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

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*

Objectives

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

1. Hyperbolicity
2. High order
3. Non-oscillatory
4. Positivity-preserving
5. High efficiency, simplicity and scalability on parallel computers

Conservation Law

The conservation law is a fundamental principle that forms the basis for modeling numerous physical processes. In the simplest terms, this law enforces the idea that, in a closed system, the overall quantity of some property can only change by adding or removing this property. Mathematically, a conservation law is expressed as

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

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

In the context of gas dynamics, the conservation of mass, momentum, and energy form a set of three coupled equations known as the 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 $e\rho(\gamma - 1) = p$
  - e is specific internal energy.
  - γ 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.

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

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

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

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
- Less computationally expensive than Finite Volume Methods
  - Particularly for high order or two/three dimensional problems [**?**]

Why High Order Schemes?

- High order schemes allow for greater accuracy per CPU cost
  - Enhances ability to solve multi-dimensional problems

Methodology

To facilitate the development of the numerical scheme, consider the discrete 1D conservation law over a domain $[x_{min}, x_{max}] \times [0, t_{max}]$.

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

where

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

Higher Order Schemes

Figure below compares 3^{rd} and 1^{st} order approximations for a simple, continuous advection problem.

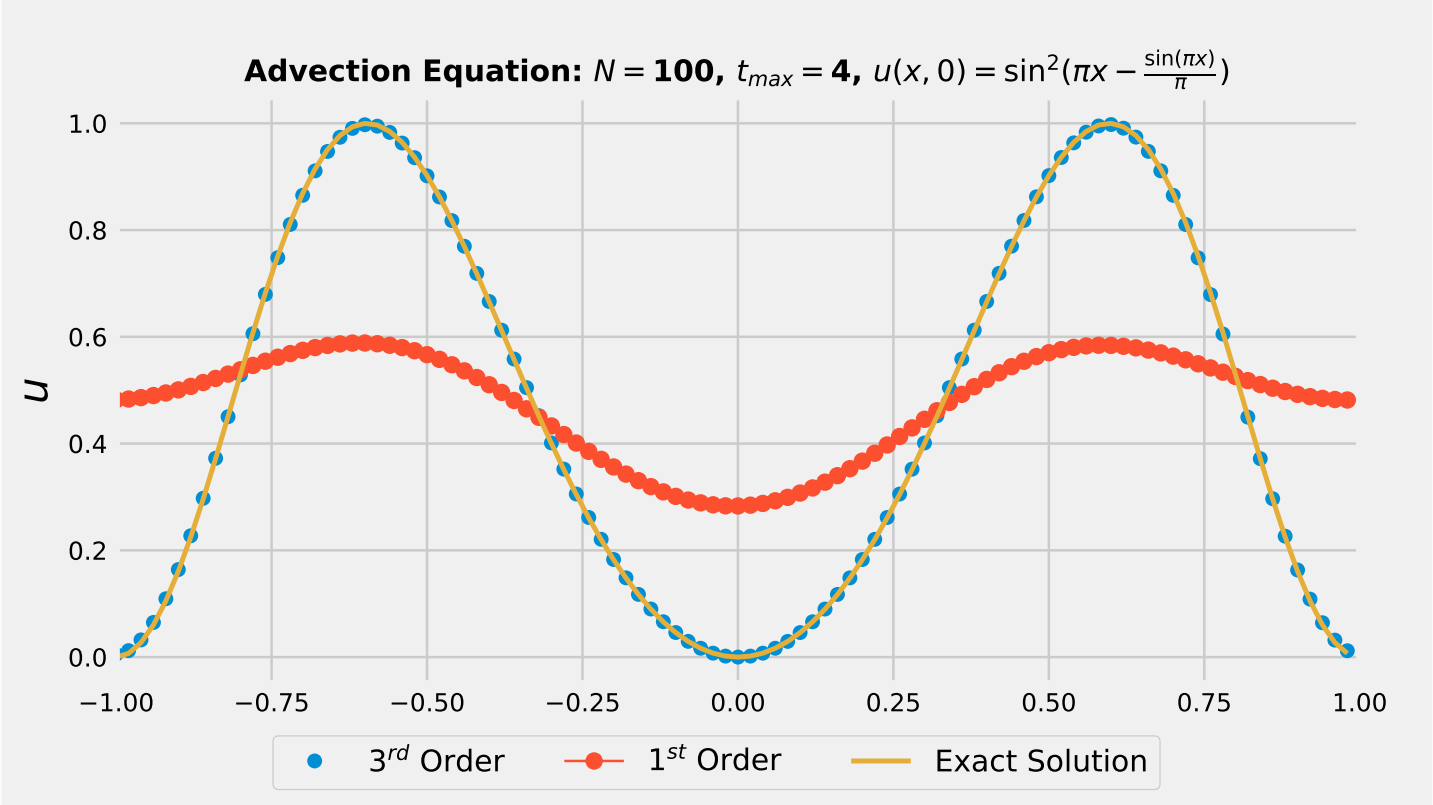

Figure 1: Comparison of First and Third Order solutions for advection equation with smooth initial condition

