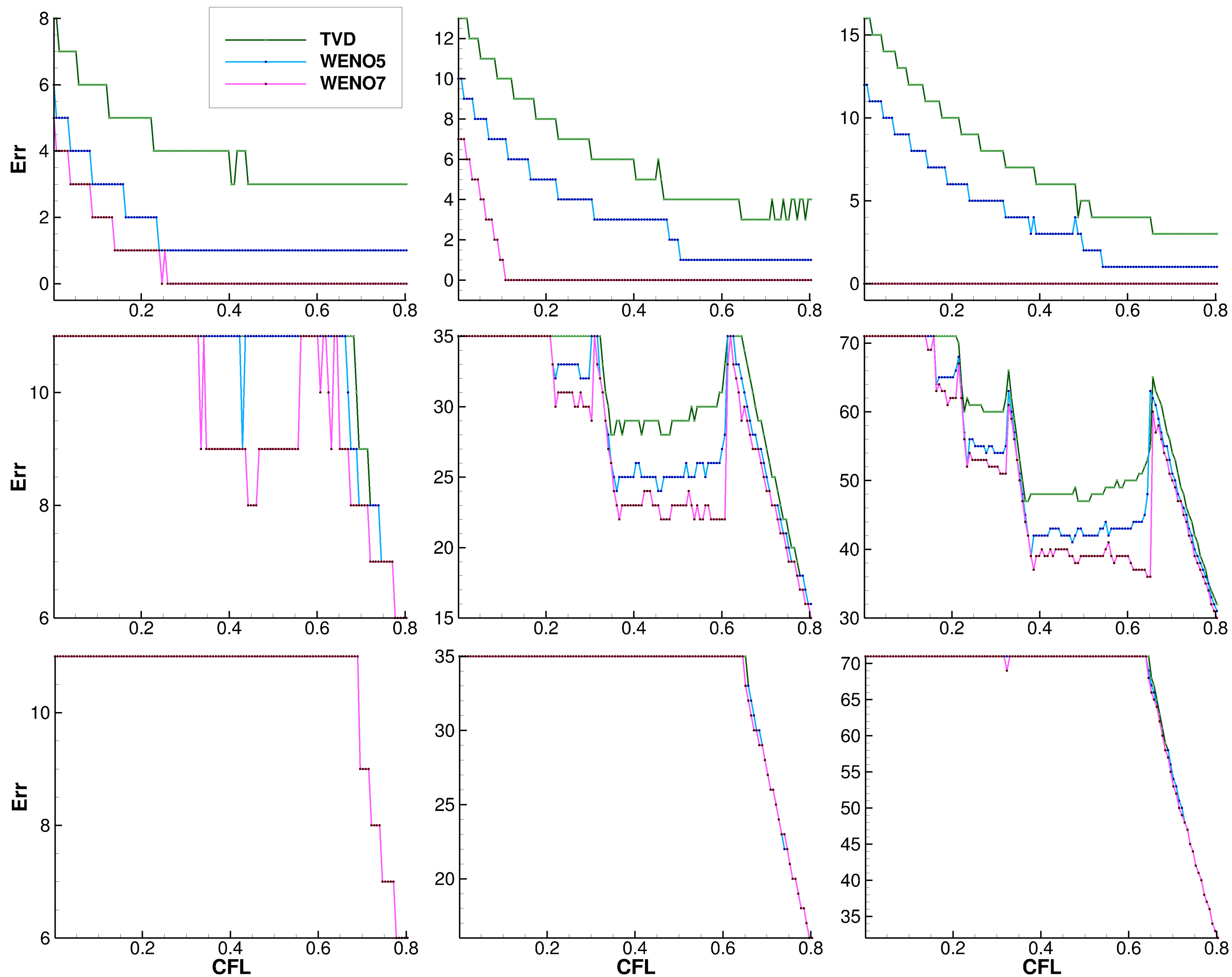
1D Detonation

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

Stiff. K_0

Stiff. $100\ K_0$

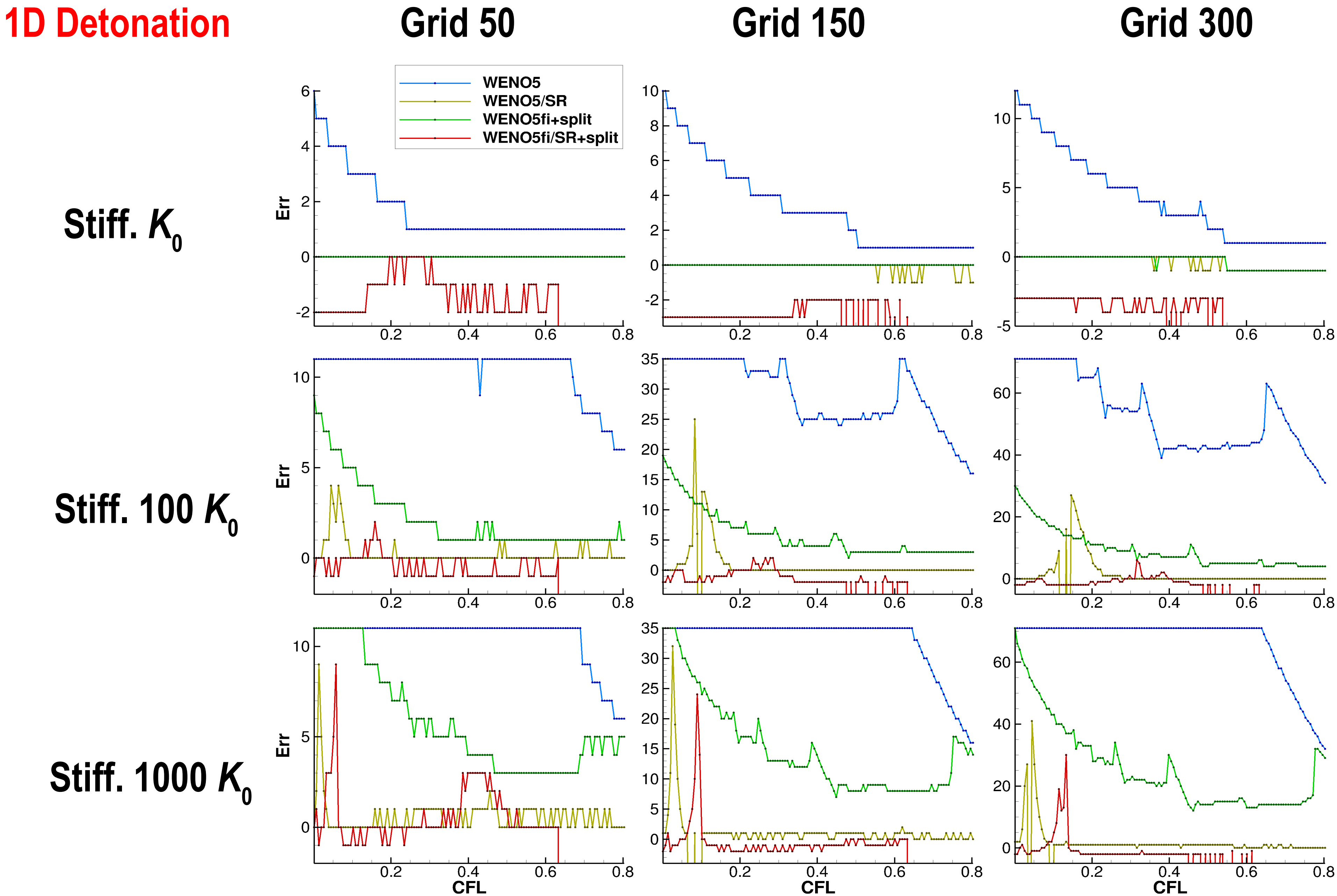
Stiff. $1000\ K_0$



Note: CFL limit based on the convection part of PDEs

Behavior of the schemes below CFL limit

(Obtaining the Correct Shock Speed)



