

# High Order Positivity Preserving Finite Difference Scheme for Compressible Two Fluid/Phase Flow Model

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Daniel Boe, Khosro Shahbazi

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South Dakota School of Mines and Technology

- Introduction - Applications, Challenges, and Objectives
- Overview of model
- Methodology
- Numerical Examples
- Conclusion

## Two phase/fluid dynamics occur in numerous fields

- Sustainable Energy / cooling systems
- Defense
- Healthcare
  - Treatment Modeling
    - Laser-activated Perfluorocarbon nanodroplets (PFCnD)
  - Cold Chain equipment
    - Portable vapor-compression systems
    - Mobile absorption based systems (Einstein refrigerator, “Icyball”)
    - Switchable adsorption/zeolite refrigeration systems
- Volcanology
  - Vulcanian eruptions

**Two phase/fluid problems are characterized by physical phenomena that pose significant challenges to numerical algorithms.**

- Highly nonlinear (shock waves, and high-intensity ultrasound waves)
- Complex wave propagation and high-frequency features
  - *Demands high fidelity numerical algorithm to accurately capture*
- Large, discontinuous jumps across shocks and even larger jumps across material interfaces
  - *Requires non-oscillatory, positivity preserving scheme to ensure physical integrity*

**Failure to maintain positivity of density and the square of sound speed leads to the simulation crashing**

**The objectives are to design, analyze and implement numerical schemes applicable to general compressible multiphase dynamics satisfying**

1. Hyperbolicity (real Eigenvalues/characteristic speeds)
2. High order
3. Non-oscillatory
4. Positivity-preserving
5. High efficiency, simplicity and scalability on parallel computers

# Conservation Law

- In a closed system, the overall quantity of some property can only change by adding or removing this property.
- Enforces fundamental principle that forms the basis for modeling numerous physical processes.

$$\frac{\partial u(x, t)}{\partial t} + \frac{\partial}{\partial x}[f(u(x, t))] = 0 \quad (1)$$

where

- $u(x, t)$  is a function describing the distribution of some physical quantity
- $f$  is a function giving the flux of the conserved quantity.

# Euler Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}[\rho v] = 0 \quad (2)$$

$$\frac{\partial}{\partial t}[\rho v] + \frac{\partial}{\partial x}[\rho v^2 + p] = 0 \quad (3)$$

$$\frac{\partial}{\partial t}[\rho(e + \frac{v^2}{2})] + \frac{\partial}{\partial x}[(\rho e + \frac{\rho v^2}{2} + p)v] = 0 \quad (4)$$

- Ideal Gas Law gives  $e\rho(\gamma - 1) = p$ 
  - $e$  is specific internal energy.
  - $\gamma$  specific heat ratio  $\frac{c_p}{c_v}$
- $\mathbf{u} = [\rho, \rho v, \rho(e + \frac{v^2}{2})]^T$ 
  - vector of *conserved* variables - specific density, specific momentum, and specific total energy.
- $\mathbf{u}_p = [\rho, v, p]^T$ 
  - vector of *primitive* variables - density, velocity, and pressure
- $\mathbf{f} = [\rho v, \rho v^2 + p, (\rho(e + \frac{\rho v^2}{2}) + p)v]^T$ 
  - vector of fluxes

# Two Fluid System

The Euler equations can be extended to a two-fluid system by adding two additional equations.

$$\frac{\partial \Gamma_1}{\partial t} + \frac{\partial}{\partial x} [v \Gamma_1] - \Gamma_1 \frac{\partial v}{\partial x} = 0 \quad (5)$$

$$\frac{\partial \Gamma_2}{\partial t} + \frac{\partial}{\partial x} [v \Gamma_2] - \Gamma_2 \frac{\partial v}{\partial x} = 0 \quad (6)$$

- $\Gamma_1 = \frac{1}{\gamma-1}$  and  $\Gamma_2 = \frac{\gamma \Pi}{\gamma-1}$  are interface capturing functions
- Stiffened Gas Equation of State:  $p = e\rho(\gamma - 1) - \gamma \Pi$ 
  - Provides a means of modeling state for both liquid and gas
  - $\Pi$  is empirical parameter
    - $\Pi = 0$  for ideal gas
    - $\Pi \approx 4(10^8)$  for liquid water