Discontinuous Solutions

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

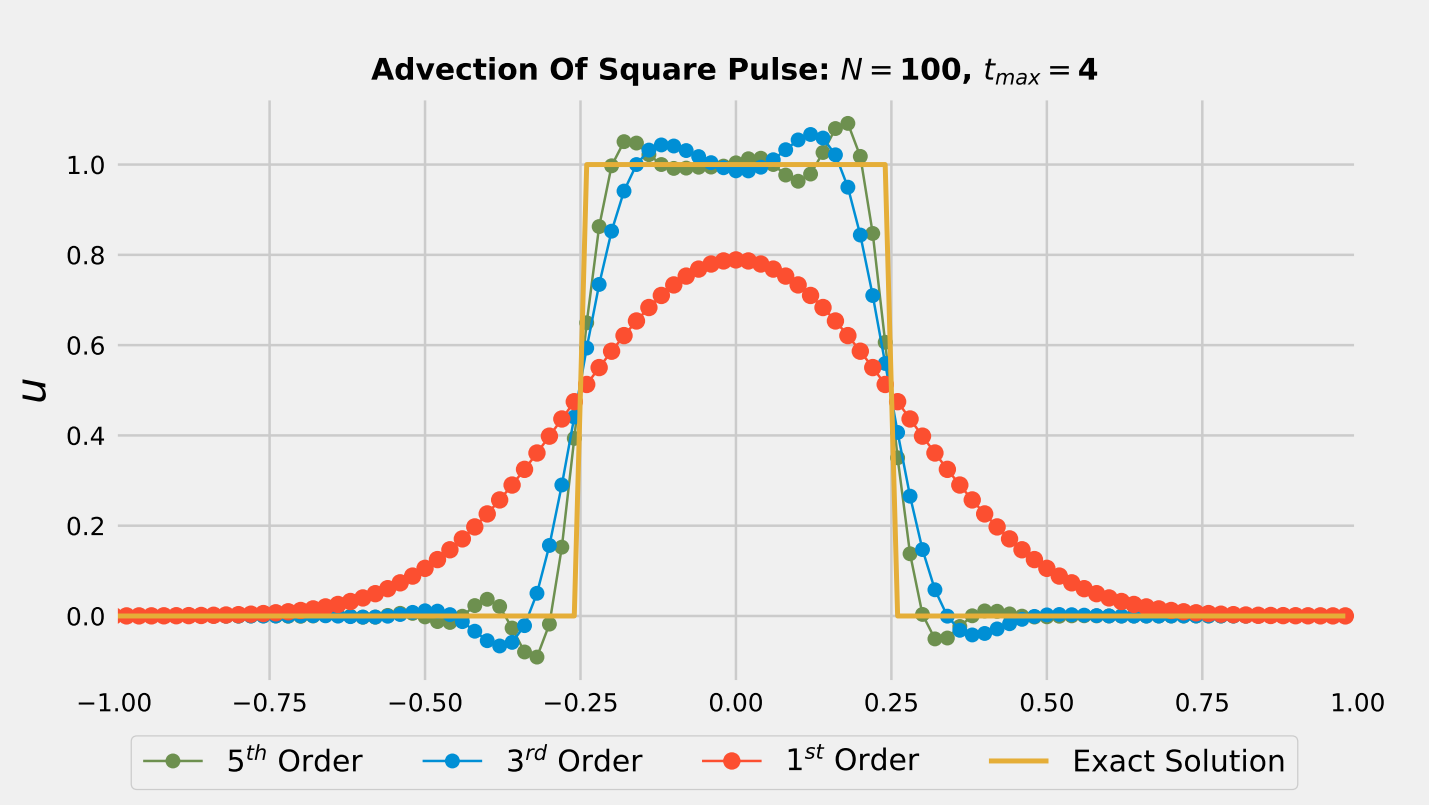

Figure 2: Comparison of First and Third Order solutions for advection equation with discontinuous initial condition

WENO Method

Assume the spatial derivative term can be written exactly as the difference of some "numerical flux function" evaluated at the cell boundaries.

$$\frac{\partial}{\partial x}[f(u_i)] = \frac{\bar{f}_{i+1/2} - \bar{f}_{i-1/2}}{h} \tag{8}$$

where

$$f(u_i) = \frac{1}{h}\int_{x-h/2}^{x+h/2} \bar{f}(\xi)d\xi \tag{9}$$

- Thus, the goal of the WENO scheme is to develop high order, non-oscillatory approximations for the numerical flux function $\bar{f}_{i\pm1/2}$
- The numerical flux function can be computed from the known flux $f(u_i)$

WENO Framework