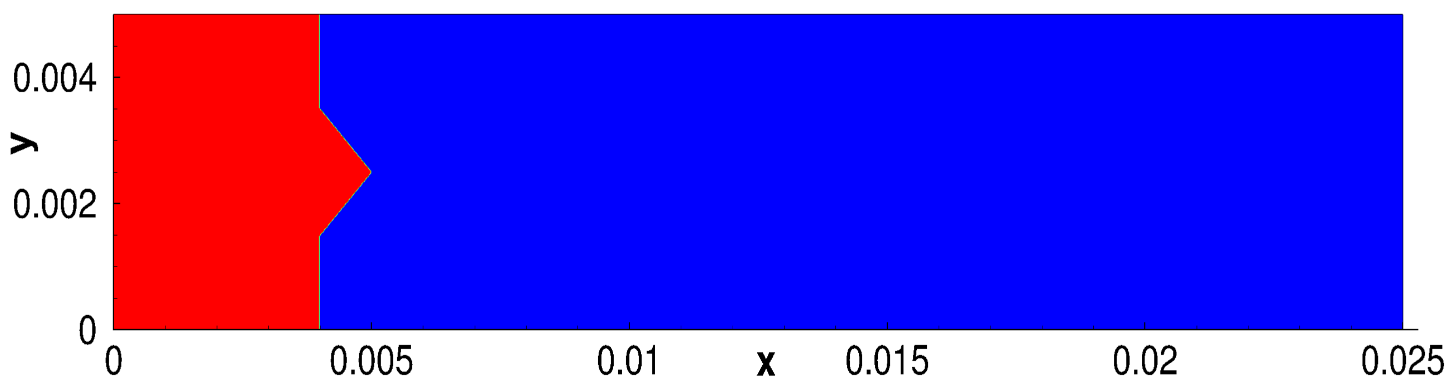
Note: CFL limit based on the convection part of PDEs

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

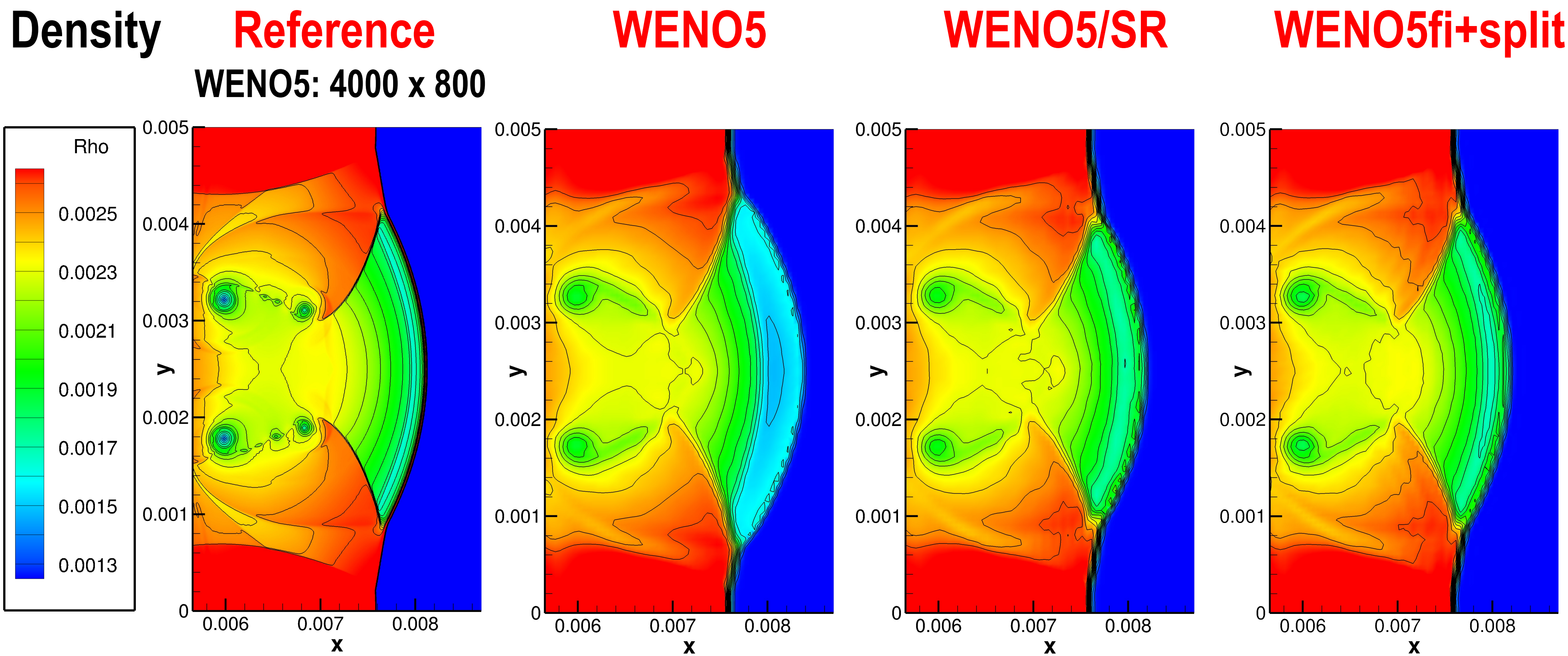
Heat release $q_0 = 0.5196\cdot 10^{10}$

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)

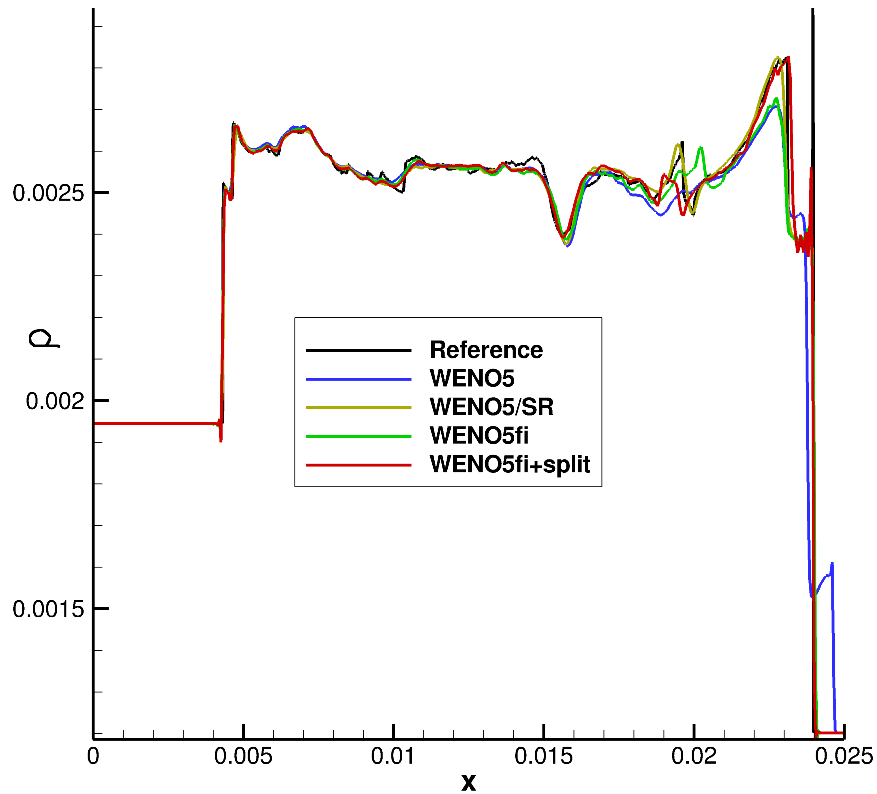
Comparison (WENO5,WENO5/SR,WENO5fi+split)