# Model Summary

We need to solve the following model subject to shocks, oscillations, and discontinuities:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}[\rho v] &= 0 \\ \frac{\partial}{\partial t}[\rho v] + \frac{\partial}{\partial x}[\rho v^2 + p] &= 0 \\ \frac{\partial}{\partial t}[\rho(e + \frac{v^2}{2})] + \frac{\partial}{\partial x}[(\rho e + \frac{\rho v^2}{2} + p)v] &= 0 \\ \frac{\partial \Gamma_1}{\partial t} + \frac{\partial}{\partial x}[v\Gamma_1] - \Gamma_1 \frac{\partial v}{\partial x} &= 0 \\ \frac{\partial \Gamma_2}{\partial t} + \frac{\partial}{\partial x}[v\Gamma_2] - \Gamma_1 \frac{\partial v}{\partial x} &= 0 \\ e\rho(\gamma - 1) - \gamma\Pi &= p\end{aligned}$$

## Why Finite Difference Schemes?

- Able to capture shock discontinuities prevalent in CFD
- Well suited for multi-scale phenomena associated with multi-phase/multi-fluid dynamics.
- Unmatched simplicity and efficiency

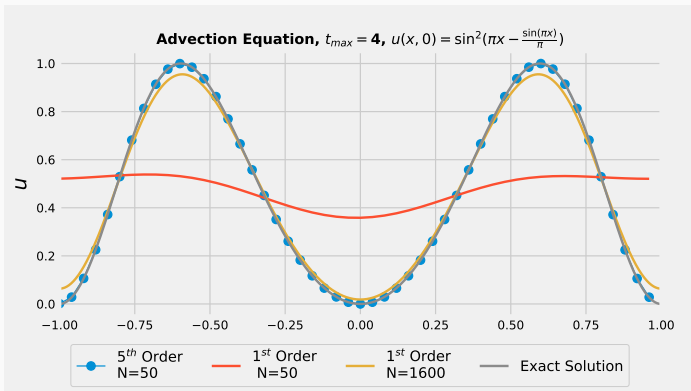
## Why High Order Schemes?

- High order schemes allow for greater accuracy per CPU cost (KS, JCP, 2017) [1, 2]
  - Enhances ability to solve multi-dimensional problems

# Higher Order Schemes

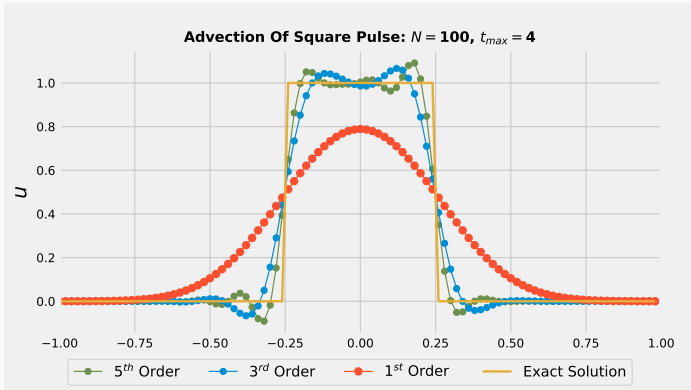
High order schemes offer superior accuracy per CPU cost

	First Order N=1600 Grid Points	Fifth Order N=50 Grid Points
$L_\infty$ Error %	4.86%	0.13%
CPU Time [sec]	0.32	0.20



# Discontinuous Solutions

For discontinuous solutions, high order methods suffer from spurious oscillations that do not diminish with grid refinement.