For an arbitrary function $u(x_i)$, we can form an r^{th} order, polynomial representation of $u(x_{i+1/2})$ as:

$$u(x_i + \tfrac{1}{2}h) \approx P_{r,k_s,i+\frac{1}{2}} = \sum_{q=0}^{q=r-1} a_{r,k_s,q}\, u_{i-k_s+q} \tag{10}$$

where $a_{r,k_s,q}$ are tabulated constants for a given order (r), stencil (k_s), and stencil cell (q).

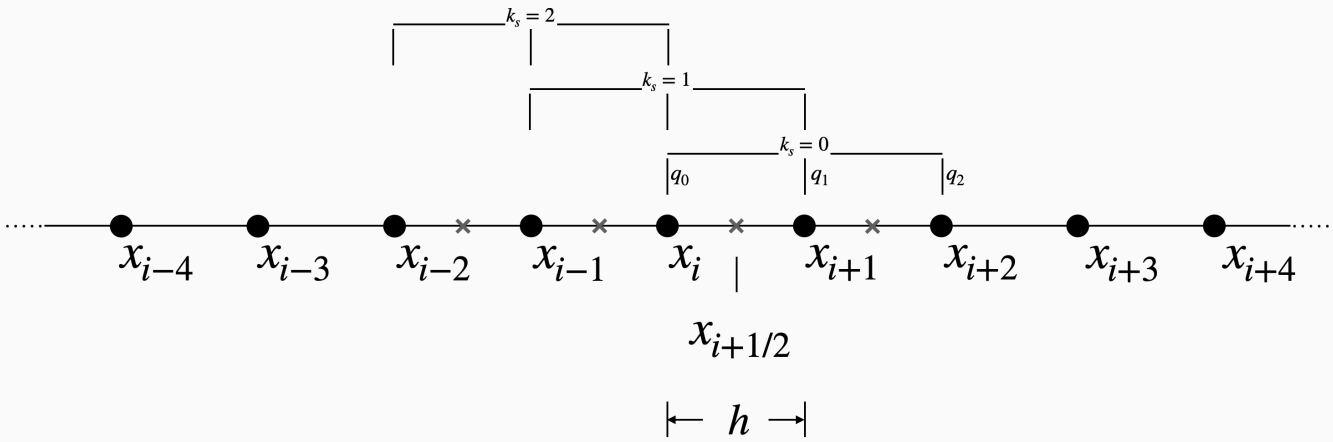

Figure 3: Illustration of candidate stencils for forming $P_{r,k_s,i+1/2}$

WENO Framework

By properly combining the polynomials associated with each candidate stencil, we can construct a $2r-1$ order approximation for $u(x_{i+1/2})$

$$P^*_{r,i+\frac{1}{2}} = \sum_{k_s=0}^{k_s=r-1} b_{r,k_s} P_{r,k_s,i+\frac{1}{2}} \tag{11}$$

Here, b_{r,k_s} are tabulated weights assigned to the local, r^{th} order polynomial associated with sub-stencil k_s.