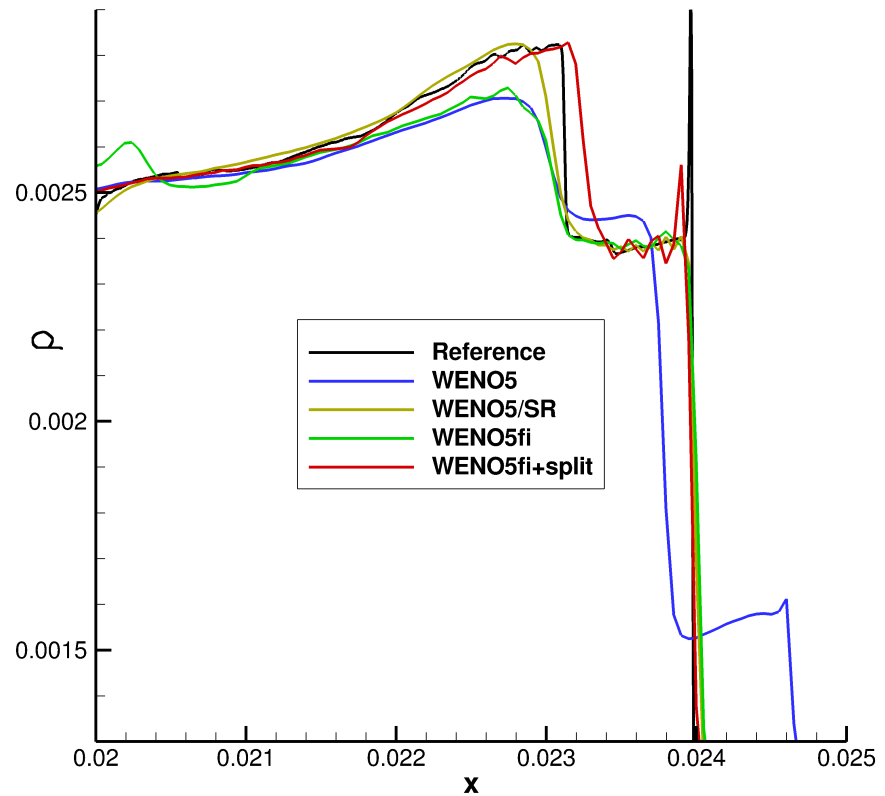


2D Detonation, 500x100 pts

WENO5,WENO5/SR,WENO5fi,WENO5fi+split

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





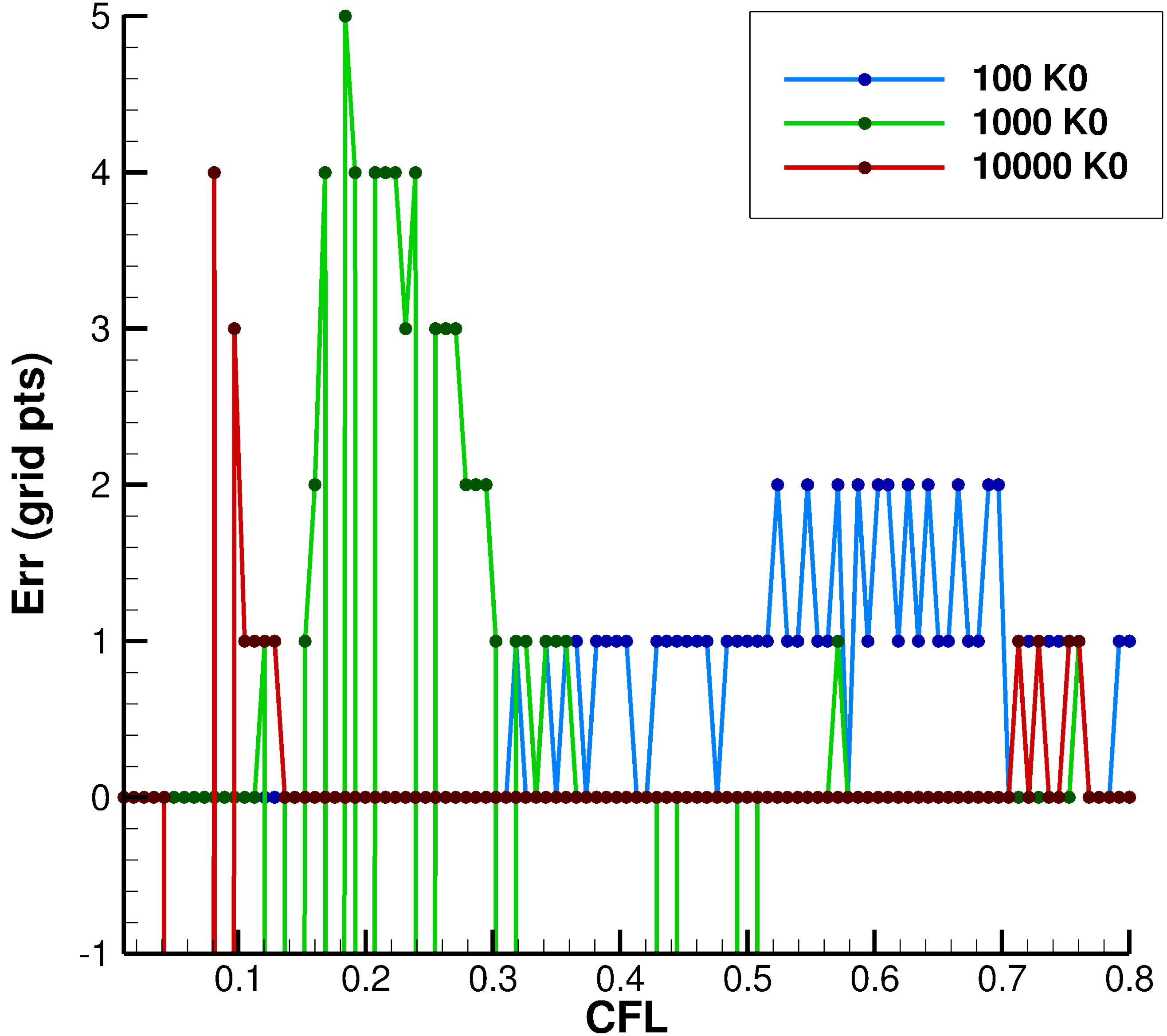
Zoom

Note: Wrong shock speed by WENO5fi using 200x40 pts

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)

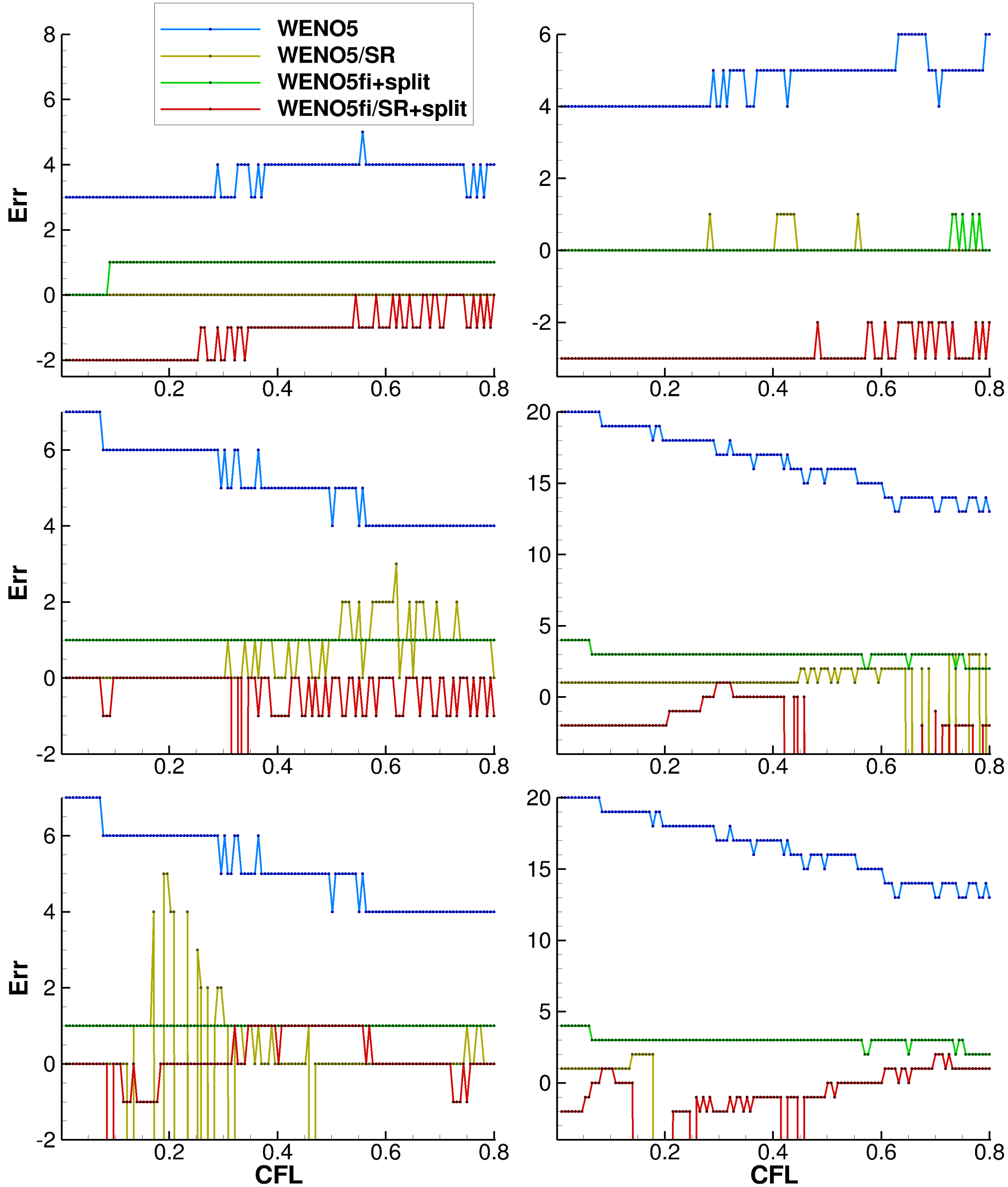
2D Detonation

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

Scheme Performance (8 Procs.)

