

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

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- 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.
 - 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.

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

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

- $\Gamma_1 = \frac{1}{\gamma-1}$ 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
 - 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:

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

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 [1, 2]
 - Enhances ability to solve multi-dimensional problems

Higher Order Schemes

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

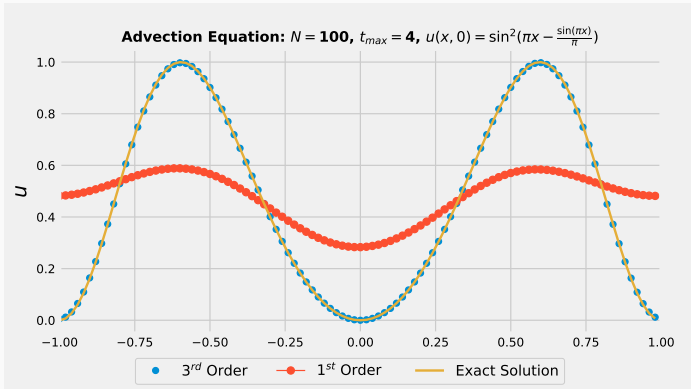


Figure 1: Comparison of First and Third Order solutions for advection equation with smooth initial condition

Discontinuous Solutions

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

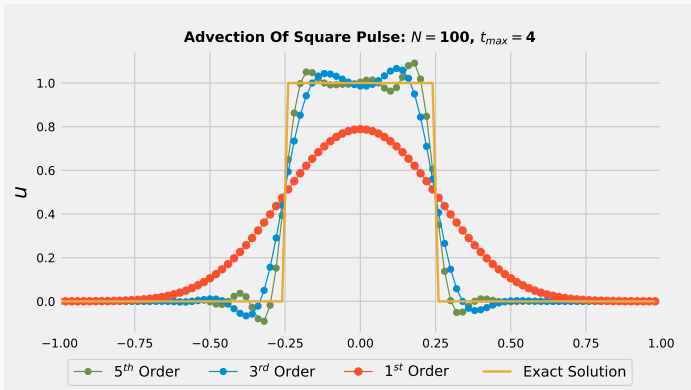


Figure 2: Comparison of First and Third Order solutions for advection equation with discontinuous initial condition

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

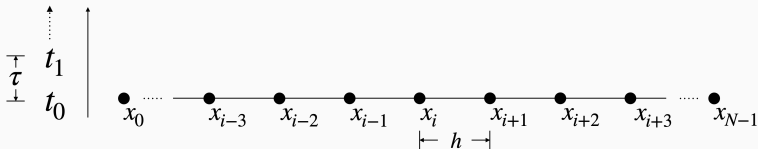
Discretization

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

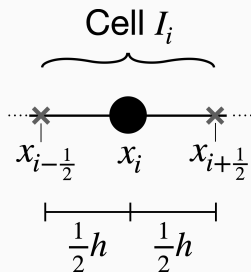
Approach

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:

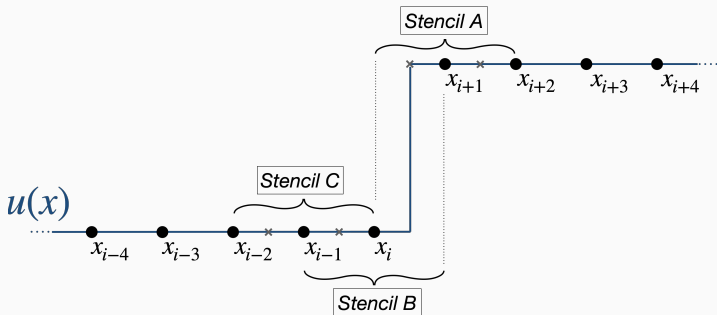
High order, non-oscillatory approximations to the cell boundary fluxes, $f(u(x_{i\pm 1/2}))$



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 tabulated constants d_j .