- The heart of WENO involves modifying the above approximation such that:
  1. If sub-stencil k_s contains a discontinuity, the weight $b_{r,k_s} \longrightarrow 0$ effectively negating the impacts of the discontinuity.
  2. If no sub-stencils contain discontinuities, the above $2r-1$ order approximation is recovered.

WENO Framework

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

$$P^{WENO}_{r,i+\frac{1}{2}} = \sum_{k_s=0}^{k_s=r-1} \omega_{r,k_s,i+\frac{1}{2}} P_{r,k_s,i+\frac{1}{2}} \tag{12}$$

where

$$\omega_{r,k_s} = \frac{\alpha_{r,k_s}}{\sum_{j=0}^{R} \alpha_{r,j}} \tag{13}$$

$$\alpha_{r,k_s} = \frac{b_{r,k_s}}{(\beta_{r,k_s,i} + 10^{-40})^r} \tag{14}$$

define the WENO weights in terms of the linear, "optimal weights" (b_{r,k_s}) and a non-linear smoothness indicator $\beta_{r,k_s,i}$ which is defined as the sum of the L^2 norms of all derivatives of the original interpolating polynomial associated with the k_s sub-stencil [1].

$$\beta_{r,k_s,i} = \sum_{l=0}^{r-1} h^{2m-1} \int_{-\frac{1}{2}h}^{\frac{1}{2}h} \left[\frac{d^m}{d\xi} P_{r,k_s,i+1/2}(\xi) \right]^2 d(\xi - x_i) \tag{15}$$

WENO Framework Summary

The WENO process can be thought of as an operator, L, that takes a function $w(x_i)$ defined on a grid $x_i \in \{x_0, x_1 \dots x_{N-1}\}$ and computes a $2r-1$ order polynomial approximation of w at the intercell points $x_{i+1/2}$.

$$L(w_i) = \hat{w}_{i+\frac{1}{2}} \approx w_{i+\frac{1}{2}}$$

The basic steps for a $2r-1$ order approximation are:

1. Calculate the r local polynomials: $P_{r,k_s,i+\frac{1}{2}} = \sum_{q=0}^{q=r-1} a_{r,k_s,q} w_{i-k_s+q}$
2. For each $P_{r,k_s,i+\frac{1}{2}}$, calculate the WENO smoothness indicators $\beta_{r,k_s,i}$.
   - These calculations are tabulated in the literature
3. Assemble the WENO weights, ω_{r,k_s}, from the constant optimal weights b_{r,k_s} and the non-linear weights $\beta_{r,k_s,i}$.
4. Calculate the WENO polynomial: $\hat{w}_{i+1/2} = \sum_{k_s=0}^{k_s=r-1} \omega_{r,k_s,i+\frac{1}{2}} P_{r,k_s,i+\frac{1}{2}}$

WENO Implementation

The WENO scheme provides a method for forming non-oscillatory approximations to the numerical flux function $\bar{f}_{i\pm1/2}$.

