High-fidelity Simulation of High Speed Multi-component Flows

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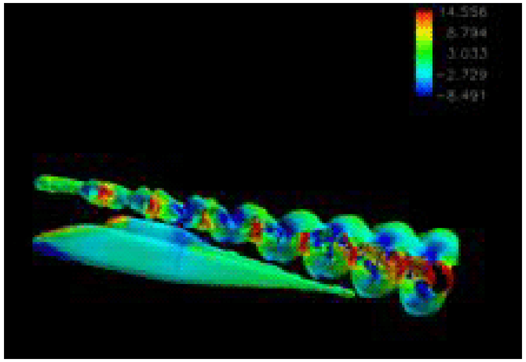
Flow Structures in Compressible Multi-component Flows

Smooth Solutions

1. Acoustic Waves
2. Turbulence
3. Vortex Dominated Flow
4. Rarefaction Fan



Vortex-dominated flow near helicopter (Advanced Dynamics Inc.)

F/A18-F in transonic flight (NASA Gallery)

Discontinuous Solutions

1. Shock Waves
2. Contact Discontinuities
3. Material Interfaces
4. Detonation Front

Difficulties in Designing Numerical Schemes in FVM

Smooth Solutions

High Order Schemes based on unlimited polynomials:

1. High-order polynomials
2. Optimized polynomials
3. Compact schemes

Sufficient

Difficulties in Designing Numerical Schemes in FVM

Discontinuous Solutions → High Order Schemes equipped Limiting Processes

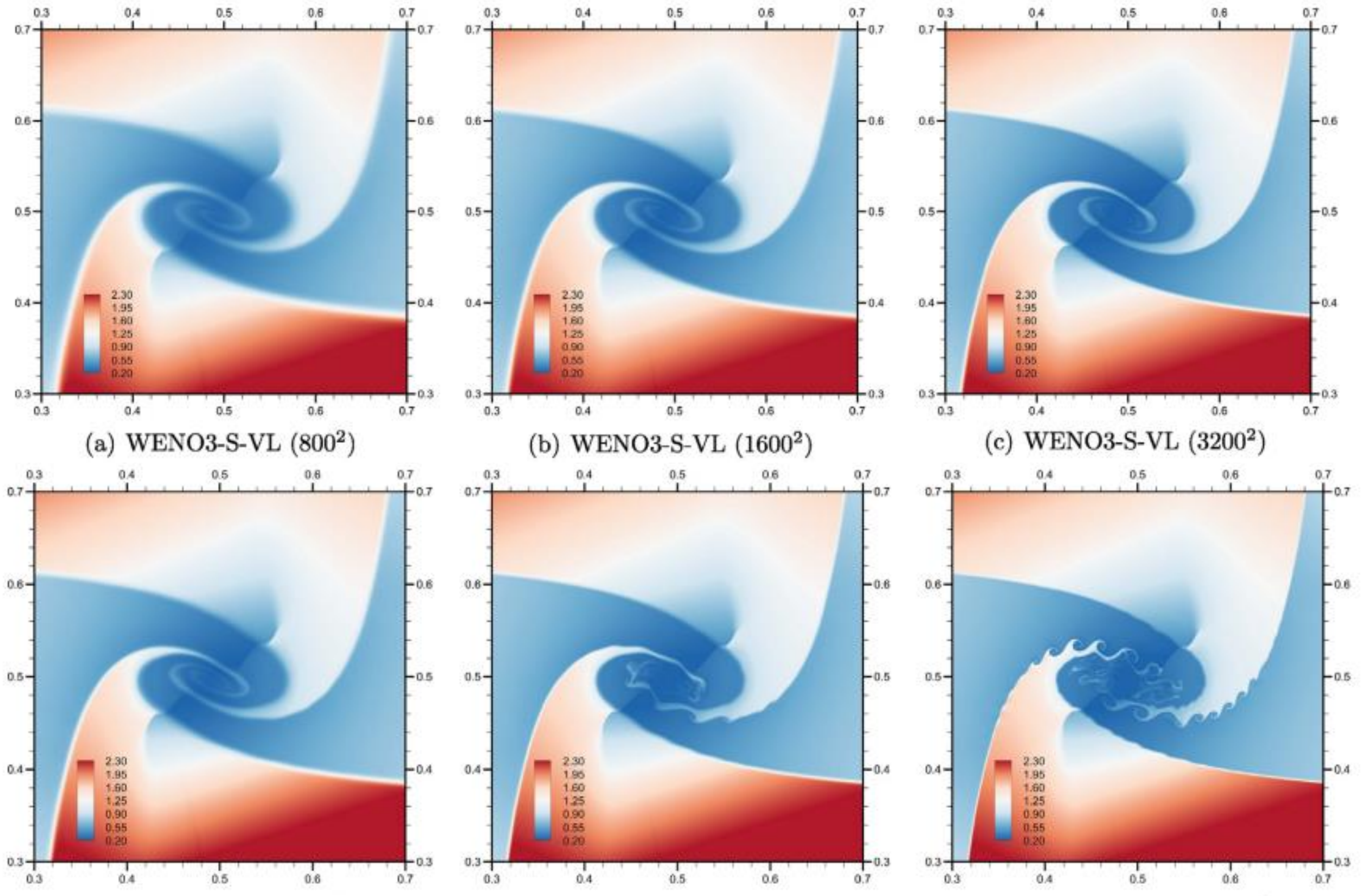
TVD ENO WENO WENOM WENOZ WENOCU TENO → years

Above schemes try to solve inbuilt paradox of current high order schemes

Numerical oscillations ⟷ Numerical dissipation

The so-called high order schemes fail in some cases

2D Riemann Problem: Kelvin-Helmholtz instability



(a) WENO3-S-VL (800^2)

(b) WENO3-S-VL (1600^2)

(c) WENO3-S-VL (3200^2)

(d) WENO5-S-VL (800^2)

(e) WENO5-S-VL (1600^2)

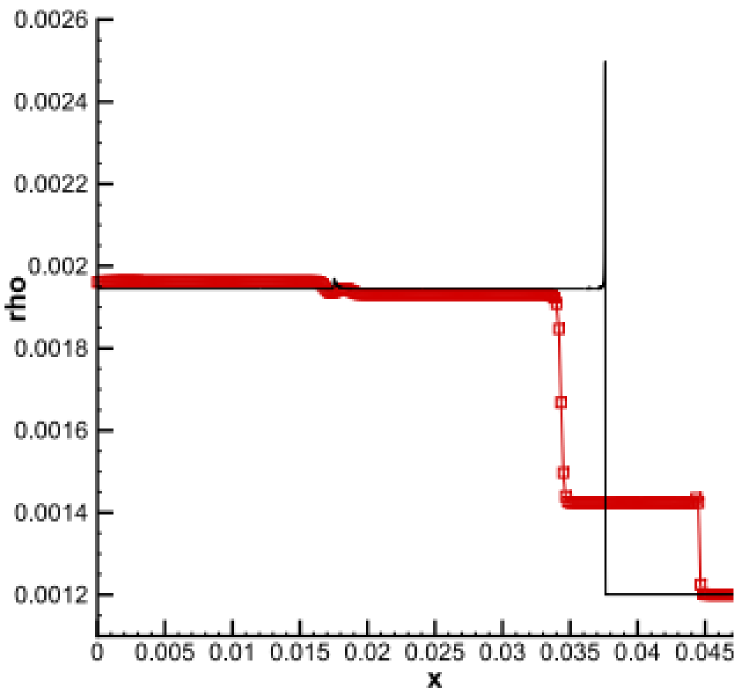
(f) WENO5-S-VL (3200^2)

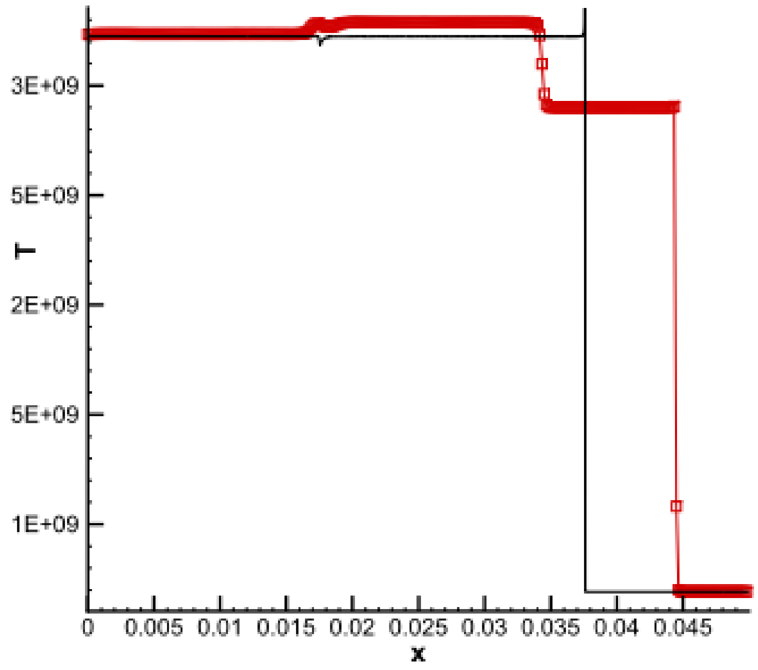
(San, *Computers & Fluids*, 2014)