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

Non-Linear Scheme for Advected Pulse

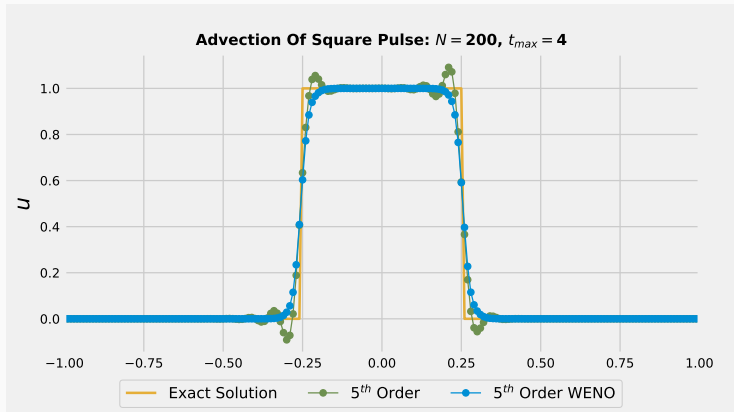


Figure 3: Comparison of linear and WENO schemes for advected pulse

Non-linear Scheme for Euler System

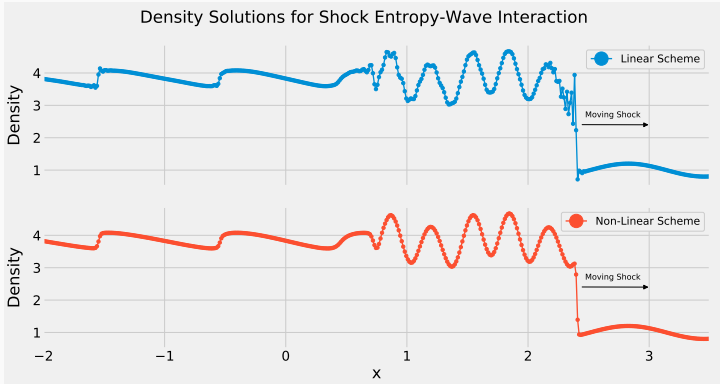


Figure 4: Comparison of linear and non-linear schemes for shock-entropy wave interaction problem

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 achieve a robust scheme, a positivity preserving method needs to be developed.

Positivity Example

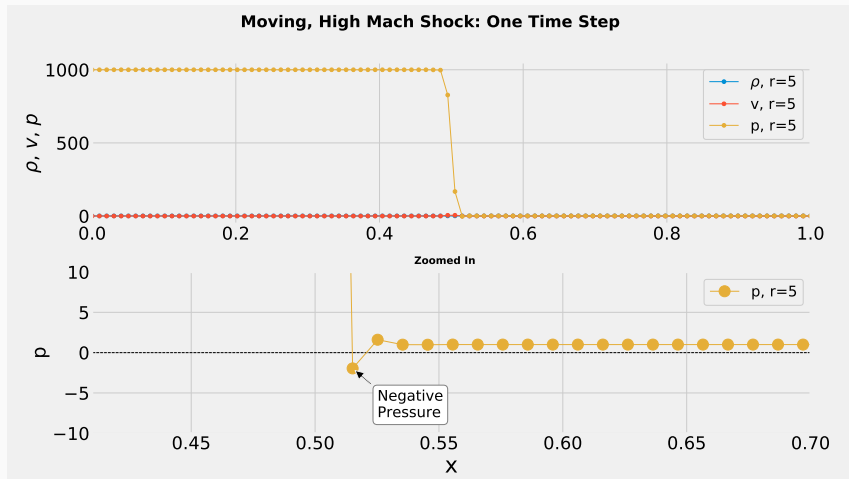


Figure 5: Example of negative pressure values for high Mach shock wave

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 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:

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

Positivity Example

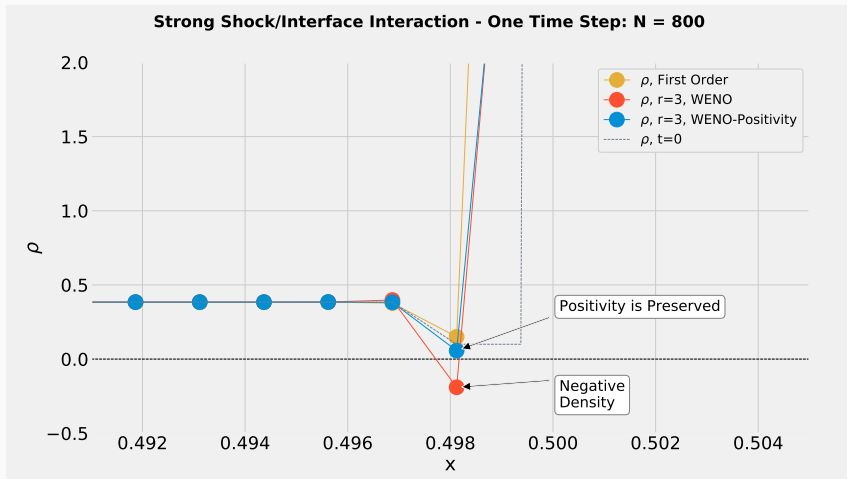


Figure 6: Impact of positivity scheme for strong shock/interface interaction

Positivity Example

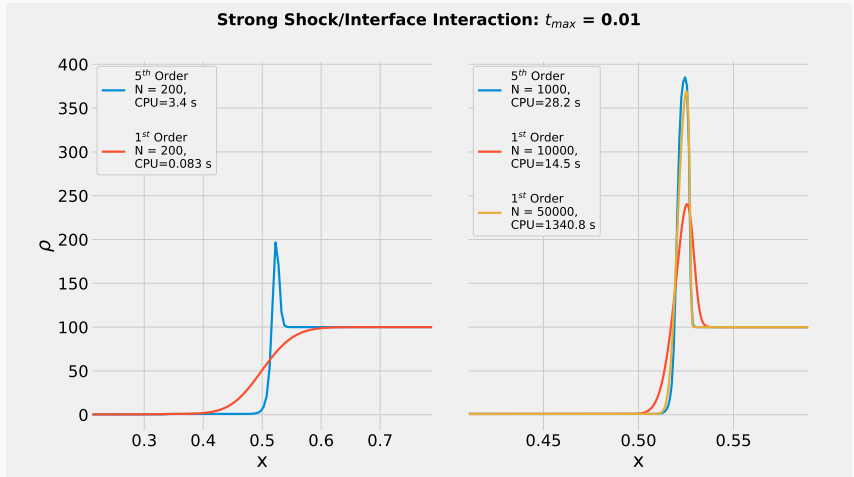


Figure 7: Example of negative pressure values for high Mach shock wave

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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:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} [\rho v_j] = 0 \quad (11)$$

$$\frac{\partial}{\partial t} [\rho v_i] + \frac{\partial}{\partial x_j} [\rho v_i v_j + p \delta_{ij}] = 0 \quad (12)$$

$$\frac{\partial}{\partial t} [\rho (e + \frac{v_j v_j}{2})] + \frac{\partial}{\partial x_j} [(\rho e + \frac{\rho v_j v_j}{2} + p) v_i] = 0 \quad (13)$$

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:

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}[f(u)] \quad (14)$$

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

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

and the flux of the conserved variables as:

$$\mathbf{f} = [\rho v, \rho v^2 + p, (\rho e + \frac{\rho v^2}{2} + p)v]^T \quad (15)$$

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

$$\mathbf{u}_p = [\rho, v, p]^T \quad (16)$$

Traditional Flux Based Approach

Traditionally, the WENO reconstruction process has been performed on the flux functions (15). This allows for the right hand side of a conservation law to be expressed exactly as:

$$\left. \frac{\partial}{\partial x} [f(u)] \right|_{x_i} = \frac{h(u_{i+1/2}) - h(u_{i-1/2})}{\Delta x} \quad (17)$$

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:

$$f(u(x)) = \frac{1}{\Delta x} \int_{x-\frac{1}{2}\Delta x}^{x+\frac{1}{2}\Delta x} h(u(\xi)) d\xi \quad (18)$$

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:

$$h \frac{\partial f}{\partial x} \Big|_{x_i} \approx (\hat{f}_{i+1/2} - \hat{f}_{i-1/2}) = \sum_{q=0}^{q=r} d_q (f_{i+q-1/2}^{WENO} - f_{i-q-1/2}^{WENO}) \quad (19)$$

With Equation 19 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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