- In general, the WENO reconstruction of the original flux f gives this high order approximation.

$$\bar{f}_{i+1/2} \approx \hat{f}_{i+1/2} = L(f(u_i))$$

- Alternately, the WENO reconstruction can be performed *directly* upon the primitive variables (or conservative variable in the scalar case).

$$\bar{f}_{i+1/2} \approx f(\hat{u}_{i+1/2}) = f(L(u_i))$$

  - With this scheme, the spatial derivative is calculated with tabulated constants (d_j) as [2]:

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

Non-Linear Scheme for Advected Pulse

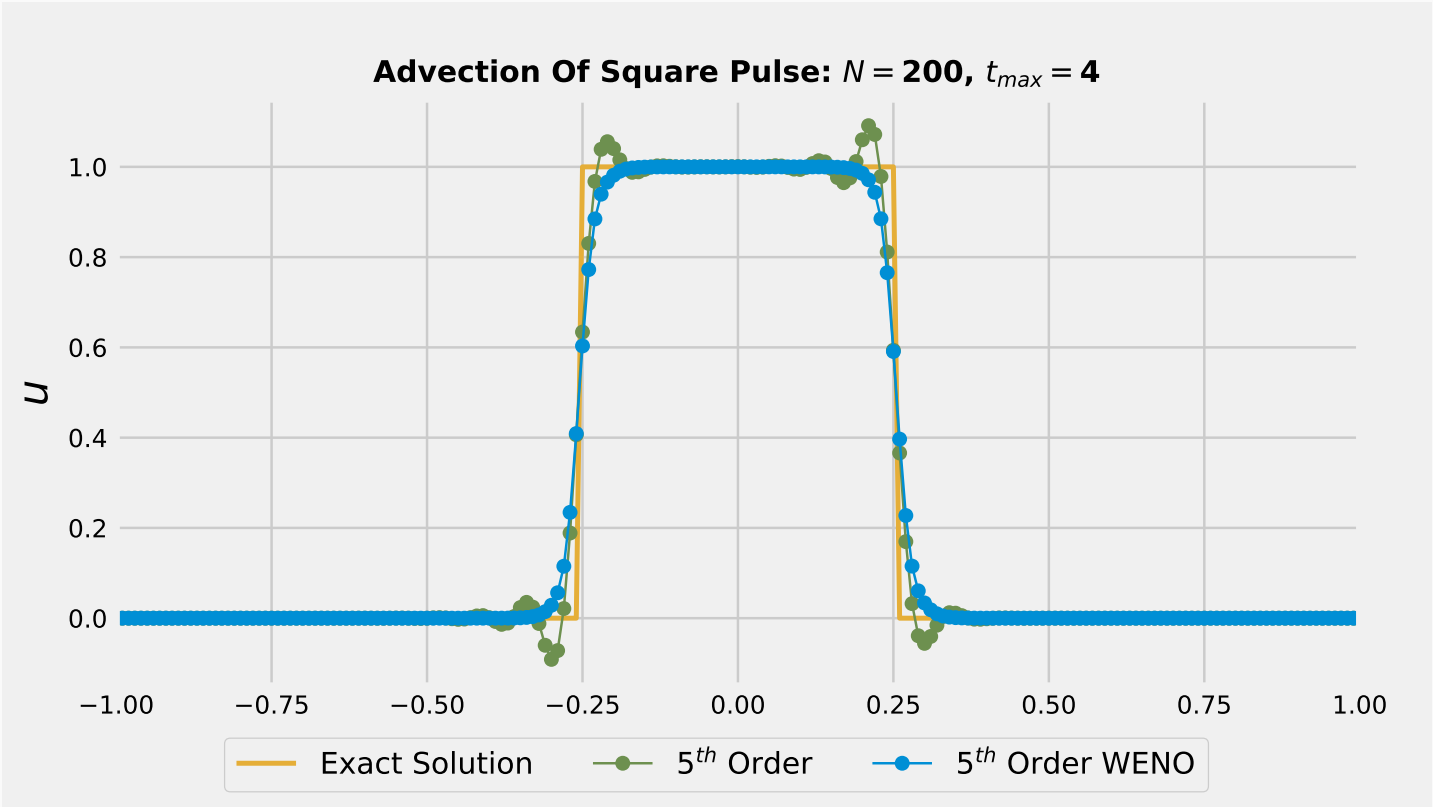

Figure 4: Comparison of linear and WENO schemes for advected pulse

