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

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Overview

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

Applications

Two phase/fluid dynamics occur in numerous fields

- Sustainable Energy
- Defense
- Volcanology
- Healthcare
  - Treatment Modeling
    - Laser-activated Perflourocarbon nanodroplets (PFCnD)
  - Cold Chain equipment
    - Mobile absorption/adsorption based systems
    - Portable vapor-compression systems
    - Refrigerant Migration

Challanges

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

Objectives

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.

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

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

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

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

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

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

Two Fluid System

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

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

$$\frac{\partial \Gamma_2}{\partial t} + \frac{\partial}{\partial x}[v\Gamma_2] - \Gamma_1 \frac{\partial v}{\partial x} = 0 \tag{6}$$

- $\Gamma_1 = \frac{1}{\gamma-1}$ and $\Gamma_2 = \frac{\gamma\Pi}{\gamma-1}$ are interface capturing functions
- Stiffened Gas Equation of State: $p = e\rho(\gamma - 1) - \gamma\Pi$
    - o Provides a means of modeling state for both liquid and gas
    - o Π 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:

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

Finite Difference Schemes

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

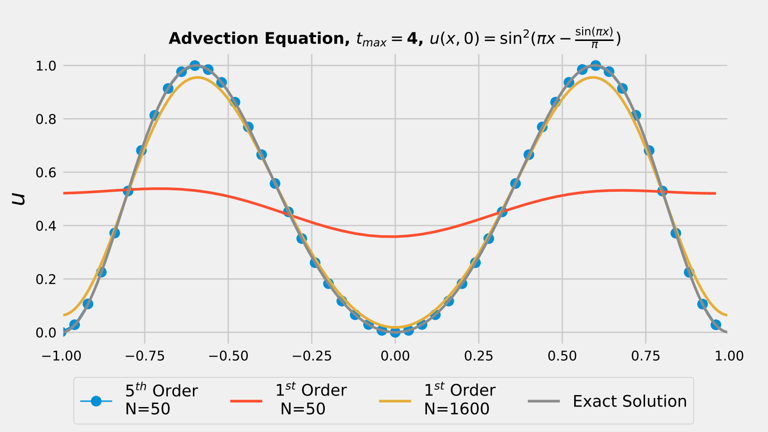
Why High Order Schemes?

- 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

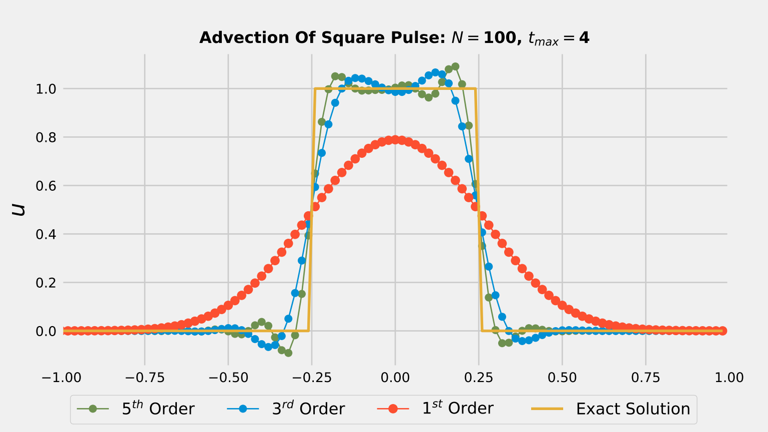
High order schemes offer superior accuracy per CPU cost

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



Discontinuous Solutions

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



Non Linear Scheme

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

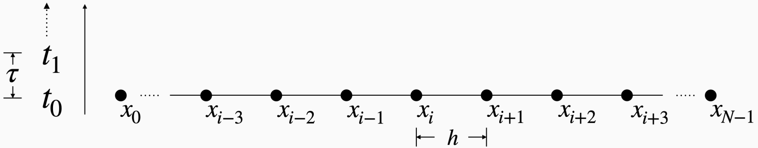
Discretization

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

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

where

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



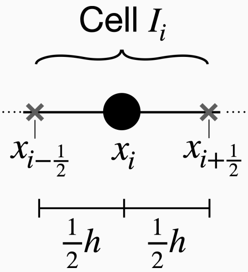
- $u_i = u(x_i)$ is the conserved variable evaluated at the gridpoint x_i at time step n
  - o $i \in \{0, 1, 2 \ldots N-1\}$ with N being the total number of cells
  - o $h = \frac{x_{max} - x_{min}}{N}$ is the step size in-between adjacent cells

Approach

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

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

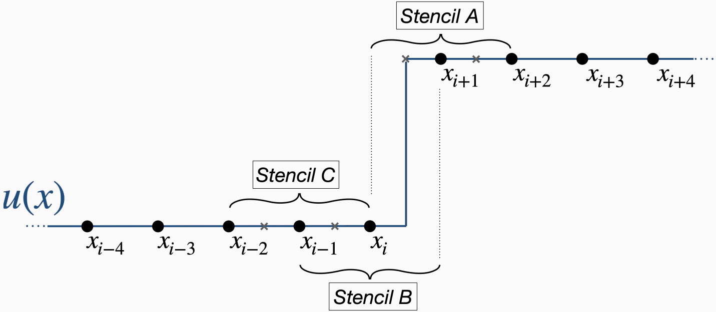
Our goal:
High order, non-oscillatory approximations to the cell boundary fluxes, $f(u(x_{i\pm 1/2}))$