**To obtain a robust algorithm, we need a globally high order, non-linear scheme that can locally adapt to discontinuous solutions**

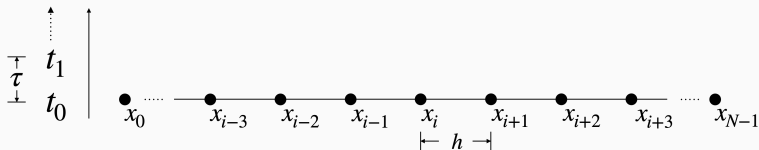
# Discretization

We seek a non-linear scheme for the discrete conservation law

$$\frac{\partial}{\partial t}[u_i^n] + \frac{\partial}{\partial x}[f(u_i^n)] = 0 \quad (7)$$

where

- Domain is  $[x_{min}, x_{max}] \times [0, t_{max}]$



- $u_i = u(x_i)$  is the conserved variable evaluated at the gridpoint  $x_i$  at time step  $n$ 
  - $i \in \{0, 1, 2 \dots N - 1\}$  with  $N$  being the total number of cells
  - $h = \frac{x_{max} - x_{min}}{N}$  is the step size in-between adjacent cells

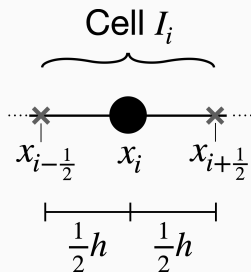
# Approach

From divergence theorem, we can relate the derivative term at  $x_i$  to the fluxes into and out of the cell  $I_i$ .

$$\frac{\partial}{\partial x}[f(u_i)] \approx \frac{\hat{f}_{i+1/2} - \hat{f}_{i-1/2}}{h}$$

**Our goal:**

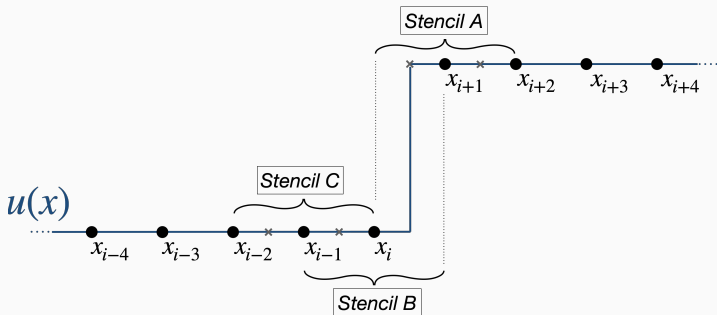
High order, non-oscillatory approximations to the cell boundary fluxes,  $f(u(x_{i\pm 1/2}))$



# The Plan

## Weighted Essentially Non Oscillatory (WENO) Method

1. Calculate local polynomial approximation at each stencil
2. Measure the smoothness of each polynomial approximation
3. Form a weighted sum of all the approximations
  - o Stencil weight is proportional to smoothness
  - o Discontinuous stencils assigned weight  $\rightarrow 0$
  - o Smooth stencils assigned an optimal weight
  - o If all stencils are smooth, overall approximation is of optimal order.





# WENO Implementation

The WENO reconstruction of  $u(x_{i+1/2})$  takes the form:

$$u(x_{i+1/2}) \approx P_{i+\frac{1}{2}}^{WENO} = \sum_{k=0}^{r-1} \omega_{k,i+\frac{1}{2}} P_{k,i+\frac{1}{2}} \quad (8)$$

where  $\omega_{k,i+\frac{1}{2}}$  is the normalization of the non-linear weights:

$$\alpha_{k,i+\frac{1}{2}} = \frac{b_{r,k}}{(\beta_{k,i+\frac{1}{2}} + 10^{-40})^r} \quad (9)$$

$b_{r,k}$  are the optimal linear weights and  $\beta_{r,k,i}$  are the smoothness indicators

$$\beta_{k,i} = \sum_{l=0}^{r-1} h^{2m-1} \int_{-\frac{1}{2}h}^{\frac{1}{2}h} \left[ \frac{d^m}{d\xi} P_{k,i+1/2}(\xi) \right]^2 d(\xi - x_i) \quad (10)$$

The WENO scheme provides a method for forming non-oscillatory approximations to primitive variables at cell boundaries.