Non-linear Scheme for Euler System

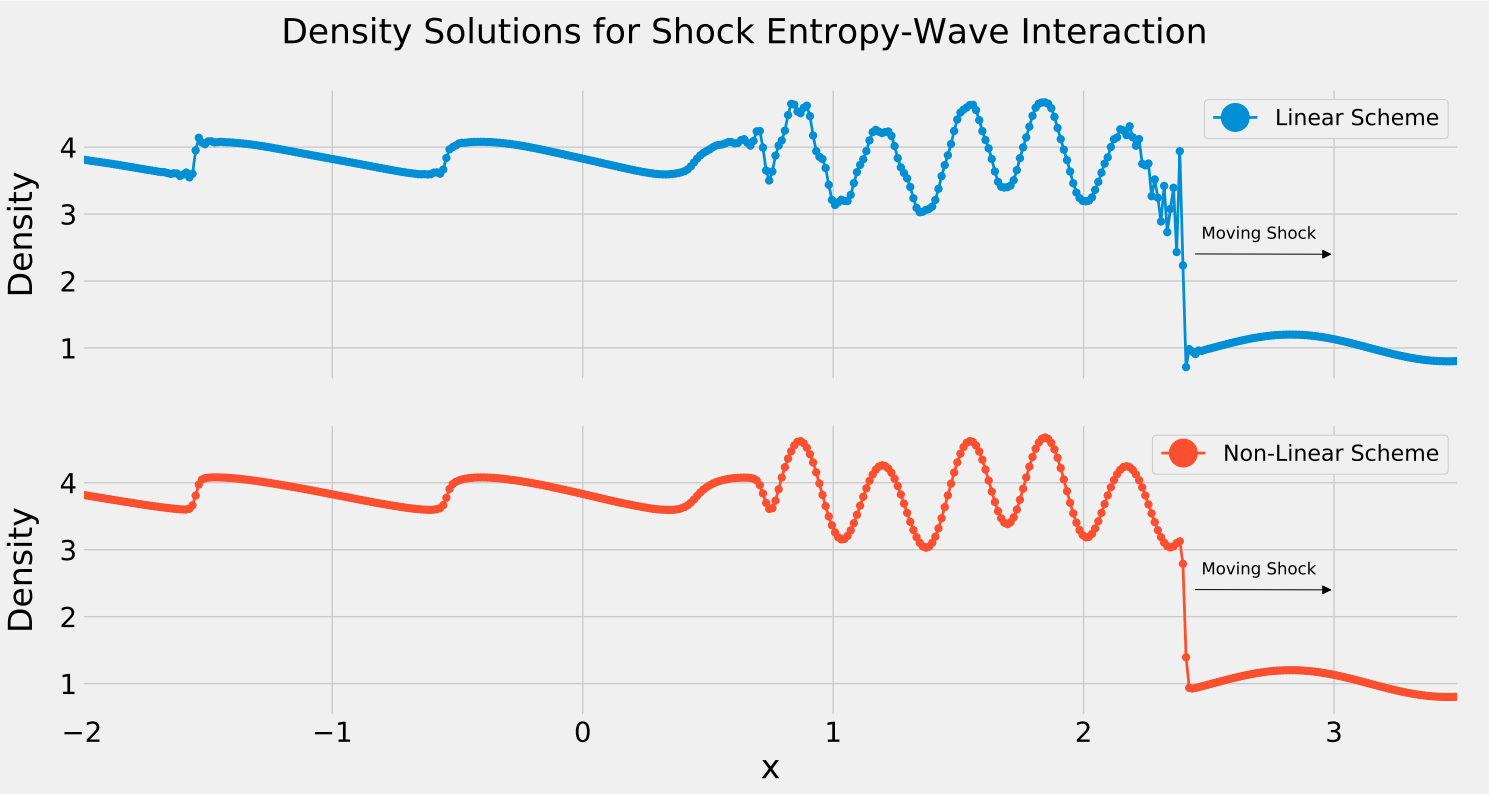

Figure 5: Comparison of linear and non-linear schemes for shock-entropy wave interaction problem

Non-linear scheme for Euler Equations

- The WENO scheme is designed to provide "essentially" non-oscillatory behavior, meaning that 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 complex speed of sound
  - Unphysical results lead to simulation crashing.
  - This issue is readily observed for problems that involve high Mach shock waves with complex interactions

To ensure the physical integrity of the solution, a positivity preserving scheme needs to be developed.