The so-called high order schemes fail in some cases

Stiff *C-J* detonation waves

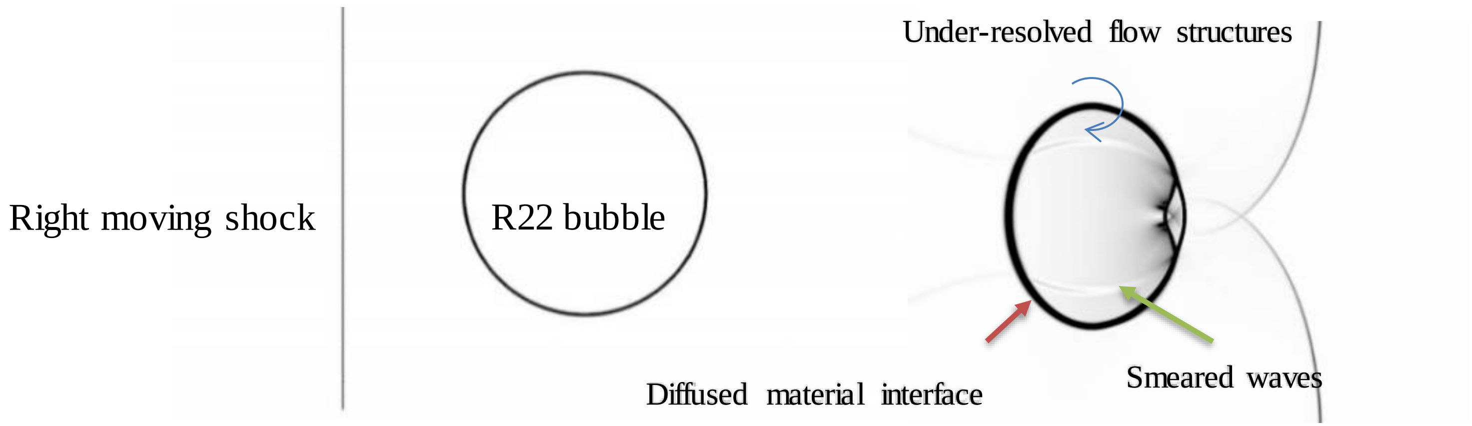
5th order WENO scheme





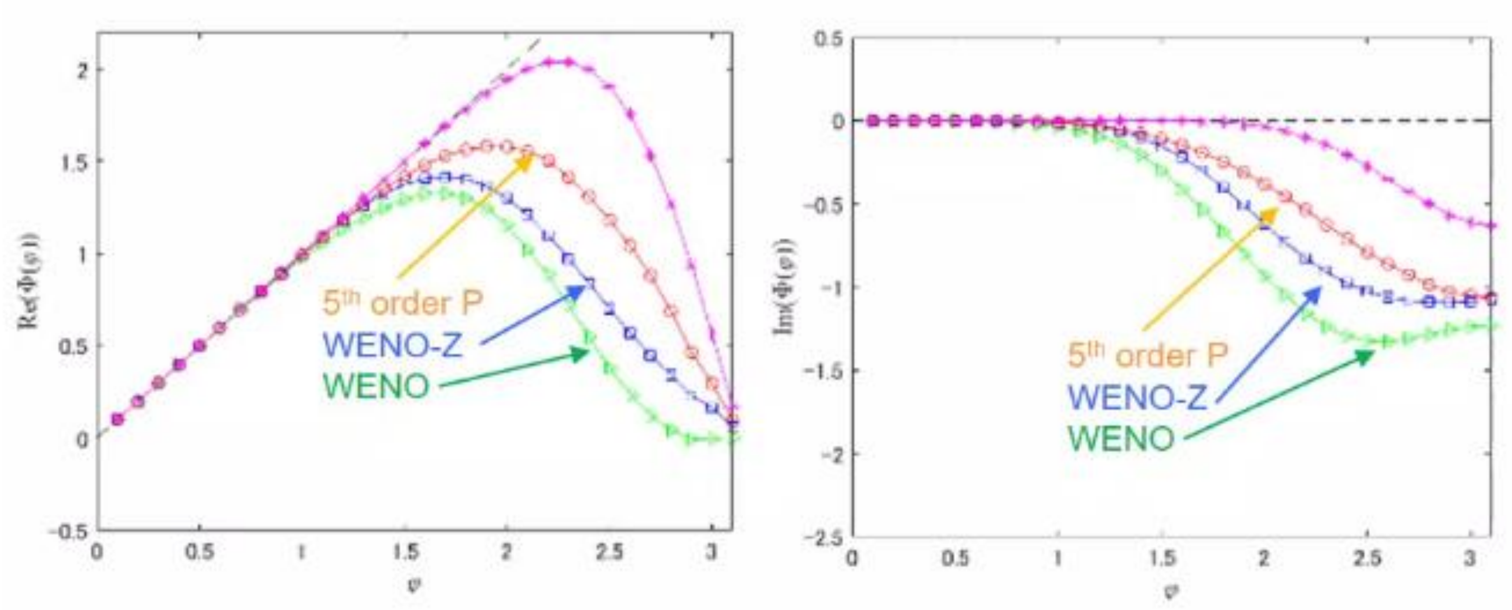
The so-called high order schemes fail in some cases

Shock-Bubble Interaction



The so-called high order schemes fail in some cases

Spectral Properties



The so-called high order schemes fail in some cases

- Fail to Resolve Discontinuous Solutions: Diffusive Interfaces, Under-resolved Flow Structures, Incorrect Wave Structures

- Fail to Preserve the Spectral Property of High Order Interpolation for Smooth Solutions.

Numerical Schemes For High-fidelity Simulations

- ➢ Less-diffusive and Less-oscillation for Discontinuous Solutions
- ➢ Retrieve the Spectral Property of High Order Interpolations

Finite Volume Method

From semi-discrete form

$$\frac{d\bar{u}_i}{dt} = -\frac{1}{\Delta x}\left(f\left(u(x_{i+\frac{1}{2}},t)\right) - f\left(u(x_{i-\frac{1}{2}},t)\right)\right)$$

to update $\bar{u}_i(t)$ from t^n to t^{n+1}

$$\bar{u}_i^{n+1} = \bar{u}_i^n - \frac{1}{\Delta x}\left(\int_{t^n}^{t^{n+1}} f\left(u(x_{i+\frac{1}{2}},t)\right)dt - \int_{t^n}^{t^{n+1}} f\left(u(x_{i-\frac{1}{2}},t)\right)dt\right)$$

Exact upto this point, but

how to calculate $\int_{t^n}^{t^{n+1}} f\left(u(x_{i+\frac{1}{2}},t)\right)dt$?

$\rightarrow$ Formulate the evolution of $u(x,t)$ at $x_{i+\frac{1}{2}}$

Approximation (Numerics)
- Find values at cell boundaries
- Determine the rule to evolve solution and flux
- Time stepping

Godunov Scheme

The central task

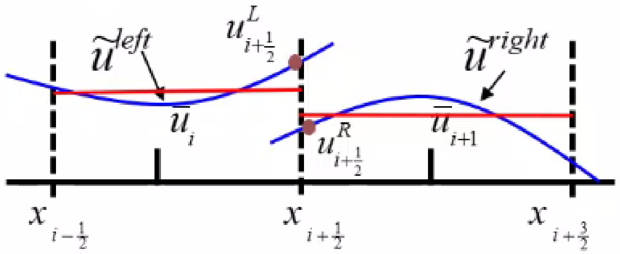
Compute numerical flux by Riemann solvers (a canonical form)

$$\hat{f}_{i+\frac{1}{2}} = \frac{1}{2}\left(f\left(u^L_{i+\frac{1}{2}}\right) + f\left(u^R_{i+\frac{1}{2}}\right)\right) - \underline{\frac{1}{2}\left|\alpha_{i+\frac{1}{2}}\right|\left(u^R_{i+\frac{1}{2}} - u^L_{i+\frac{1}{2}}\right)}$$

Efforts to improve solution quality have been made to

(1) <u>Reconstruction:</u>

find $u^L_{i+\frac{1}{2}}$ and $u^R_{i+\frac{1}{2}}$ from interpolations based on known DOFs



A jump between $u^L_{i+\frac{1}{2}}$ and $u^R_{i+\frac{1}{2}}$ inevitable to Godunov FVM

We focus on this

$\Rightarrow$ A key to determine accuracy and solution quality

(2) <u>Riemann solver (flux formulation):</u>

formulate $\alpha_{i+\frac{1}{2}}$ with desired properties

$\Rightarrow$ Flux vector spliting, Roe, HLL, HLLC, AUSM, GRP, GKS, . . .

Reconstruction Functions

Assume we know to some extent the structures of solution
Use the best suited reconstruction to fit solution structure

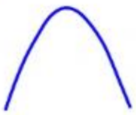
Solution structures(roughly) :

① Smooth solution →

② Discontinuous solution →

Reconstruction function:

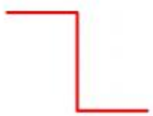
① Polynomial type



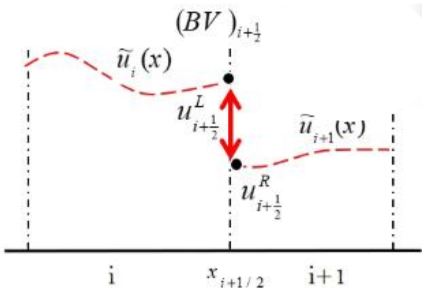
....

② Something else

(e.g. THINC)



Need an algorithm to decide which one to use



Revisit the Riemann solver

The Riemann solvers (a canonical form)

$$\hat{f}_{i+\frac{1}{2}} = \frac{1}{2}\left(f(u^L_{i+\frac{1}{2}}) + f(u^R_{i+\frac{1}{2}})\right) - \frac{1}{2}\left|\alpha_{i+\frac{1}{2}}\right|\left(u^R_{i+\frac{1}{2}} - u^L_{i+\frac{1}{2}}\right)$$

$\rightarrow (BV)_{i+\frac{1}{2}}$ Boundary Variation

Central scheme   Effective dissipation

$$\mapsto \frac{1}{2}\left|\alpha_{i+\frac{1}{2}}\right|(BV)_{i+\frac{1}{2}}$$

It suggests that minimizing BV effectively reduces numerical dissipation

BVD algorithm is to choose the reconstruction functions that can minimize the BV and fit the solution structures.