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
    - Stencil weight is proportional to smoothness
    - Discontinuous stencils assigned weight $\rightarrow 0$
    - Smooth stencils assigned an optimal weight
    - 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:

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

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

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

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

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

WENO Summary

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

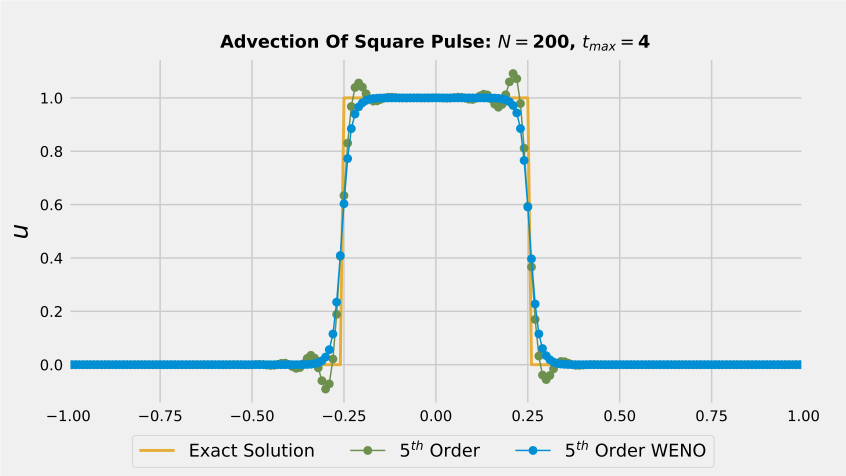
$$\hat{u}_{i+\frac{1}{2}} \approx u(x_i + \tfrac{1}{2}h)$$

The derivative is then approximated to high order using constants d_j introduced and tabulated to 9^{th} order by Shahbazi (Computers and Fluids, 2019) and extended to 13^{th} order (DB and KS, unpublished).

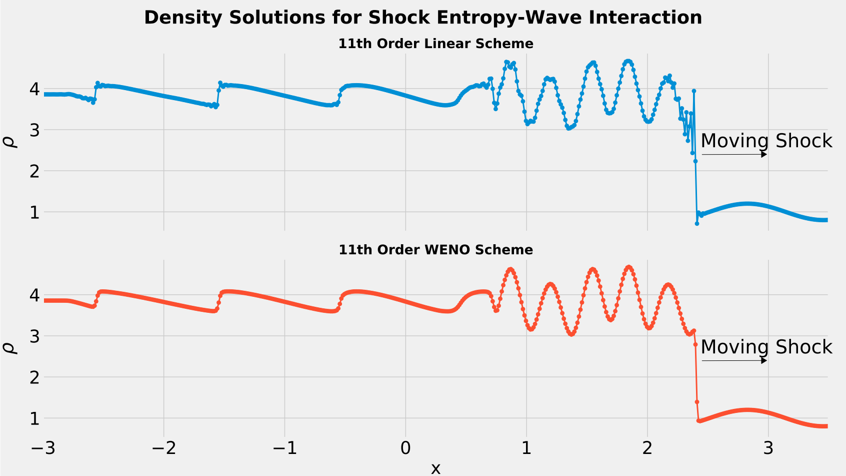
$$h\frac{\partial f}{\partial x}\bigg|_{x_i} \approx \sum_{j=1}^{j=\text{ceil}(\frac{r}{2})} d_j\left(f(\hat{u}_{i+j-1/2}) - f(\hat{u}_{i-j-1/2})\right)$$

Non-Linear Scheme for Advected Pulse

WENO scheme significantly reduces the spurious oscillations



Non-linear Scheme for Euler System

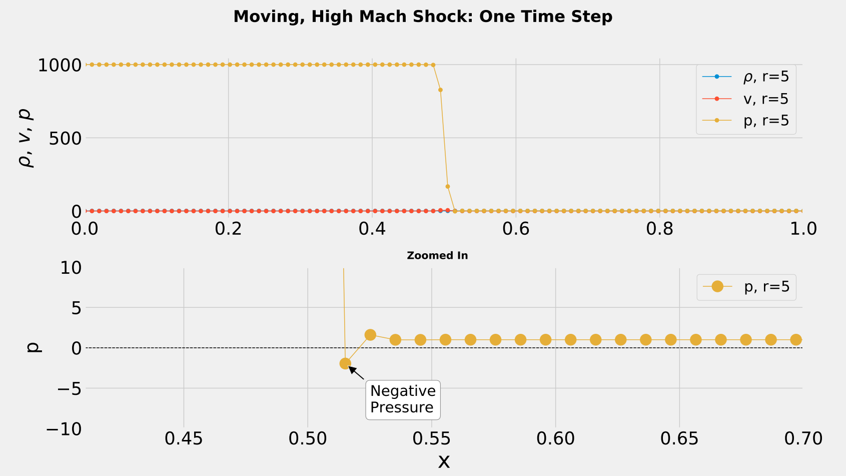


Non-linear scheme for Euler Equations

- The WENO scheme is designed to provide "essentially" non-oscillatory behavior; small oscillations may be remain.
- 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.*