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

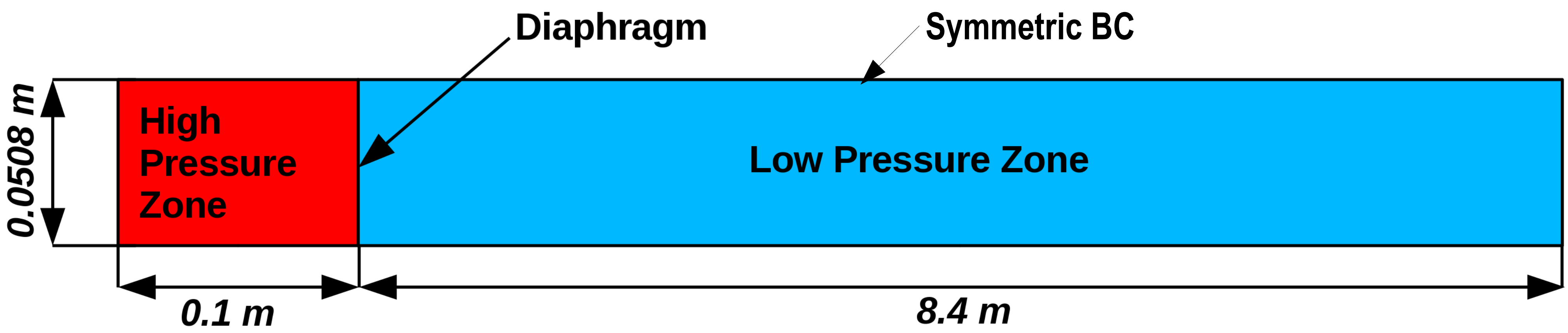
	WENO5	WENO5/SR	WENO5fi+split	WENO5fi/SR+split
CPU eff, iterations/sec	630	610	1720	1590
Discontinuity location error (grid points)	10	0	0	-3

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

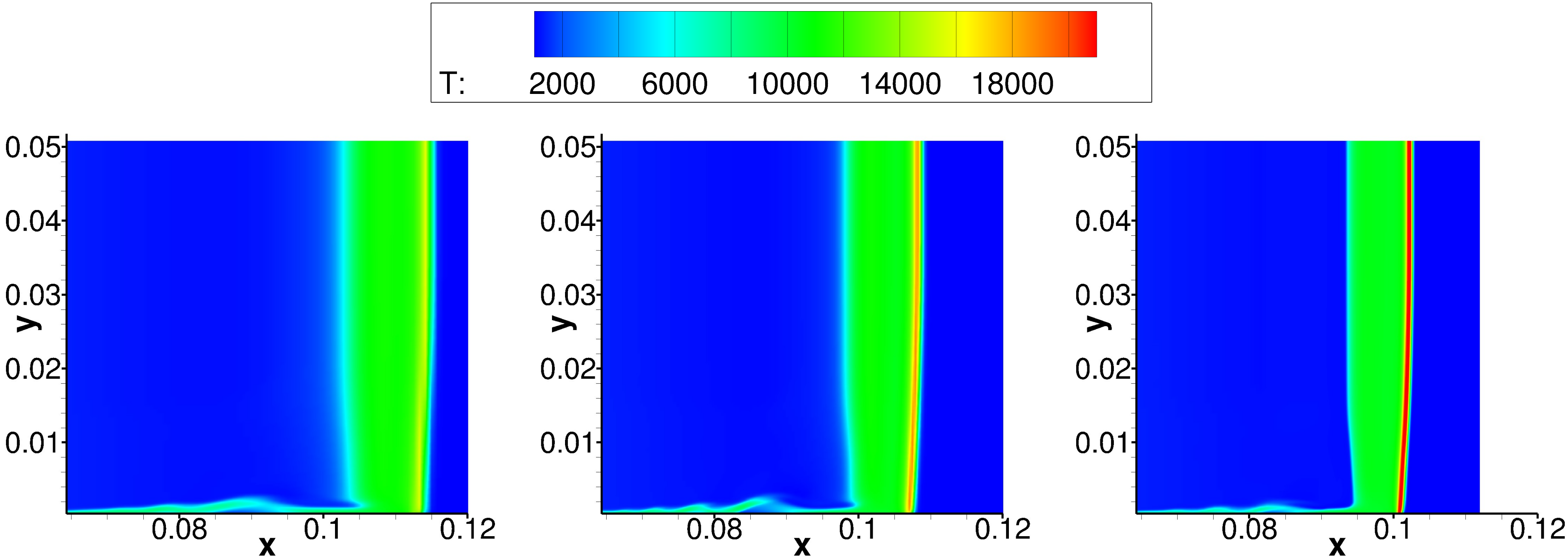
Low Pressure Zone

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 in x	Uniform in x	Cluster near shock in x
Tmax = 15,800 K	Tmax = 18,800 K	Tmax = 21,700 K

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

Concluding Remarks & Future Plans

- **Studies show the danger in practical simulations for the subject flow without better knowledge of scheme behavior**

  Added Issues not addressed:
  Pointwise evaluation of source terms, Roe average state & ODE solvers

- **Containment of numerical dissipation on schemes can delay the onset of wrong propagation speed**

  > *WENO5/SR performs better than WENO5fi+split & WENO5fi/SR+split*

  > *For turbulence with strong shocks WENO5fi+split & WENO5fi/SR+split provide better dissipation control for turbulence*

Future Plans

- **Non-pointwise evaluation of source terms**
- **Correct spurious oscillation near discontinuities due to standard Roe average state**
- **Stiff ODE solver with adaptive error control to alleviate temporal stiffness** *(interfere with the subcell resolution step)*

Note: Spurious numerics due to spatial discretization is more difficult to contain

Thank you!

References

- Bao, W. & Jin, S. 2001 The random projection method for stiff detonation capturing. SIAM J. Sci. Comput. Vol. 23, No. 3, 1000–10026.
- B.Sjögreen & H.C.Yee 2009 Variable high order multiblock overlapping grid methods for mixed steady and unsteady multiscale viscous flows. Commun. Comput. Phys. 5, 730–744.
- Chorin, A. 1976 Random choice solution of hyperbolic systems. J. Comput. Phys. 22, 517-533.
- Ducros, F., Laporte, F., Soul`eres, T., Guinot, V., Moinat, P. & Caruelle, B. 2000 High-order fluxes for conservative skew-symmetric-like schemes in structured meshes: Application to compressible flows. J. Comp. Phys. 161, 114–139. Harten, A. 1989 Eno schemes with subcell resolution. J. Comp. Phys. 83, 148–184.
- Helzel, C., LeVeque, R. & Warneke, G. 1999 A modified fractional step method for the accurate approximation of detonation waves. SIAM J. Sci. Stat. Comp. 22, 1489–1510.
- Kailasanath, K., Oran, E., Boris, J. & Young, T. 1985 Determination of detonation cell size and the role of transverse waves in two-dimensional detonations. Combust. Flame 61, 199–209.
- LeVeque, R. & Yee, H. 1990 A study of numerical methods for hyperbolic conservation laws with stiff source terms. J. Comp. Phys. 86, 187–210.
- Olsson, P. & Oliger, J. 1994 Energy and maximum norm estimates for nonlinear conservation laws. Tech. Rep. 94.01. RIACS.