BVD Admissible Reconstruction Functions

- Pure (Taylor) high-order polynomial
- Optimized polynomials (Li et al, 2005, ...)
- Compact schemes (Fu et al, 1997, Ren et al, 2003,...)
- ...

Unlimited-polynomial
Group 1

- MUSCL scheme (van Leer, 1977,79)

  $\tilde{u}_i(x_{i\pm\frac{1}{2}}) = \bar{u}_i + \sigma_i(x_{i\pm\frac{1}{2}} - x_i)$
- ENO scheme (Harten et al. 1987)
- WENO scheme (Jiang & Shu, 1996,...)

  $\tilde{u}_i(x_{i\pm\frac{1}{2}}) = \sum_{k=0}^{K} \omega_k u^{(k)}_{i\pm\frac{1}{2}}$, ω_k: nonlinear weights
- WENO-Z, TENO,... schemes and others (Borges et al, 2008, Shen, Fu et al, 2017,...)
- ...

Group 2
Limited-polynomial

BVD Admissible Reconstruction Functions

- Hyperbolic(Marquina, 1994),
- Logarithmic(Artebrant & Schroll, 2006),
- Hyperbolic tangent (THINC scheme, Xiao et al, 2005, ...)

Group 3

Non-polynomial

THINC

$$\tilde{u}_i(x) = \bar{u}_{\min} + \frac{\bar{u}_{\max}}{2}\left(1 + \theta\ \tanh\left(\beta\left(\frac{x - x_{i-1/2}}{\Delta x_i} - \tilde{x}_i\right)\right)\right)$$

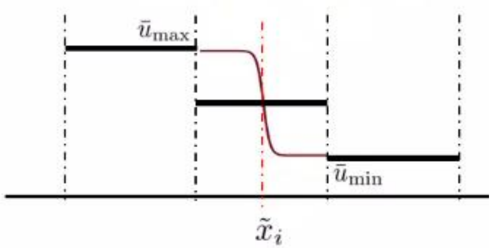
where $\bar{u}_{\min} = \min(\bar{u}_{i-1}, \bar{u}_{i+1})$, $\bar{u}_{\max} = \max(\bar{u}_{i-1}, \bar{u}_{i+1}) - \bar{u}_{\min}$

$\theta = \text{sgn}(\bar{q}_{i+1} - \bar{q}_{i-1})$, β: jump thickness

$\tilde{x}_i$: the location of the jump center, computed by

$$\frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{u}_i(x)dx = \bar{u}_i$$

THINC: a non-polynomial reconstruction



BVD Selecting Algorithm

BVD algorithm (TBV minimizing) example(1)

1. Prepare two BVD-admissible reconstructions, $\tilde{u}_i^{<1>}$ and $\tilde{u}_i^{<2>}$, with $\tilde{u}_i^{<1>}$ being higher order and $\tilde{u}_i^{<2>}$ more monotone;

2. Compute the TBVs of the target cell $\mathcal{I}_i$ using $\tilde{u}_i^{<\xi>}$ and $\tilde{u}_{i\pm1}^{<\xi>}$ for $\mathcal{I}_i$ and its two neighboring cells $(I_{i\pm1})$ with $<\xi>$ being $<1>$ and $<2>$ respectively,

$$\underline{TBV_i^{<1>} = |\tilde{u}_{i-1}^{<1>}(x_{i-\frac{1}{2}}) - \tilde{u}_i^{<1>}(x_{i-\frac{1}{2}})| + |\tilde{u}_i^{<1>}(x_{i+\frac{1}{2}}) - \tilde{u}_{i+1}^{<1>}(x_{i+\frac{1}{2}})|}$$

and

$$\underline{TBV_i^{<2>} = |\tilde{u}_{i-1}^{<2>}(x_{i-\frac{1}{2}}) - \tilde{u}_i^{<2>}(x_{i-\frac{1}{2}})| + |\tilde{u}_i^{<2>}(x_{i+\frac{1}{2}}) - \tilde{u}_{i+1}^{T}(x_{i+\frac{1}{2}})|.}$$

3. Given TBVs for both $\tilde{u}_i^{<1>}(x)$ and $\tilde{u}_i^{<2>}(x)$, $TBV_i^{<1>}$ and $TBV_i^{<2>}$, choose the reconstruction function for cell $\mathcal{I}_i$ by

$$\tilde{u}_i(x) = \begin{cases} \tilde{u}_i^{<2>} & \text{if } TBV_i^{<2>} < TBV_i^{<1>}, \\ \tilde{u}_i^{<1>} & \text{otherwise} \end{cases} .$$

Without any threshold

BVD algorithm (TBV minimizing) example(2)

Prepare K reconstruction functions $\hat{u}_i^{<k>}(x), k = 1, 2, \cdots K$

with different order and different monotonicity;

- $\tilde{u}_i^{<1>}(x) = \hat{u}_i^{<1>}(x)$
- for $(k = 2; k \leq K; k^{++})$

  $\{$

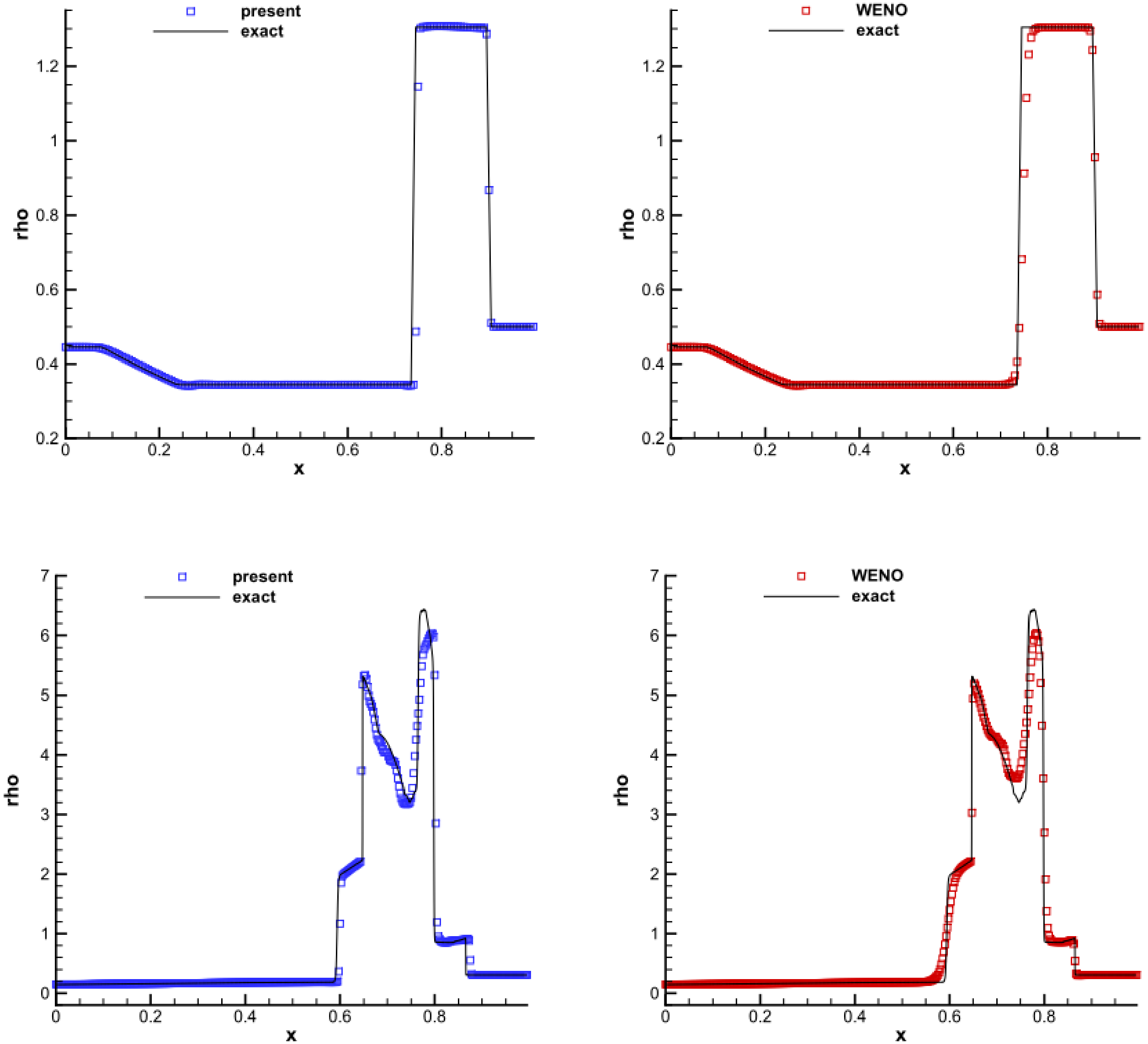
  $$\tilde{u}_i^{<k>}(x) = \mathcal{BVD}_k\left(\tilde{u}_i^{<k-1>}(x), \hat{u}_i^{<k>}(x)\right)$$