Positivity Example

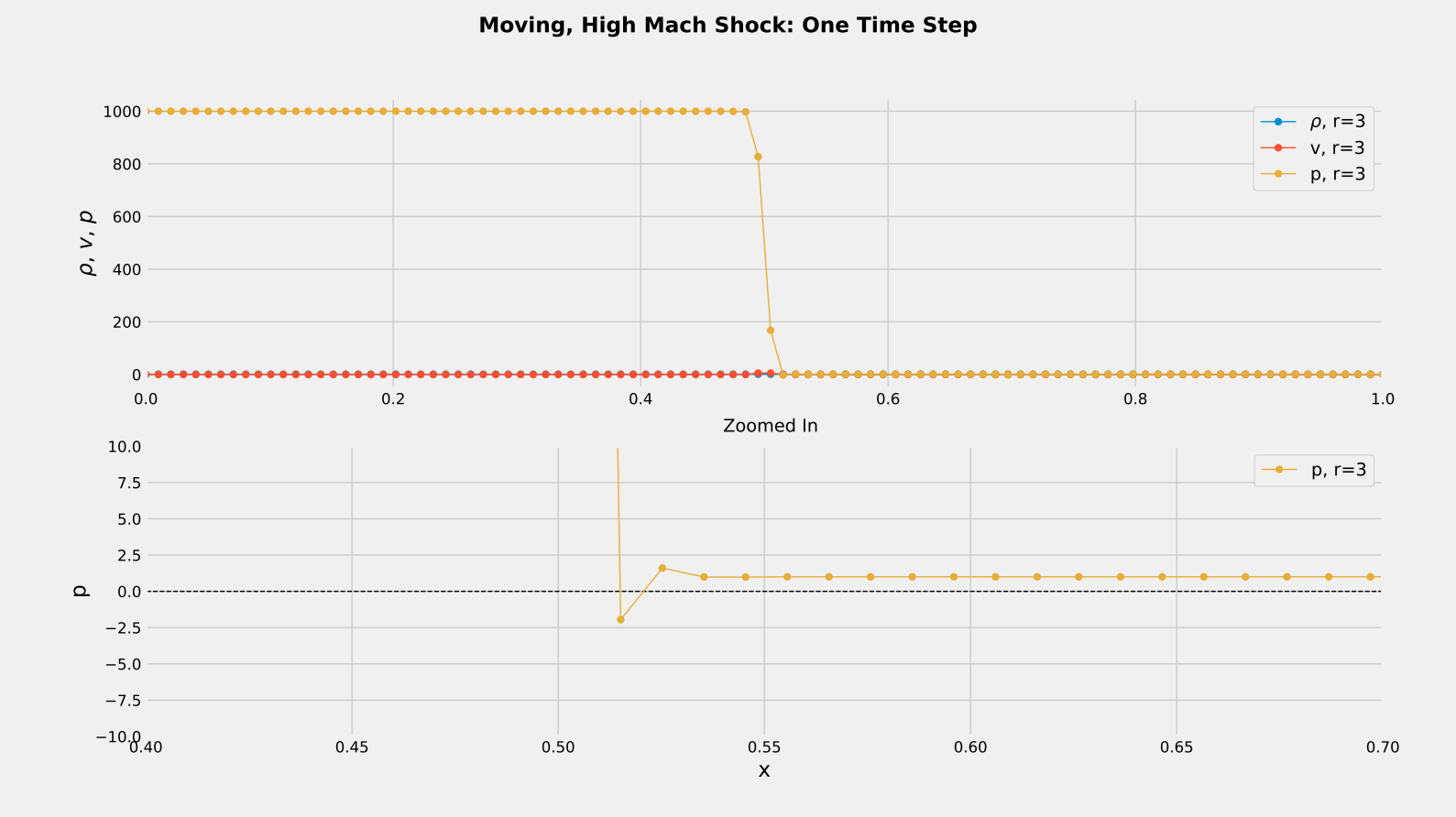

Figure 6: Example of negative pressure values for high Mach shock wave

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 as [4, 3]:

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

- $\theta_{i+1/2} \in [0, 1]$ 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 function (e.g. density) $\theta_{i+1/2}$ are found using 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:

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

Two-fluid Positivity

The two fluid model poses some additional challenges to the positivity scheme.