References

- Shu, C.-W. & Osher, S. 1989 Efficient implementation of essentially non-oscillatory shock-capturing schemes, ii. J. Comp. Phys. 83, 32–78.
- Sjögreen, B. & Yee, H. 2009 On skew-symmetric splitting and entropy conservation schemes for the euler equations. In Proceedings of the 8th European Conference on Numerical Mathematics & Advanced Applications (ENUMATH 2009). Uppsala University, Uppsala, Sweden.
- Sjögreen, B. & Yee, H. C. 2004 Multiresolution wavelet based adaptive numerical dissipation control for shock-turbulence computation. J. Scient. Computing 20, 211–255.
- Strang, G. 1968 On the construction and comparison of difference schemes. SIAM J.Numer. Anal. 5, 506–517.
- Tosatto, L. & Vigevano, L. 2008 Numerical solution of under-resolved detonations. J. Comp. Phys. 227, 2317–2343.
- Wang, W., Shu, C., Yee, H. & Sjögreen, B. 2012 High order finite difference methods with subcell resolution for advection equations with stiff source terms. J. Comput. Phys. 231, 190–214.
- Wang, W., Yee, H., Sjögreen, B., Magin, T. & Shu, C. 2011 Construction of low dissipative high-order well-balanced filter schemes for nonequilibrium flows. J. Comput. Phys. 230, 4316–4335.
- Yee, H. & Sjögreen, B. 2007 Development of low dissipative high order filter schemes for multiscale navier-stokes/mhd systems. J. Comput. Phys. 225, 910–934.

References

- Yee, H., Sandham, N. & Djomehri, M. 1999a Low dissipative high order shockcapturing methods using characteristic-based filters. J. Comput. Phys. 150, 199–238.
- Yee, H. & Sjögreen, B. 2010 High order filter methods for wide range of compressible flow speeds. Proceedings of ICOSAHOM 09 (International Conference on Spectral and High Order Methods). June 22-26, 2009, Trondheim, Norway
- Yee, H. & Sjögreen, B. 2011 Local flow sensors in controlling numerical dissipations for a wide spectrum of flow speed and shock strength. In preparation.
- Yee, H., Sjögreen, B., Shu, C., Wang, W., Magin, T. & Hadjadj, A. 2011 On numerical methods for hypersonic turbulent flows. In Proceedings of ESA 7th Aerothermodynamics Symposium. Site Oud Sint-Jan, Brugge, Belgium.
- Yee, H. & Sweby, P. 1997 Dynamics of numerics & spurious behaviors in cfd computations. In Keynote paper, 7th ISCFD Conference. Beijing, China, rIACS Technical Report 97.06, June 1997.
- Yee, H., Torczynski, J., Morton, S., Visbal, M. & Sweby, P. 1999b On spurious behavior of cfd simulations. Int. J. Num. Meth. Fluids 30, 675–711.
- Yee, H., Vinokur, M. & Djomehri, M. 2000 Entropy splitting and numerical dissipation. J. Comput. Phys. 162, 33–81.
- H.C. Yee, P.K. Sweby & D.F. Griffiths, 1990 Dynamical Approach Study of Spurious Steady-State Numerical Solutions for Nonlinear Differential Equations, Part I: The Dynamics of Time Discretizations and Its Implications for Algorithm Development in Computational Fluid Dynamics. NASA TM-102820, April 1990; J. Comput. Phys., 97 (1991) 249-310.

EAST Problem. Governing equations

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

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

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

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

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

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

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

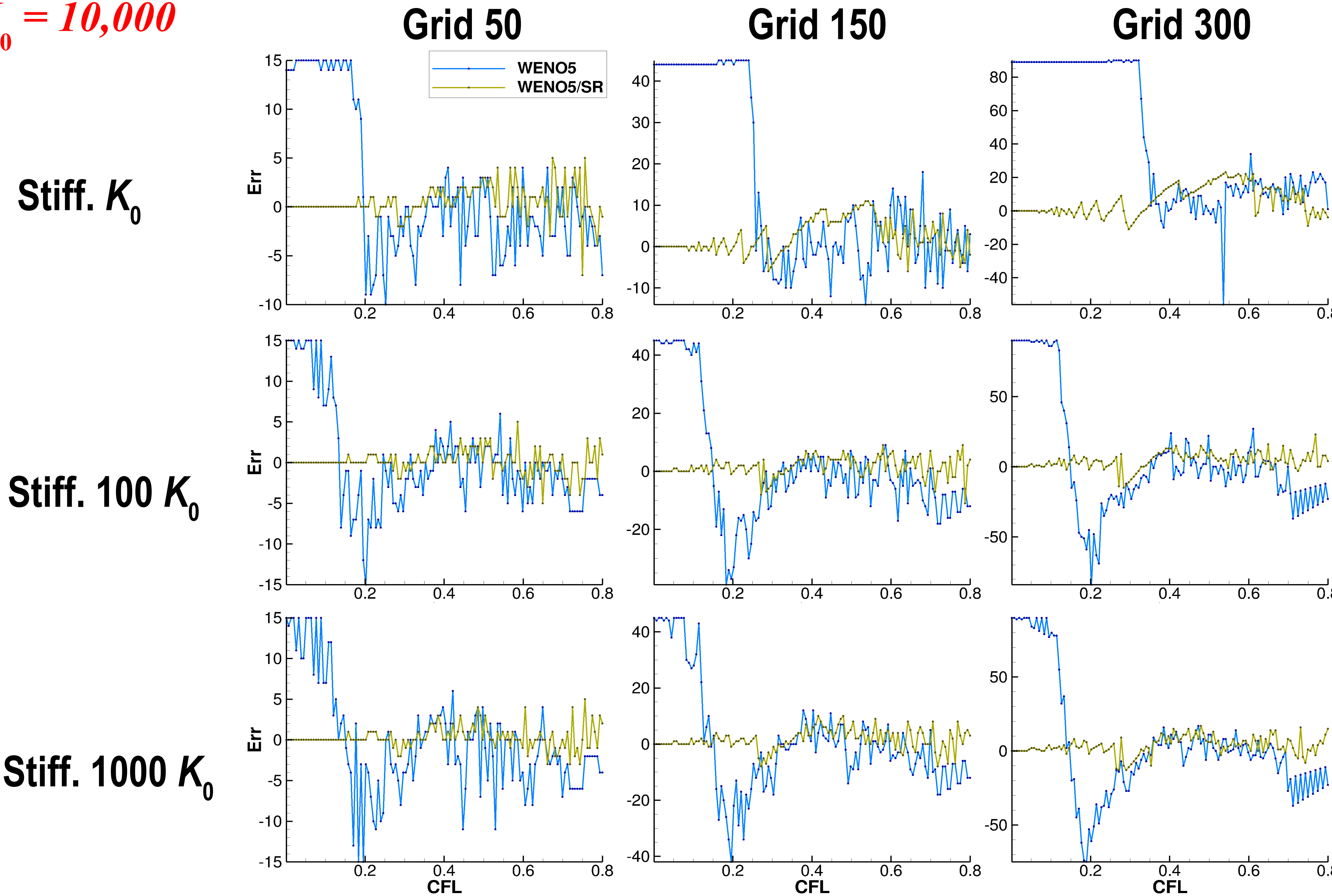
Scalar Case Behavior of WENO5 & WENO5/SR below CFL limit

(Obtaining the Correct Discontinuity Speed)

Source term:

$S = K_0(1\text{-}u)(u\text{-}0.5)u$

$K_0 = 10{,}000$



Note: CFL limit based on the convection part of PDE

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

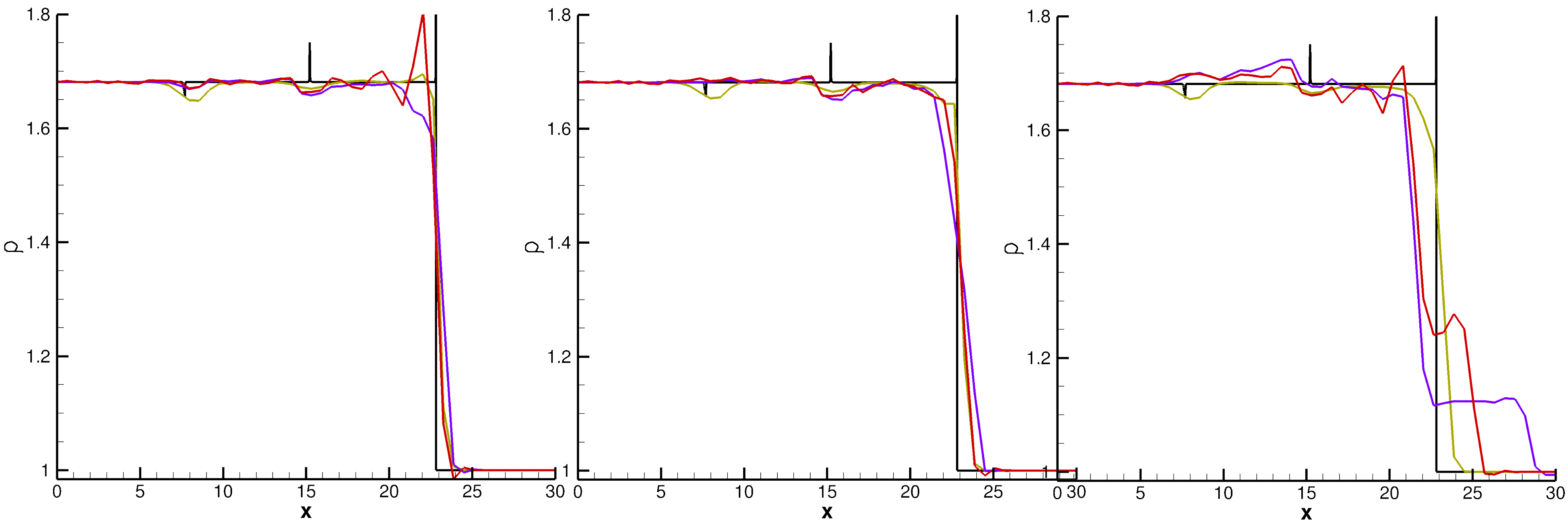
R – Reaction operator

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

1D C-J Detonation: Stiffness Dependence

$K_0 = 16418$ **10** K_0 **100** K_0



WENO5/SR: WENO5 + subcell resolution

WENO5fi+split: $\kappa = 0.4$

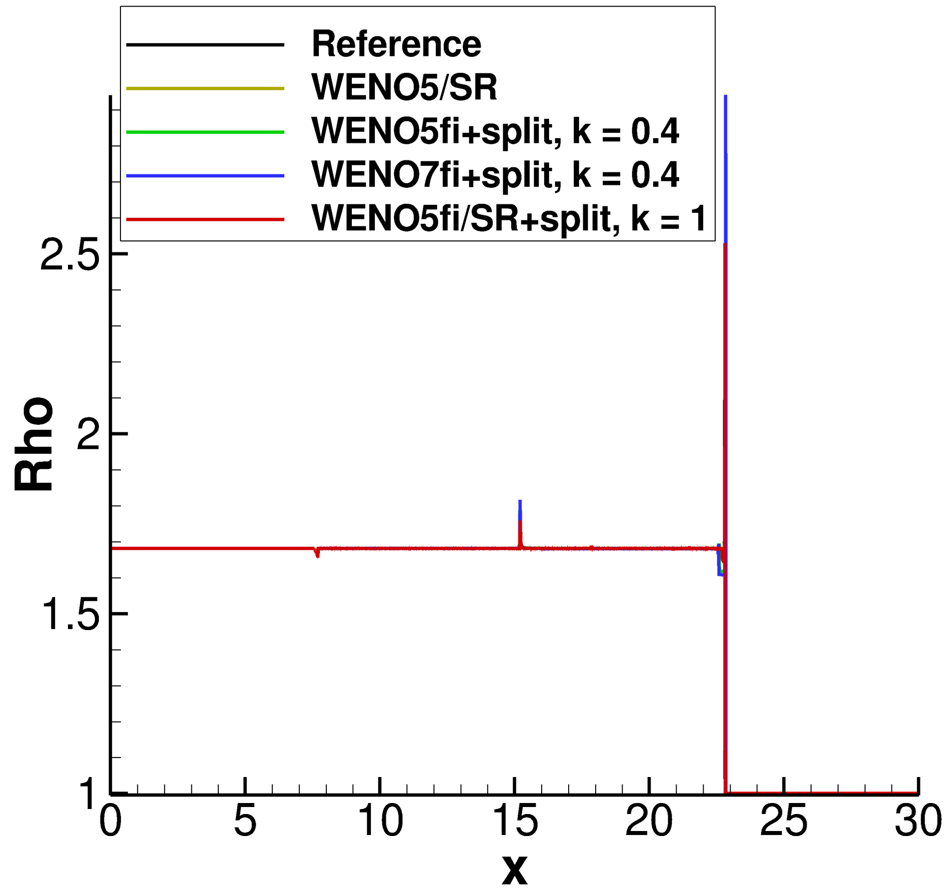
WENO5fi+split: $\kappa = \kappa_0 f(M)$

Reference – WENO5, grid 10,000

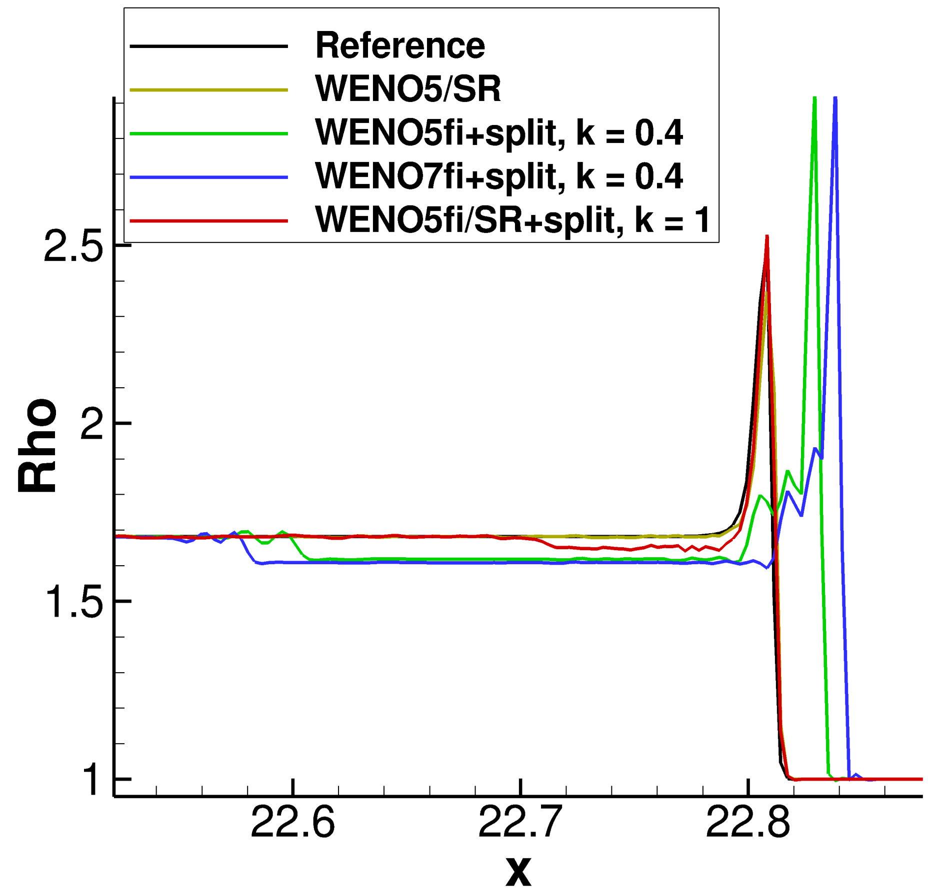
1D C-J Detonation (grid 10,000)