  $\}$
- $\tilde{u}_i(x) = \tilde{u}_i^{<K>}(x)$

Without any threshold

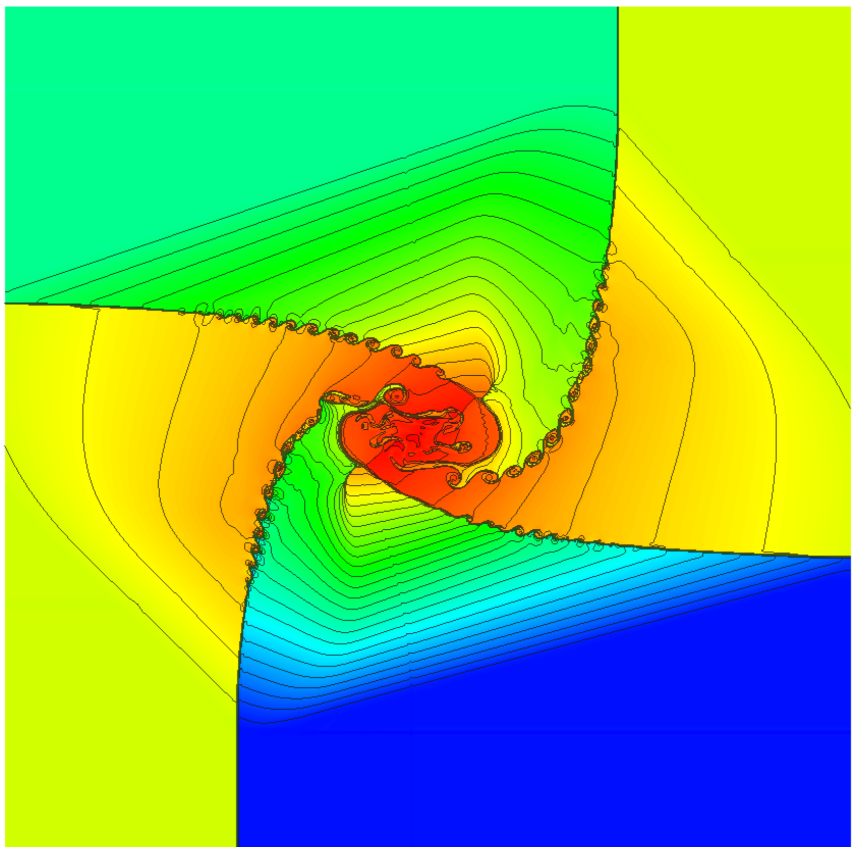
MUSCL-THINC-BVD

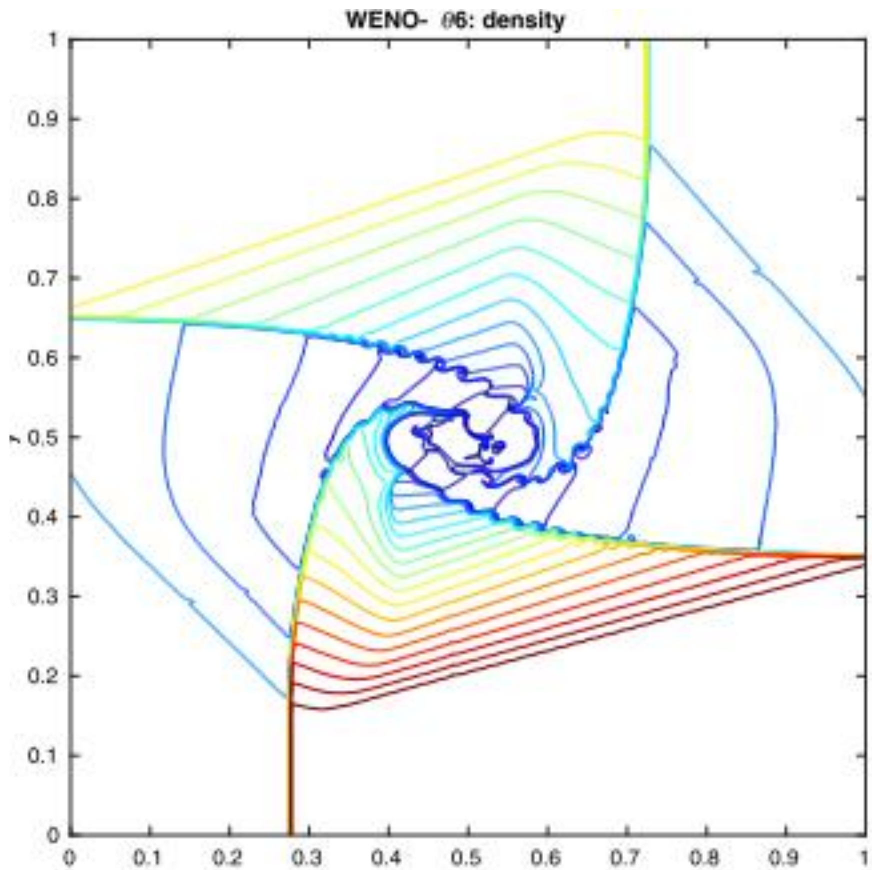
Shock-tube:



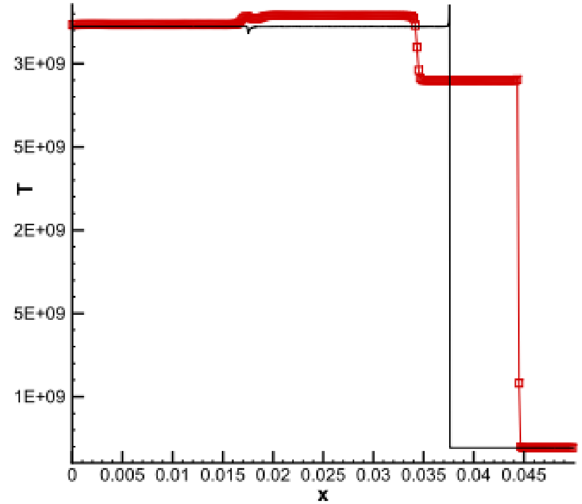
MUSCL-THINC-BVD

2D Riemann Problems:

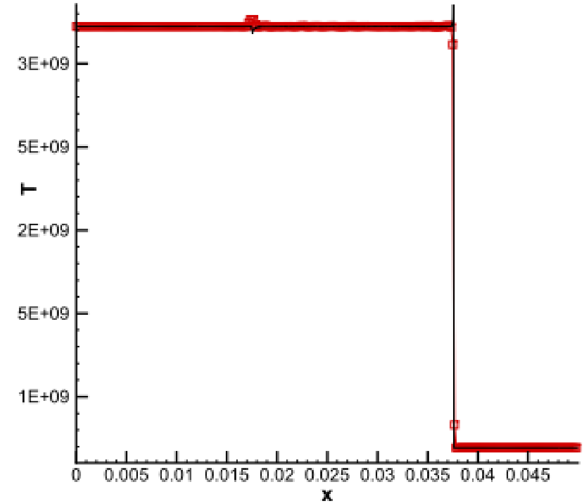




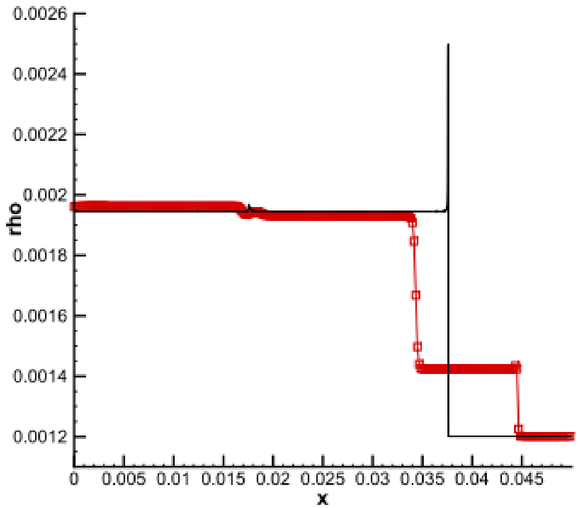
C-J detonation wave with the Heaviside model