- The two order parameter equations contain source terms

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High Level Description of Method

Euler Equations of Gas Dynamics

To demonstrate the mechanisms of a non-linear scheme, consider the three-dimensional Euler Equations of gas dynamics:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}[\rho v_j] = 0 \tag{16}$$

$$\frac{\partial}{\partial t}[\rho v_i] + \frac{\partial}{\partial x_j}[\rho v_i v_j + p\delta_{ij}] = 0 \tag{17}$$

$$\frac{\partial}{\partial t}[\rho(e + \tfrac{v_j v_j}{2})] + \frac{\partial}{\partial x_i}[(\rho e + \tfrac{\rho v_j v_j}{2} + p)v_i] = 0 \tag{18}$$

where e is the specific internal energy. In addition to these three equations, an additional property relation (e.g. Ideal Gas Law) is utilized in order to obtain a solvable system.

Numerical Interpretation of Euler System

Each one of the Euler Equations is just a conservation law of the form:

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}[f(u)] \tag{19}$$

enforced upon mass, momentum, and energy, respectively. We define a vector of conserved variables as:

$$\mathbf{u} = [\rho, \rho v, \rho(e + \tfrac{v^2}{2})]^T$$

and the flux of the conserved variables as:

$$\mathbf{f} = [\rho v, \rho v^2 + p, (\rho e + \frac{\rho v^2}{2} + p)v]^T \tag{20}$$

Finally, we can define the primitive variables as the quantities from which the conservation variables are constructed

$$\mathbf{u}_p = [\rho, v, p]^T \tag{21}$$

Traditional Flux Based Approach

Traditionally, the WENO reconstruction process has been performed on the flux functions (20). This allows for the right hand side of a conservation law to be expressed exactly as:

$$\frac{\partial}{\partial x}[f(u)]\bigg|_{x_i} = \frac{h(u_{i+1/2}) - h(u_{i-1/2})}{\Delta x} \tag{22}$$

where h is defined to be some function that gives $f(u(x))$ when averaged over the interval $x \in [x - \frac{1}{2}\Delta x, x + \frac{1}{2}\Delta x]$, that is:

$$f(u(x)) = \frac{1}{\Delta x}\int_{x-\frac{1}{2}\Delta x}^{x+\frac{1}{2}\Delta x} h(u(\xi))d\xi \tag{23}$$

Since, $f(u(x_i))$ is known, the values $h(u_{i\pm 1/2}) \approx P_{WENO,2r-1}(x_{i+\frac{1}{2}})$ can be approximated using the WENO scheme to yield a high order approximation to the spatial derivative term in the conservation law. However, as shown by Shahbazi [2], this approach can fail to preserve the non-oscillatory property for certain multi-fluid flow problems. To combat this, a new method based upon the WENO reconstruction of primitive variables was proposed.

Primitive Variable Reconstruction Approach

The key difference between the traditional WENO method and the scheme proposed by Shahbazi [2] lies in how the spatial derivatives are calculated. In the traditional approach, the derivatives are calculated using the WENO reconstruction directly on the flux functions. In the new method, the derivatives are approximated to order $2r$ by performing the WENO reconstruction on the primitive variables and then forming the flux functions directly from these approximated values. Here, the derivative term is calculated as:

$$h\frac{\partial f}{\partial x}\bigg|_{x_i} \approx (\hat{f}_{i+1/2} - \hat{f}_{i-1/2}) = \sum_{q=0}^{q=r} d_q (f^{WENO}_{i+q-1/2} - f^{WENO}_{i-q-1/2}) \tag{24}$$

With Equation 24 giving a high order approximation for the right hand side of each governing equation, a High-order Runge-Kutte method can be utilized to integrate in time.

Thank You

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