Grid Refinement Study

Density

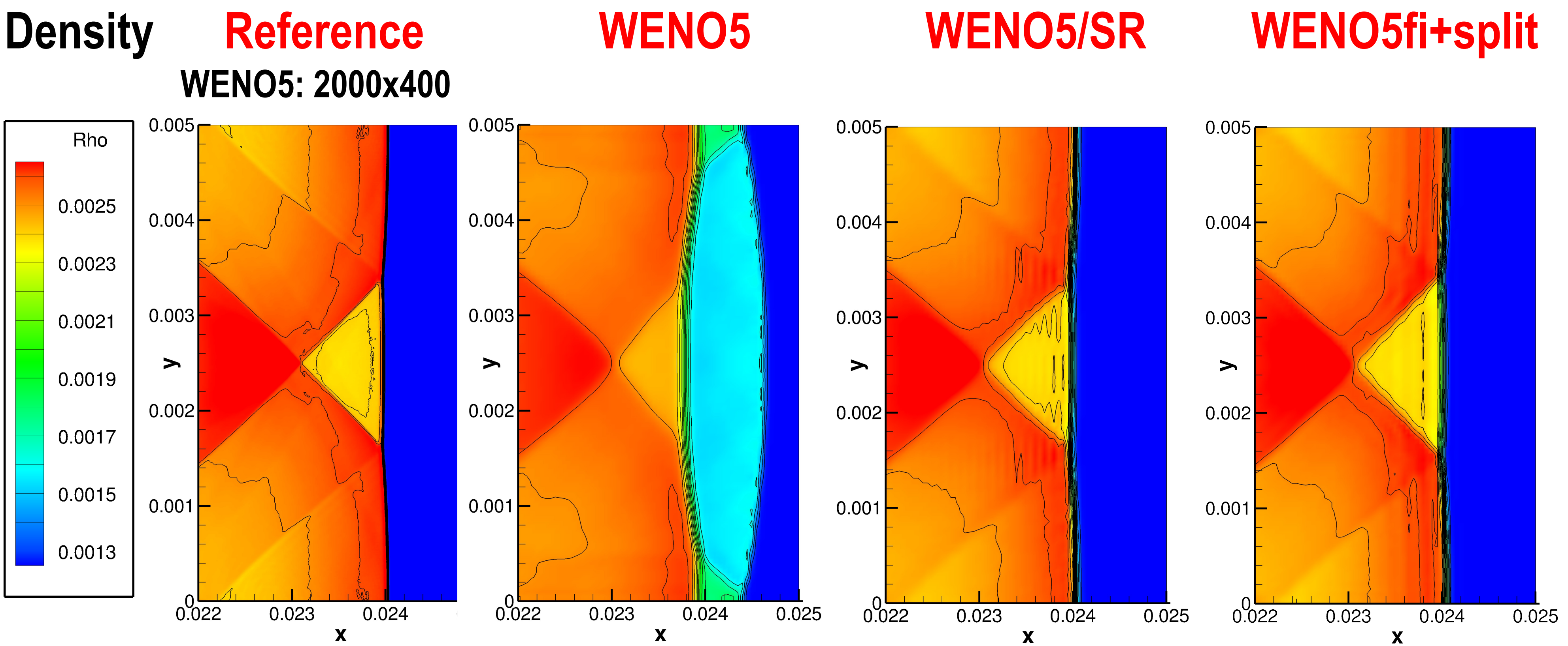


Density Zoom



2D Detonation, t=1.7e-7 s (500x100 pts)

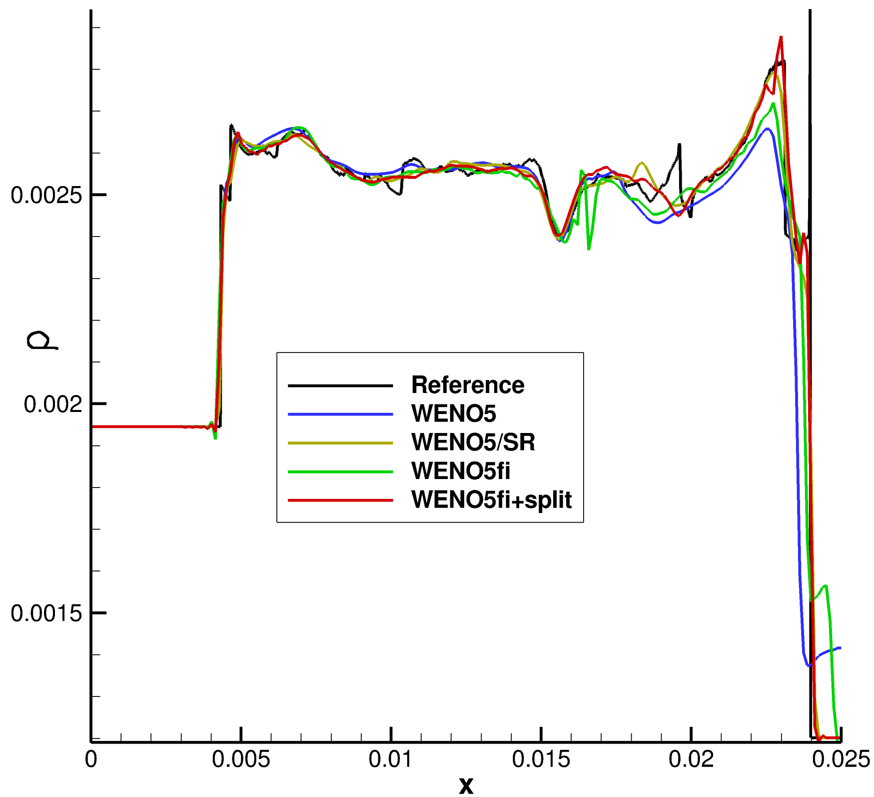
Comparison (WENO5,WENO5/SR,WENO5fi+split)