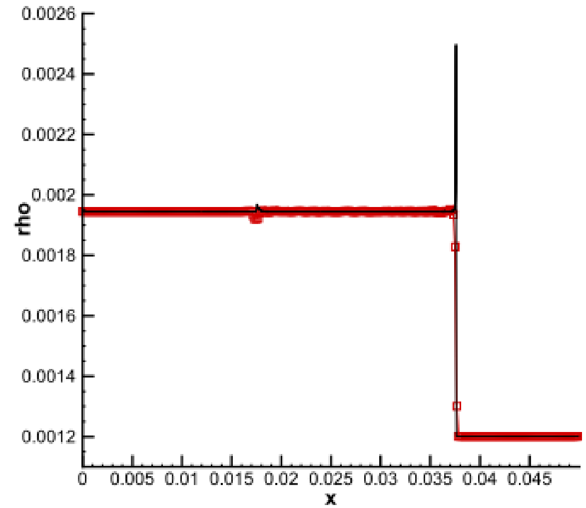


5th WENO

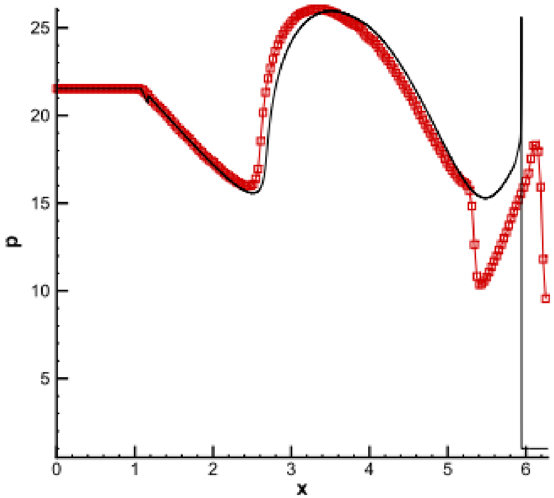


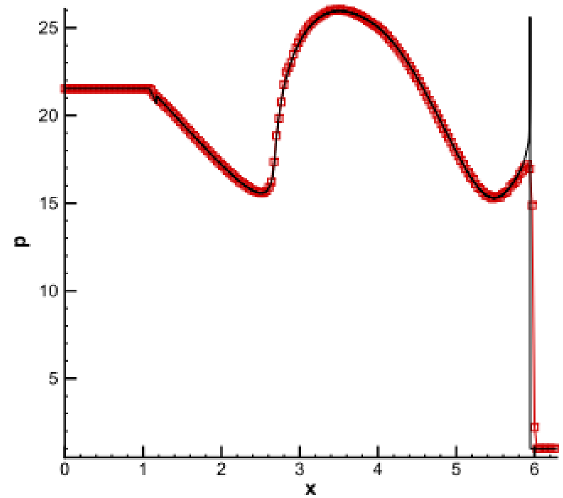
MUSCL-THINC-BVD





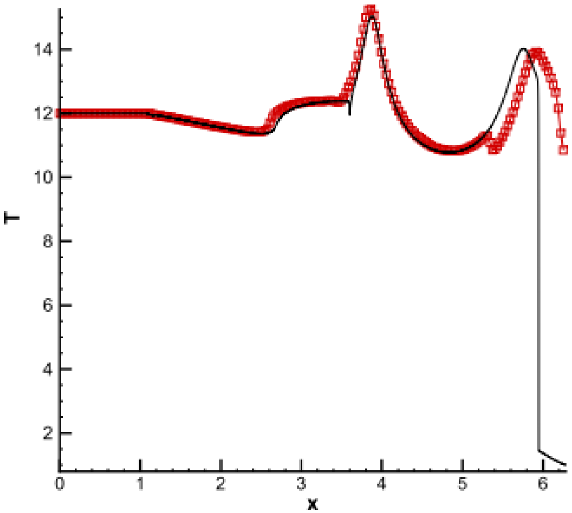
Interaction between a detonation wave and an oscillatory profile

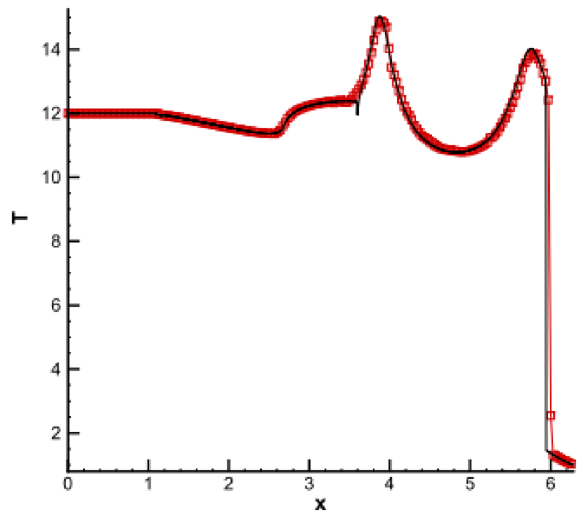




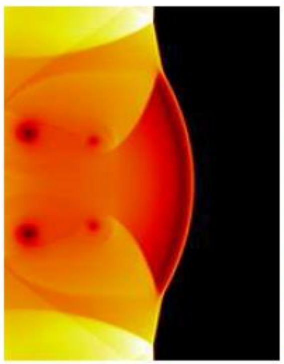
5th WENO

MUSCL-THINC-BVD

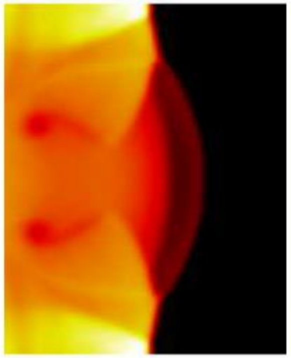




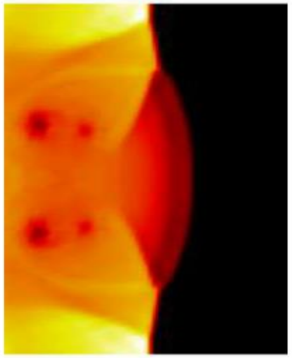
MUSCL-THINC-BVD



Reference

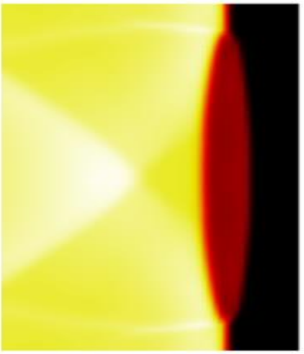


5^{th} WENO



MUSCL-THINC-BVD

Reference



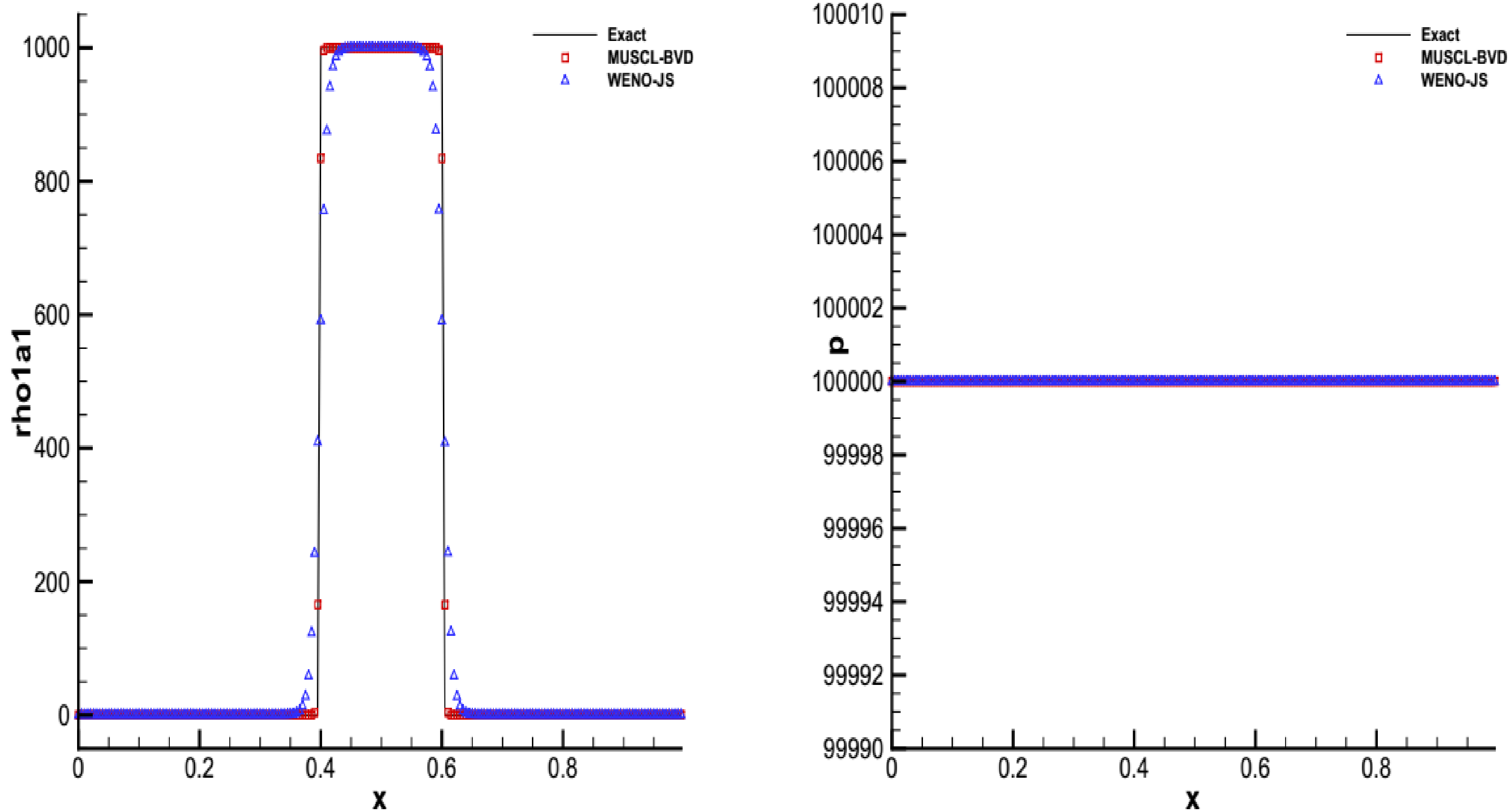
5^{th} WENO

MUSCL-THINC-BVD

MUSCL-THINC-BVD

Liquid-Gas Advection

Passive advection of a square liquid column with constant pressure and velocity while there is a jump about volume fraction and density