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:

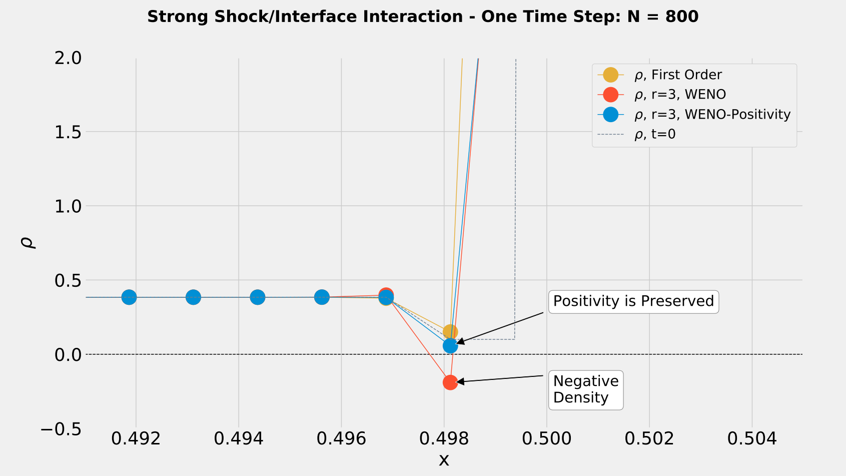
$$\frac{\partial}{\partial x}[f(u_i)] \approx \frac{\tilde{H}_{i+1/2} - \tilde{H}_{i-1/2}}{h}$$

Numerical Example

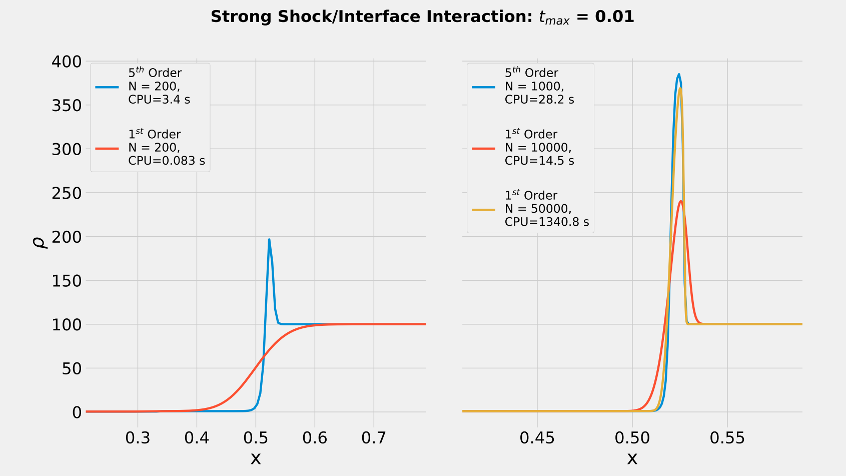
Here we consider a particularly challenging problem that contains a strong shock interacting with a density interface:

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

Positivity Example



Positivity Example



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 $\frac{p+\Pi}{\gamma-1}$
    - o Ensures speed of sound is a real number

Two-Fluid Positivity Implementation

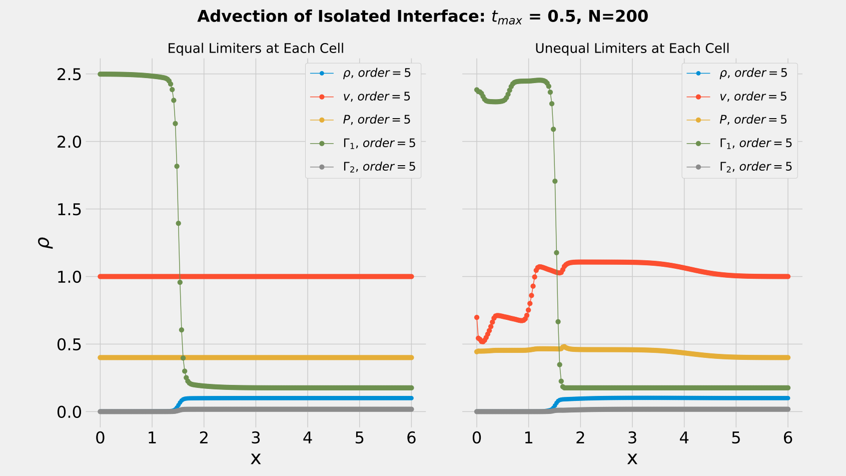
Two-fluid positivity is implemented using the flux limiting technique to form modified fluxes:

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

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



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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