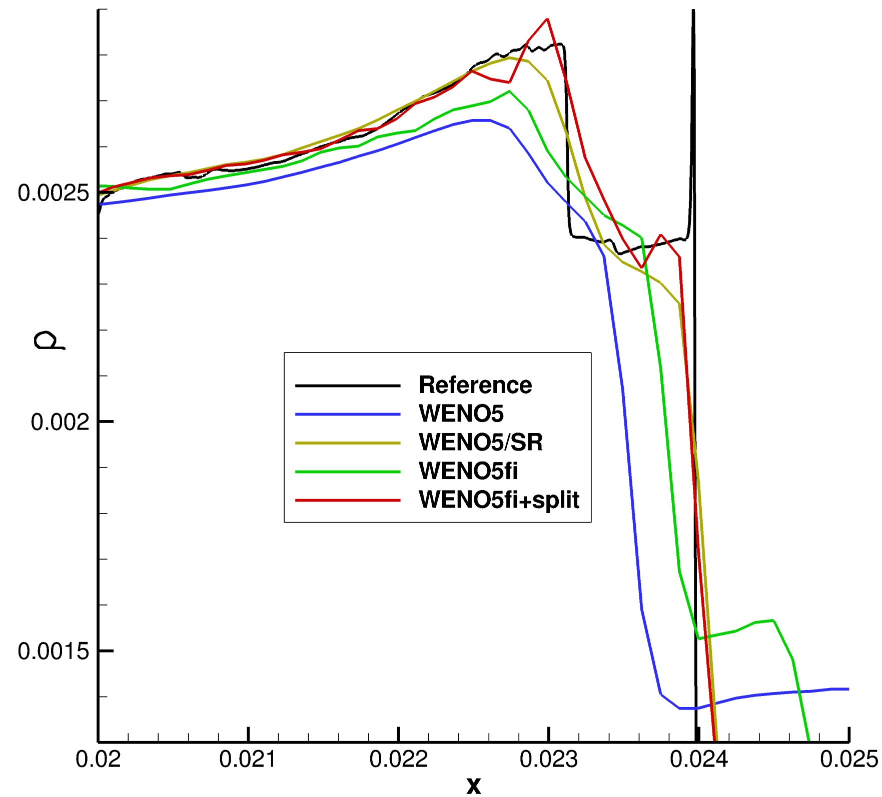


2D Detonation, 200x40 pts

WENO5,WENO5/SR,WENO5fi,WENO5fi+split

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



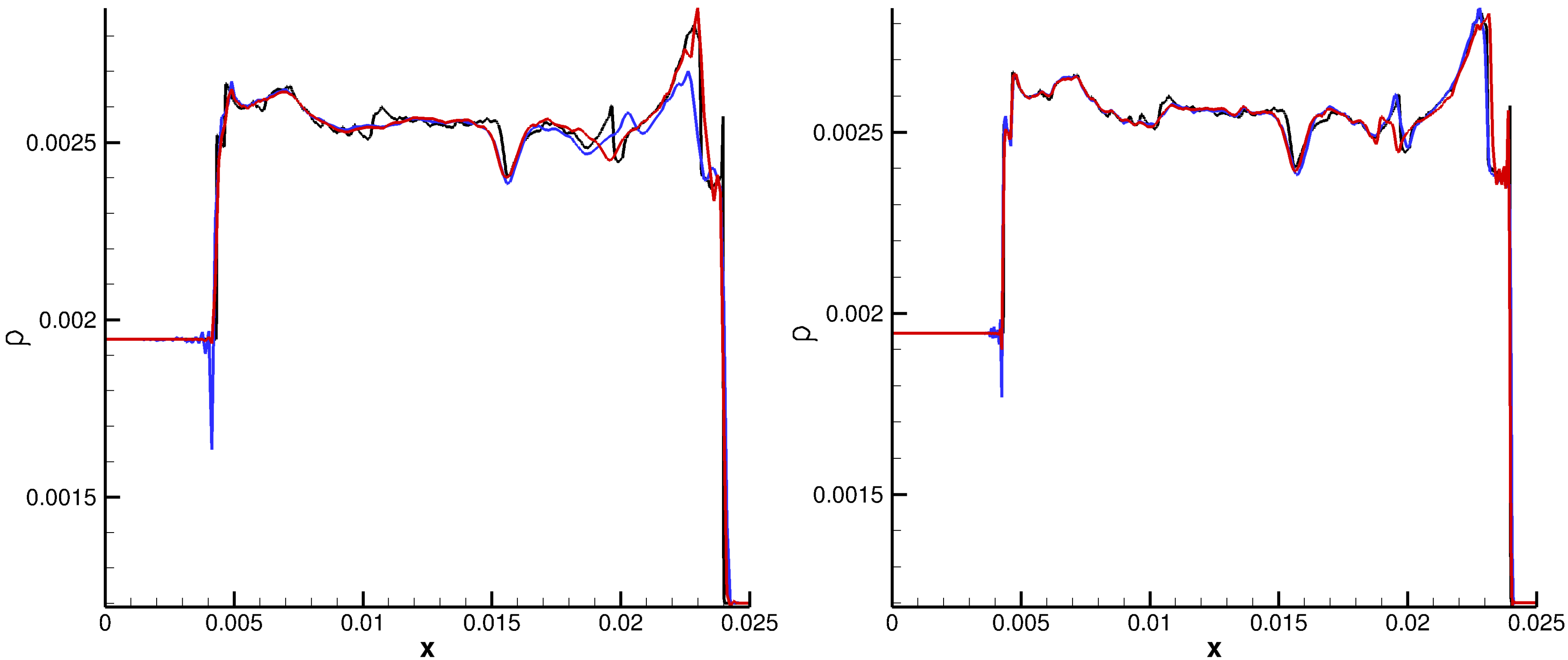


Zoom

Global vs Local $\kappa_{j+1/2}^{m}$ of Filter Scheme

(Controlling Amount of Numerical Dissipation)

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



200x40 **500x100**

WENO5fi+split, κ = *const*

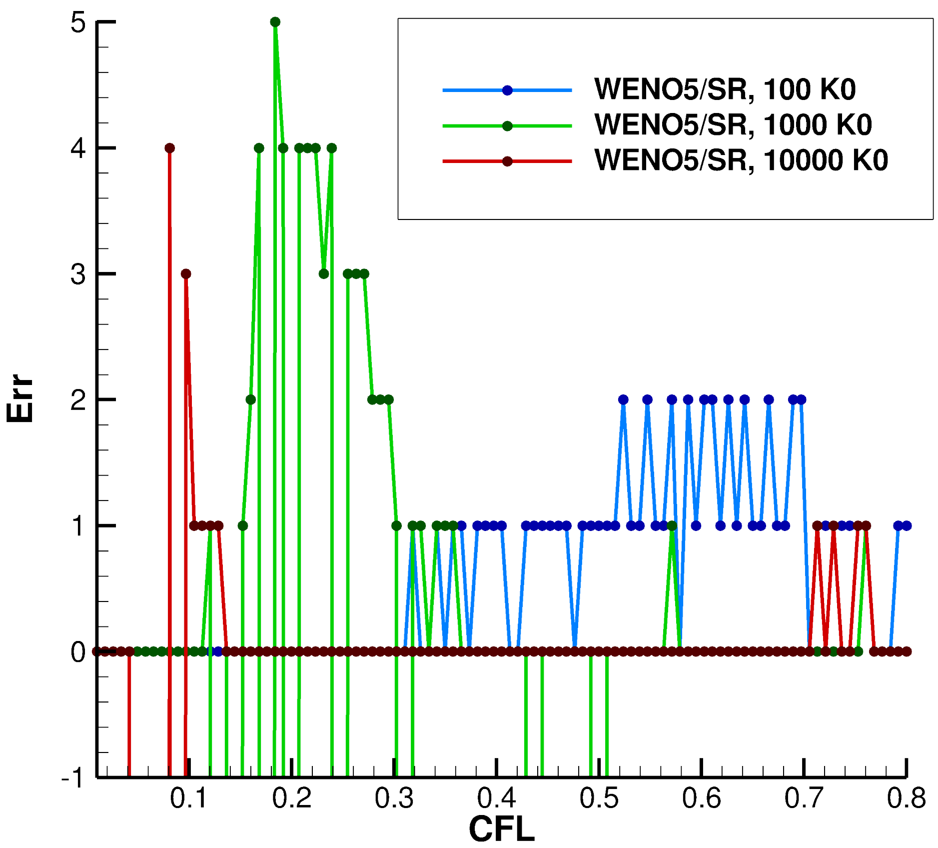
WENO5fi+split, $\kappa = \kappa_0 f(M)$

Behavior of the schemes below CFL limit

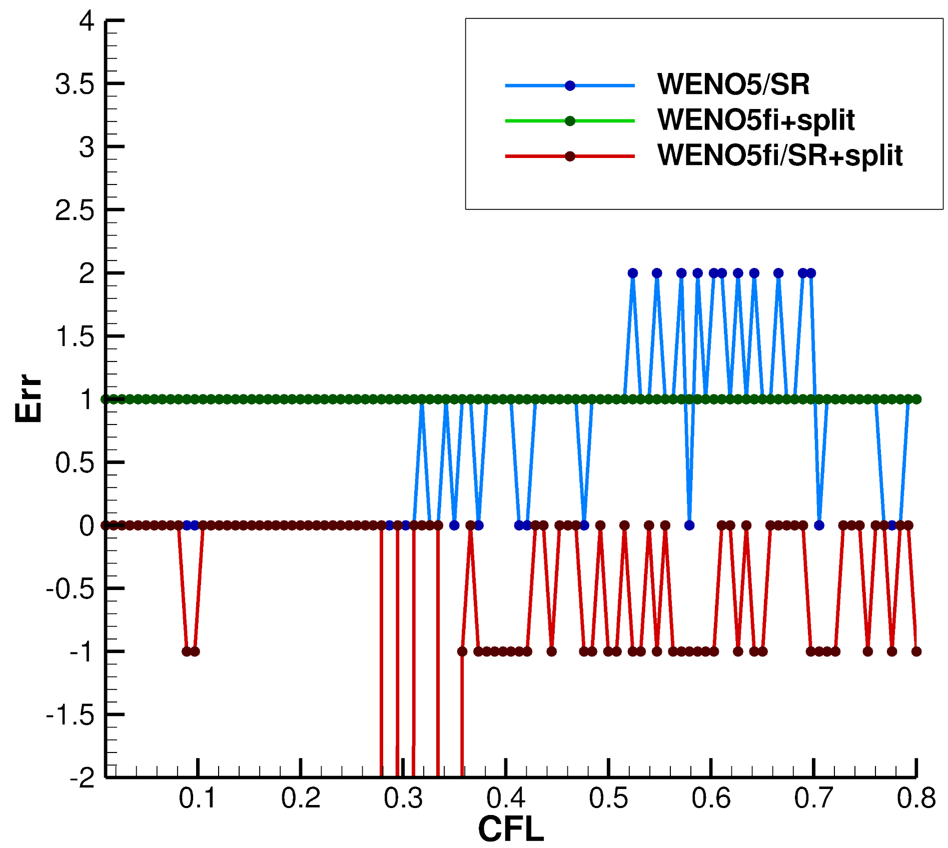
(Obtaining correct shock speed)

2D Detonation, 200x40 pts

WENO5/SR, 3 stiff. coeff.



100 K_0



ADPDIS3D Solver

(Solver for Present Study, Sjögreen, Yee & Collaborators)

- Features
  - Fortran/C (core solver), C++ (high level API, IO)
  - Single-block and Overset Grids
  - Variable High Order Overset Finite Difference Methods
  - Parallel IO
- Computational kernels
  - Navier-Stokes (DNS & LES)
  - Magneto Hydro Dynamics
  - Chemically Reactive Non-equilibrium Flows & Combustion