WENO-JS	9.90s
MUSCL-BVD	4.23s

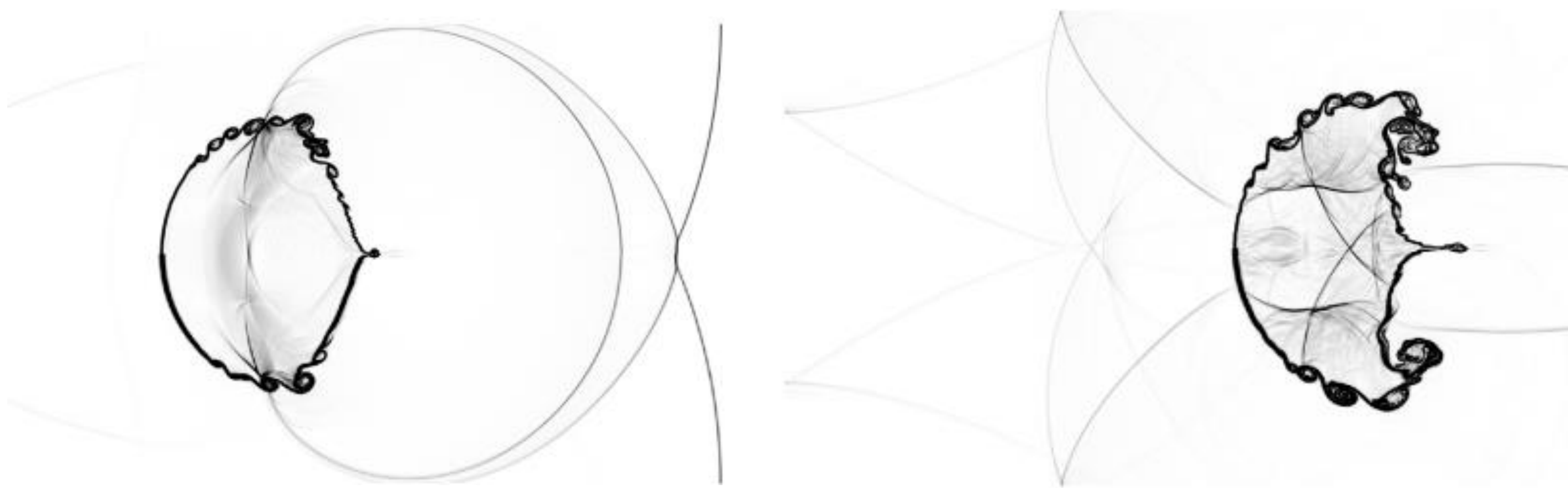
MUSCL-THINC-BVD

Shock-Bubble Interaction

BVD

MUSCL

BVD



WENO

MUSCL-THINC-BVD

Shock-Bubble Interaction

Anti-diffusion
(So, *JCP*, 2012)

Same Grids Resolution

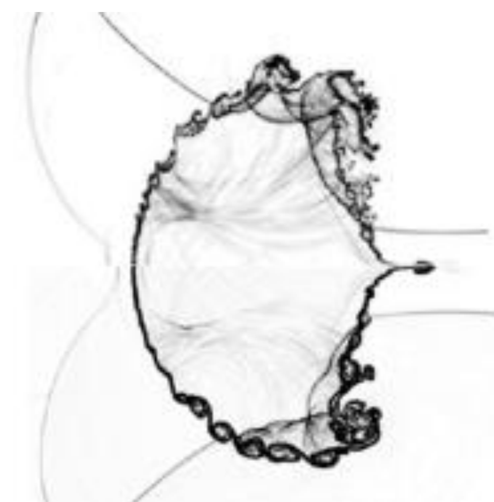
MUSCL-THINC-BVD

Multi-scale
(Luo, *JCP*, 2016)

1150 along diameters

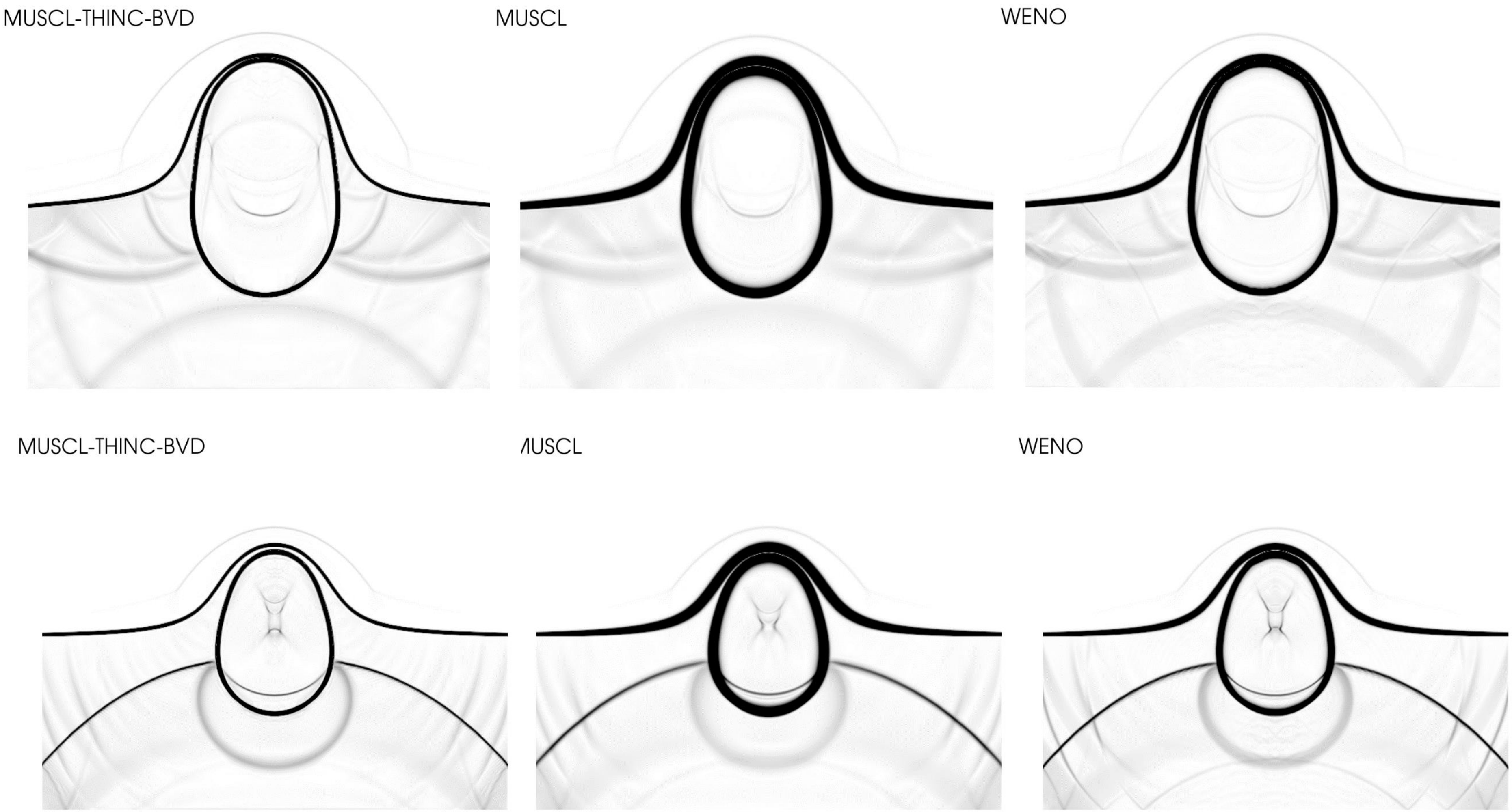
400 along diameters

MUSCL-THINC-BVD



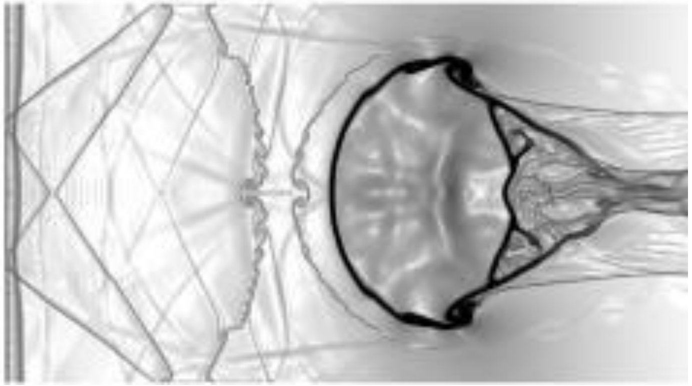
MUSCL-THINC-BVD

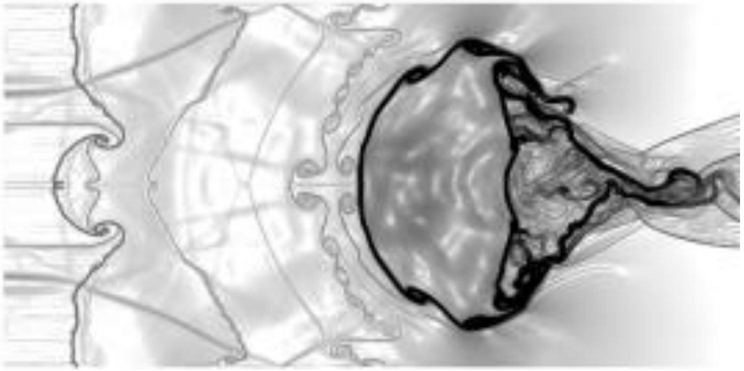
Under Water Explosion



MUSCL-THINC-BVD

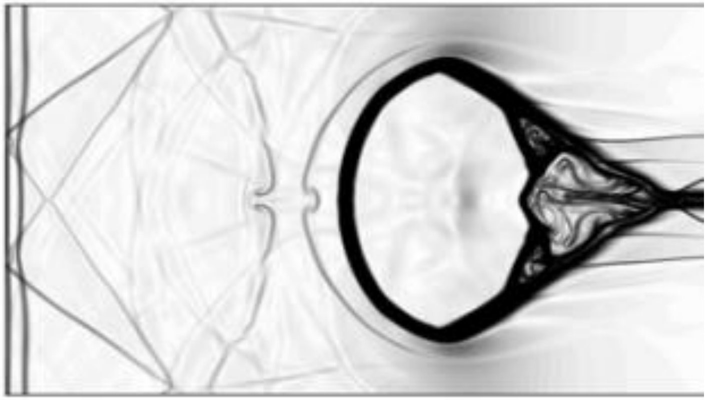
Top: MUSCL-THINC-BVD





Under the same grids number

Bottom: 5th WENO + artificial interface compression (Shukla, *JCP*, 2010)