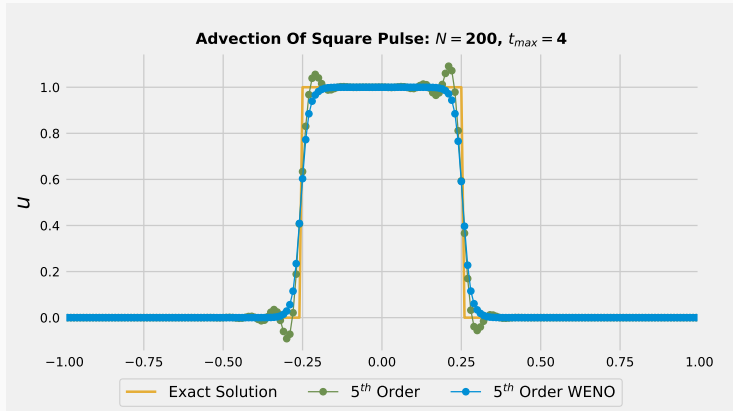
$$\hat{u}_{i+\frac{1}{2}} \approx u(x_i + \frac{1}{2}h)$$

The derivative is then approximated to high order using constants  $d_j$  introduced and tabulated to 9<sup>th</sup> order by Shahbazi (Computers and Fluids, 2019) and extended to 13<sup>th</sup> order (DB and KS, unpublished).

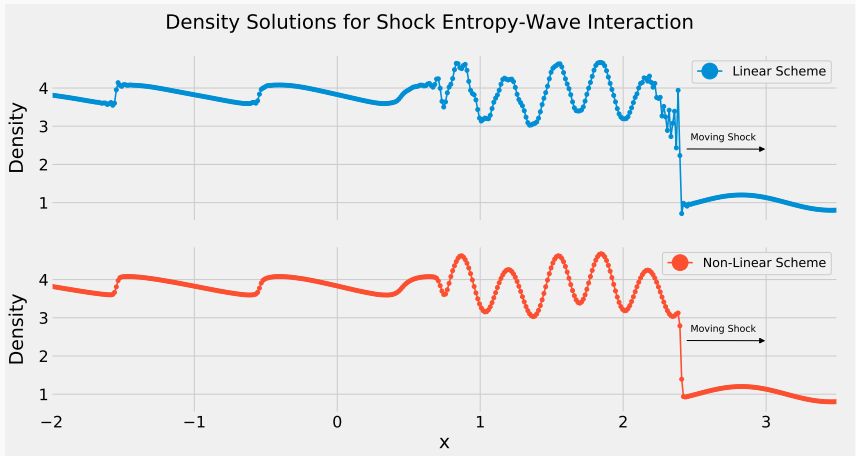
$$h \frac{\partial f}{\partial x} \Big|_{x_i} \approx \sum_{j=1}^{j=\text{ceil}(\frac{r}{2})} d_j (f(\hat{u}_{i+j-1/2}) - f(\hat{u}_{i-j-1/2}))$$