MUSCL-THINC-BVD Unstructured Grids

Under Water Explosion

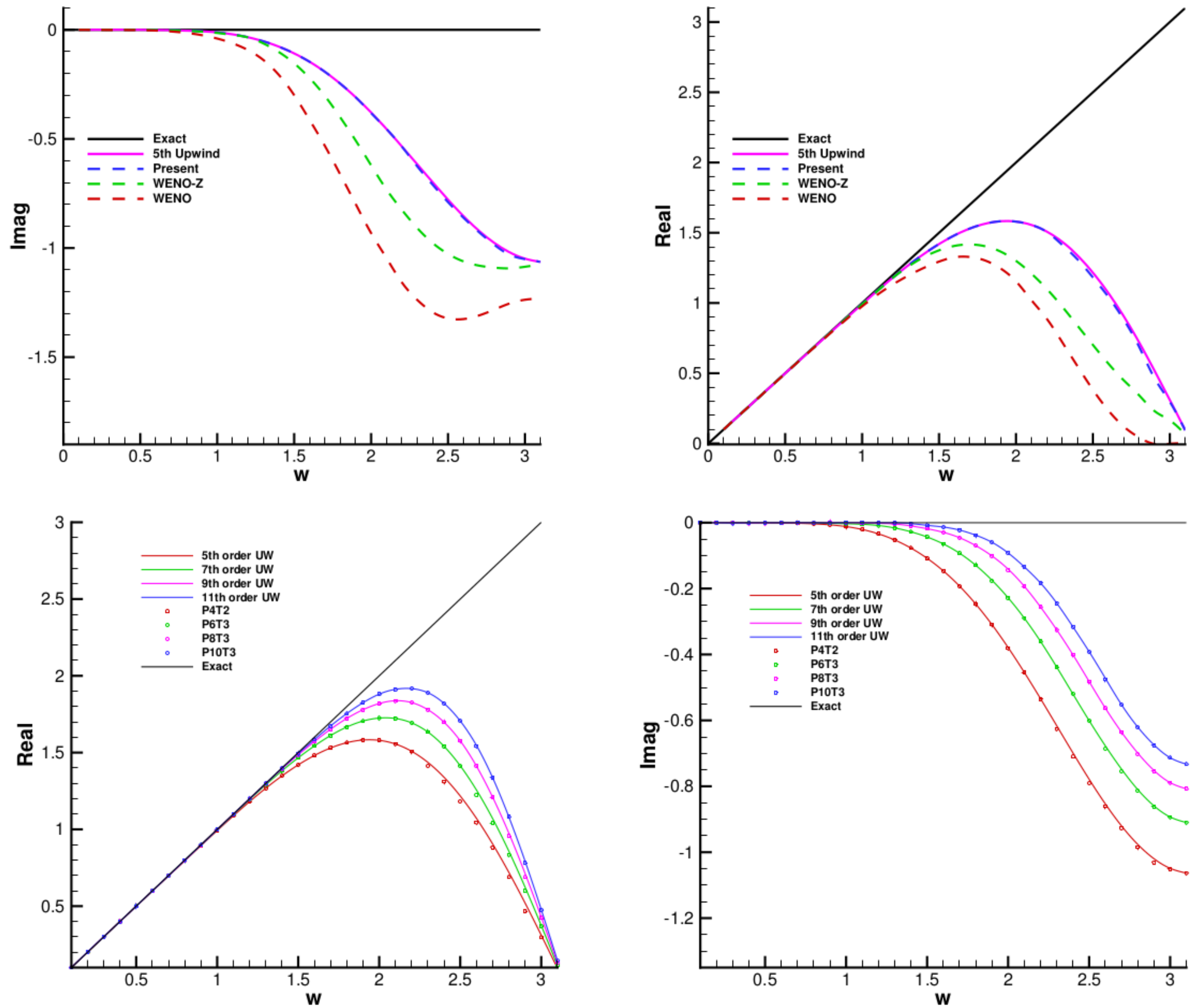
Conclusions

Low-order non-oscillatory schemes + THINC + BVD algorithm can achieve higher resolution across discontinuities.

PnTm-BVD Schemes

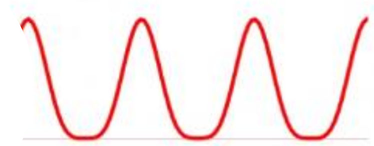
Unlimited upwind-biased n degree polynomial + THINC with m level + BVD algorithm

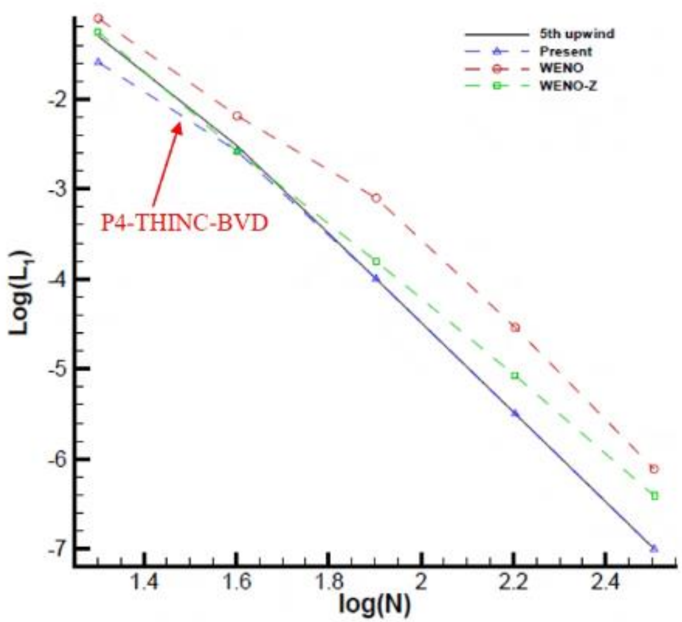
P4T2-BVD



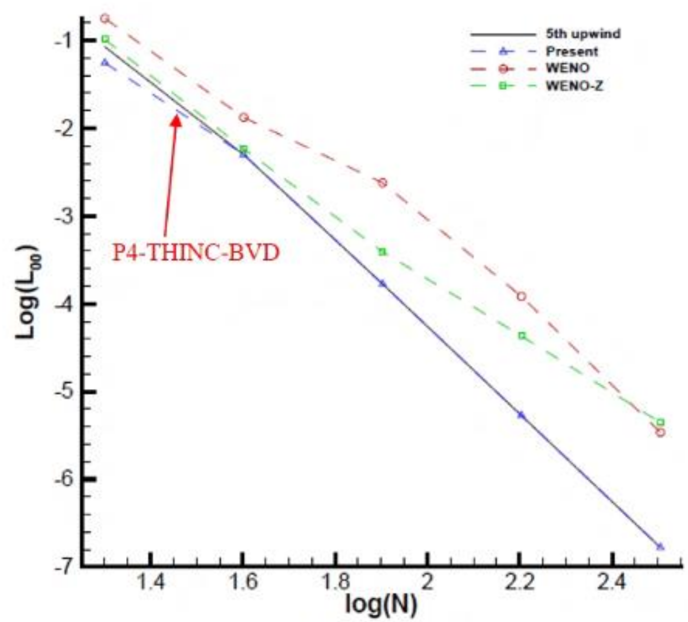
A more challenge test for convergence rate