# Non-Linear Scheme for Advected Pulse

WENO scheme significantly reduces the spurious oscillations



# Non-linear Scheme for Euler System

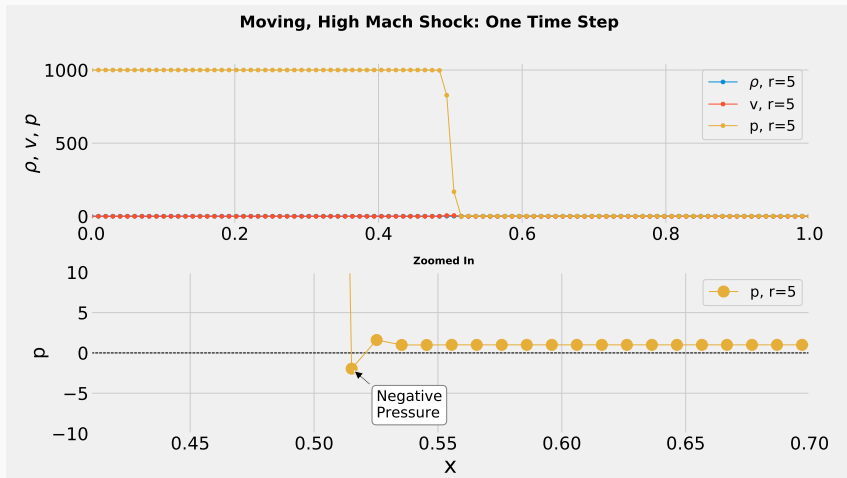


# Non-linear scheme for Euler Equations

- The WENO scheme is designed to provide “essentially” non-oscillatory behavior,
- Some relatively insignificant, small oscillations may be remain.
- In many cases, these small oscillations have no impact on the overall solution; however for certain scenarios, they can pose problems.
- For the Euler system, slight oscillations can result in negative density and/or pressure values which imply a non-real speed of sound
  - *Complex sound speed results in simulation crashing.*
  - This issue is readily observed for problems that involve high Mach shock waves with complex interactions

**To achieve a robust scheme, we need to enforce the positivity of density and pressure**

# Positivity Example



# Positivity Preserving Scheme

A positivity preserving scheme can be developed by combining the high order fluxes with the first order fluxes whenever necessary to prevent the solution from obtaining unphysical values.

- $h_{i+1/2}$ : flux from first order method
- $H_{i+1/2}$ : High order, WENO flux

The high order WENO approximation is of the form:

$$\frac{\partial}{\partial x}[f(u_i)] = \frac{H_{i+1/2} - H_{i-1/2}}{h} + \mathcal{O}(h^{2r-1})$$

The first order approximation is:

$$\frac{\partial}{\partial x}[f(u_i)] = \frac{h_{i+1/2} - h_{i-1/2}}{h} + \mathcal{O}(h)$$

## Positivity Preserving Scheme

The positivity preserving scheme is realized by forming a modified flux (Xu, Mathematics of Computation, 2014):

$$\tilde{H}_{i+1/2} = h_{i+1/2} + \theta_{i+1/2}(H_{i+1/2} - h_{i+1/2})$$

- $\theta_{i+1/2} \in [0, 1]$  are locally defined flux limiters.
- $\theta_{i+1/2} = 1$  gives pure high order approximation
- $\theta_{i+1/2} = 0$  gives first order
- For linear functions (e.g. density)  $\theta_{i+1/2}$  are found by a sequence of 4 logical statements at each  $i$ .
- Non-linear functions, e.g. pressure, require a root finding routine

The modified, high order, positivity preserving approximation is thus:

$$\frac{\partial}{\partial x}[f(u_i)] \approx \frac{\tilde{H}_{i+1/2} - \tilde{H}_{i-1/2}}{h}$$

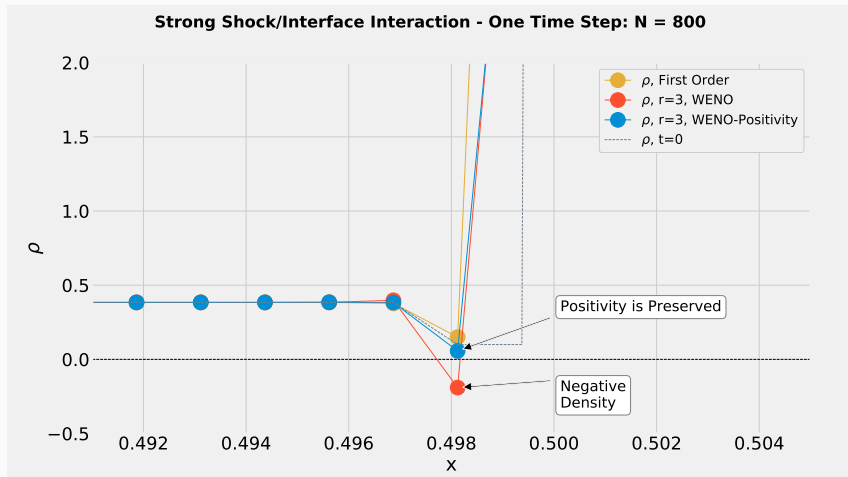


## Numerical Example

Here we consider a particularly challenging problem that contains a strong shock interacting with a density interface:

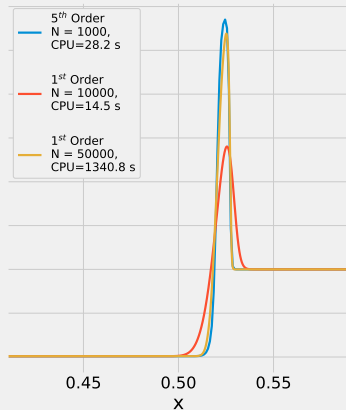
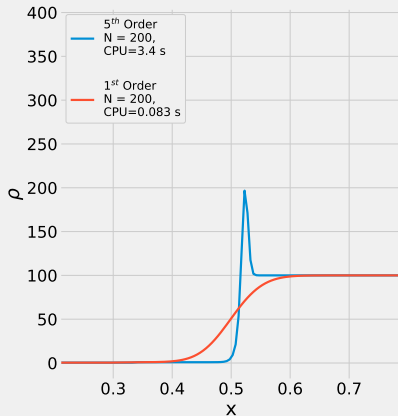
$$(\rho, v, p) = \begin{cases} (0.384, 27.086, 100.176) & 0 \leq x < (0.5 - 2h) \\ (0.1, 0, 1) & (0.5 - 2h) \leq x \leq 0.5 \\ (100, 0, 1) & 0.5 < x \leq 1 \end{cases}$$

# Positivity Example



# Positivity Example

**Strong Shock/Interface Interaction:  $t_{max} = 0.01$**



# Two-fluid Positivity

To retain positivity within the two-fluid model we need to enforce the following (KS, unpublished):

- Upper and lower bounds of order parameters
- Positivity of density
- Positivity of a modified pressure  $\frac{p+\Pi}{\gamma-1}$ 
  - Ensures speed of sound is a real number

## Two-Fluid Positivity Implementation

Two-fluid positivity is implemented using the flux limiting technique to form modified fluxes:

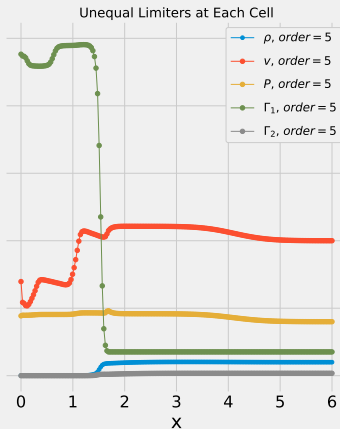
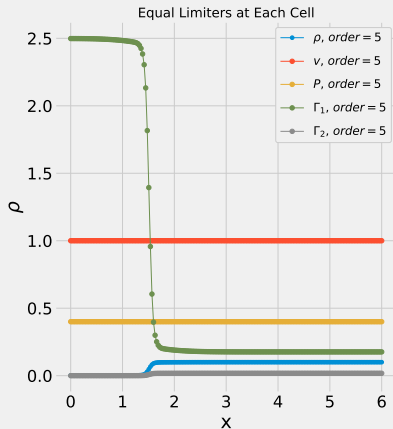
$$\tilde{H}_{i+1/2} = h_{i+1/2} + \theta_{i+1/2}(H_{i+1/2} - h_{i+1/2})$$

Because of the source terms in the order parameter equations, at each cell, we need to add the restriction of equal limiters (DB and KS, unpublished)

$$\theta_{i+\frac{1}{2}} = \theta_{i-\frac{1}{2}}$$

# Two Fluid Positivity Example

**Advection of Isolated Interface:  $t_{max} = 0.5$ ,  $N=200$**



## Conclusions and Ongoing Work

- A WENO finite difference scheme for two/phase fluid flow (KS, Computers and Fluids, 2019)
- Addition of positivity preservation for Euler System (DB and KS, unpublished)
- Extend positivity preserving method to two-fluid problems

# Acknowledgment

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K. Shahbazi.

**Robust second-order scheme for multi-phase flow computations.**

*Journal of Computational Physics*, 339:163–178, 2017.



K. Shahbazi.

**High-order finite difference scheme for compressible mult-component flow computations.**

*Computers and Fluids*, 190:425–439, 2019.