$$q(x) = \sin^4(\pi x), \quad x \in [-1, 1]$$



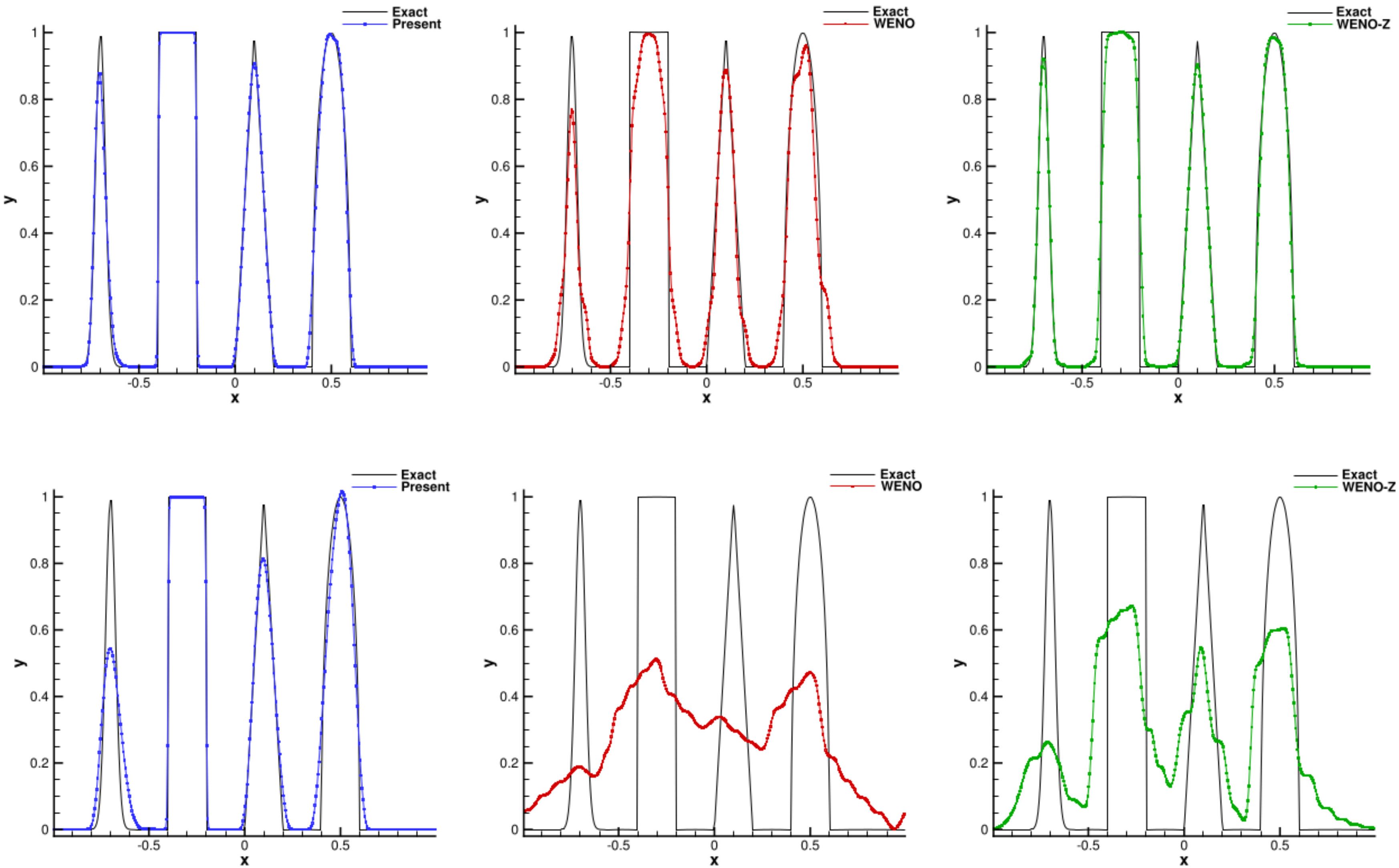


L_1 errors



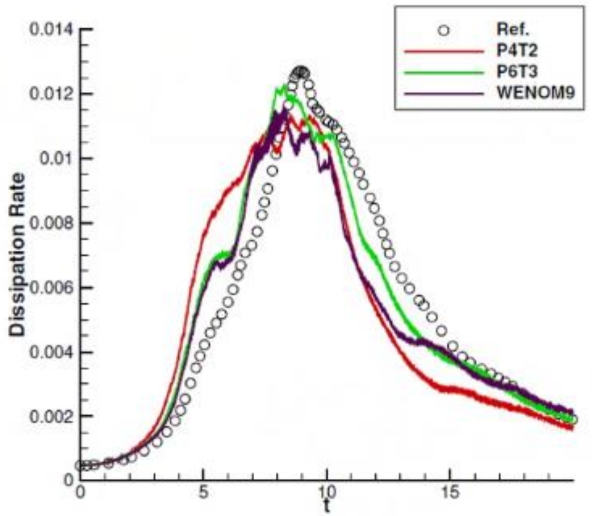
L_∞ errors

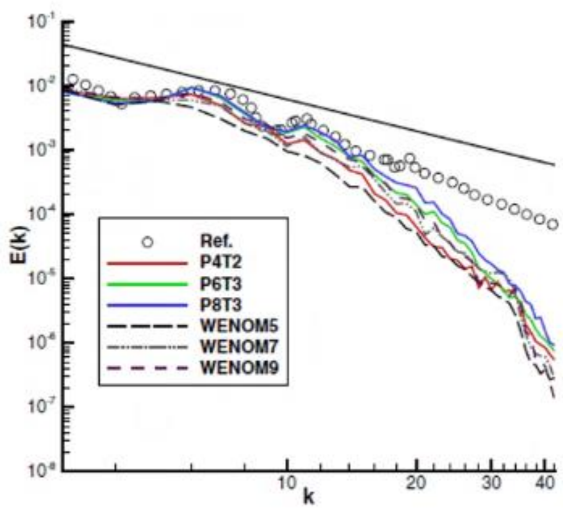
Advection of Complex Profiles

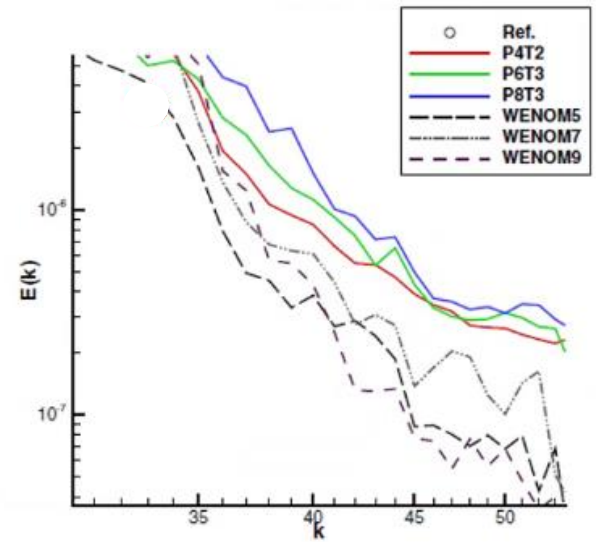


Viscous incompressible flow

Taylor-Green vortex problem with Re = 1600

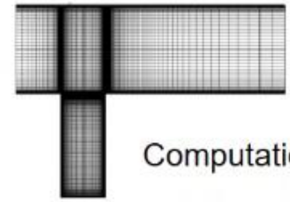






Transonic flow past a deep cavity

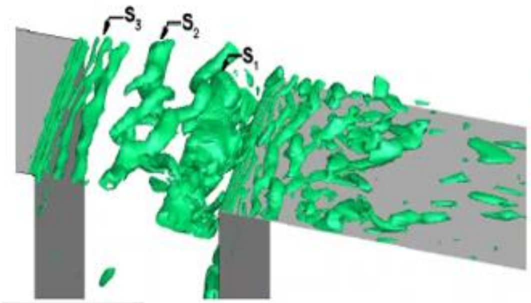
Jiang, et al (CiCP, 2020)



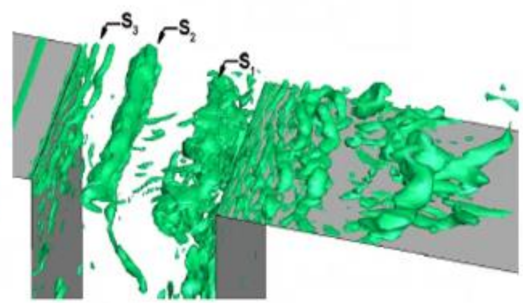
Computational Mesh

$M_\infty = 0.8$ and $Re_\infty = 8.6 \times 10^5$

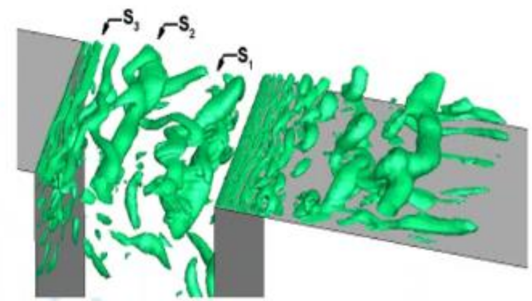
Q-criterion



BVD (0.75M cells)

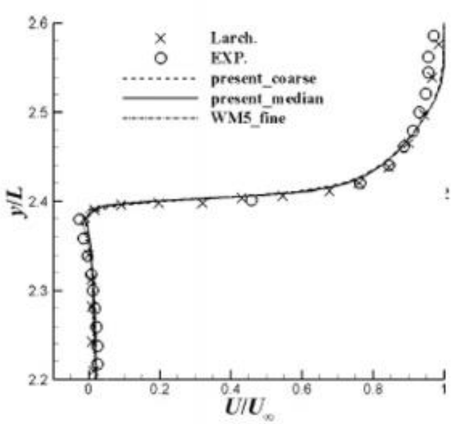


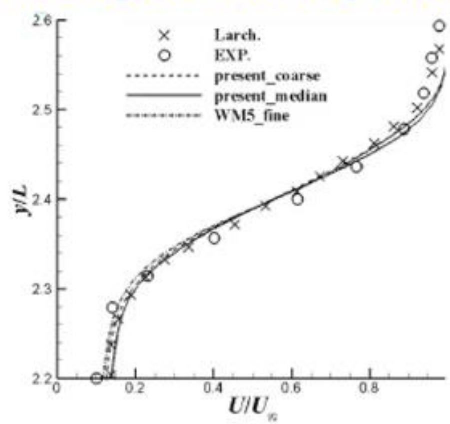
BVD (1.2M cells)

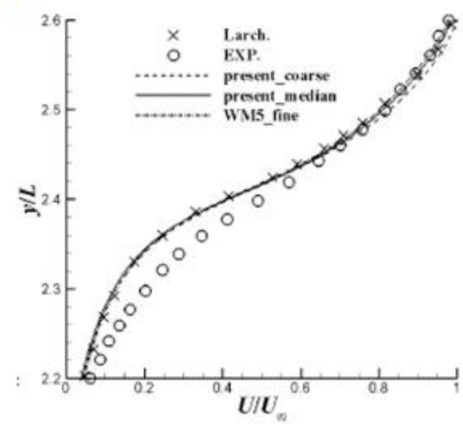


WENOM5 (2.0M cells)

Averaged x-velocity component







Conclusions

PnTm-BVD schemes can retrieve the spectral property of the underlying high order interpolations, and solve both discontinuous and smooth solutions with high-fidelity.

Chamarthi, A. S., & Frankel, S. H. (2021). High-order central-upwind shock capturing scheme using a Boundary Variation Diminishing (BVD) algorithm. *Journal of Computational Physics, 427*, 110067.