High Order, Non-linear Finite Difference Schemes

Thesis Research - Overview

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Overview

- Introduction - discussion of the conservation law its applications
- Overview of finite difference methods
- The WENO scheme
- A positivity preserving WENO scheme
- Numerical Examples
- Conclusion

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 equations.

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

$$\frac{\partial \Gamma_2}{\partial t} + v\frac{\partial \Gamma_2}{\partial x} = 0 \tag{6}$$

- 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 (0 for ideal gasses)
- $\Gamma_1 = \frac{1}{\gamma - 1}$
- $\Gamma_2 = \frac{\gamma\Pi}{\gamma - 1}$

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

Review of Finite Difference Methods

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

Finite Difference Schemes

The Taylor Series expansion $u(x)$ centered about x_i evaluated at $x = x_i + jh$ is:

$$u(x_i + jh) = u(x_i) + (jh)\left.\frac{du}{dx}\right|_{x_i} + \frac{(jh)^2}{2!}\left.\frac{d^2u}{dx^2}\right|_{x_i} + \frac{(jh)^3}{3!}\left.\frac{d^3u}{dx^3}\right|_{x_i} + \mathcal{O}(h^4) \tag{8}$$

taking $j = 1$, we have

$$u(x_i + h) = u(x_i) + (h)\left.\frac{du}{dx}\right|_{x_i} + \frac{1}{2!}\left.\frac{d^2u}{dx^2}\right|_{x_i} + \mathcal{O}(h^3) \tag{9}$$

Truncating the higher order terms and solving for the derivative gives:

$$\left.\frac{du}{dx}\right|_{x_i} \approx \frac{u(x_i + h) - u(x_i)}{h} = \frac{u_{i+1} - u_i}{h} \tag{10}$$

which is a first order, *forward* finite difference approximation.

- It is a forward-biased approximation because we utilize a point (x_{i+1}) that falls after or downwind of x_i on the grid.
- Taking $j = -1$ would give a backwards finite difference formula.
- Subtracting the backwards scheme from the forward scheme would cancel the second derivative term to give a second order approximation.

Higher Order Schemes

High order finite difference approximations can be obtained by evaluating the Taylor expansion at multiple points surrounding x_i and combining each approximation such that the $2^{nd}, 3^{rd}, 4^{th} \ldots$ order terms cancel.

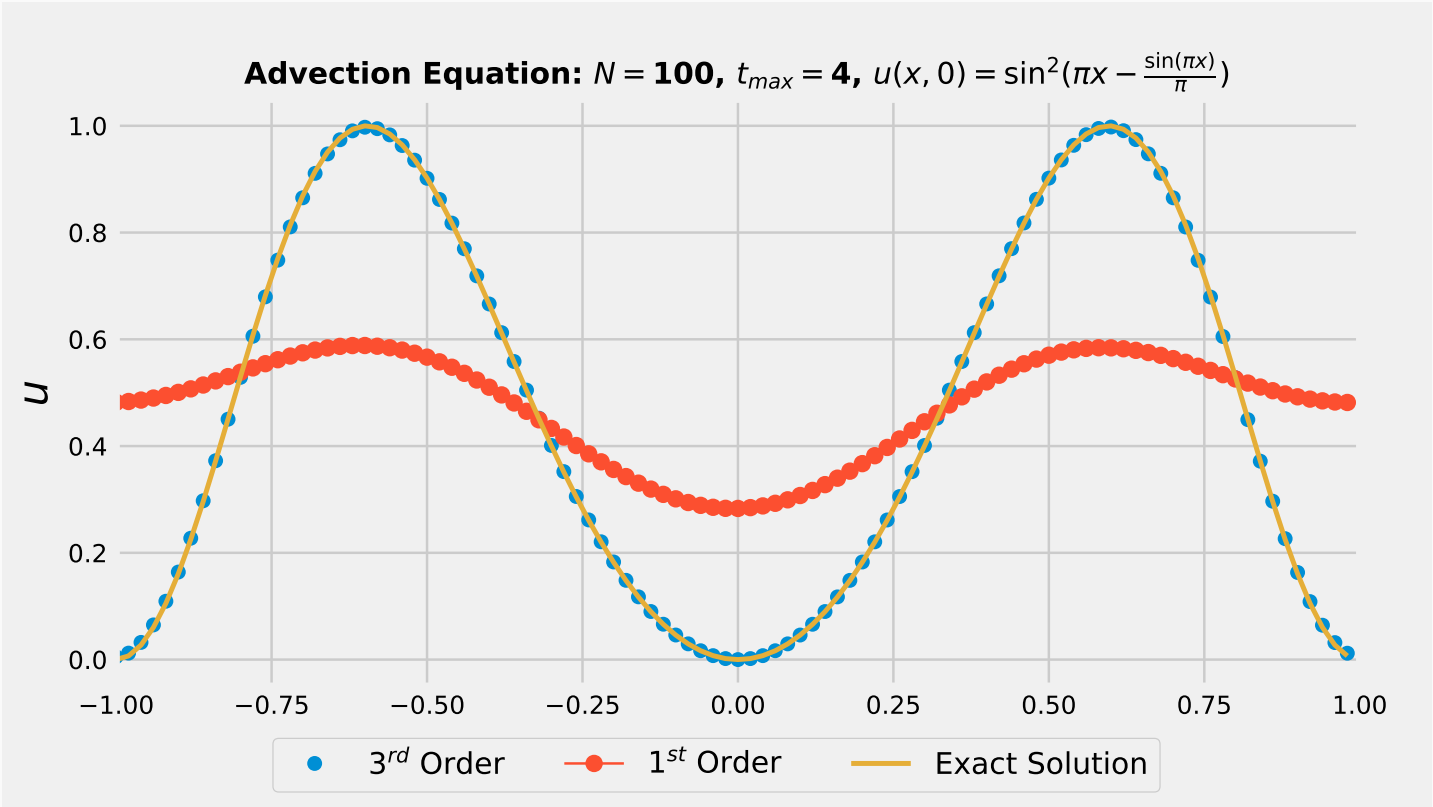

Figure 1: Comparison of First and Third Order solutions for advection equation with smooth initial condition

Discontinuous Solutions

- High order methods work great provided the solution is continuous.
- For discontinuous solutions, high order methods suffer from spurious oscillations that do not diminish with grid refinement.

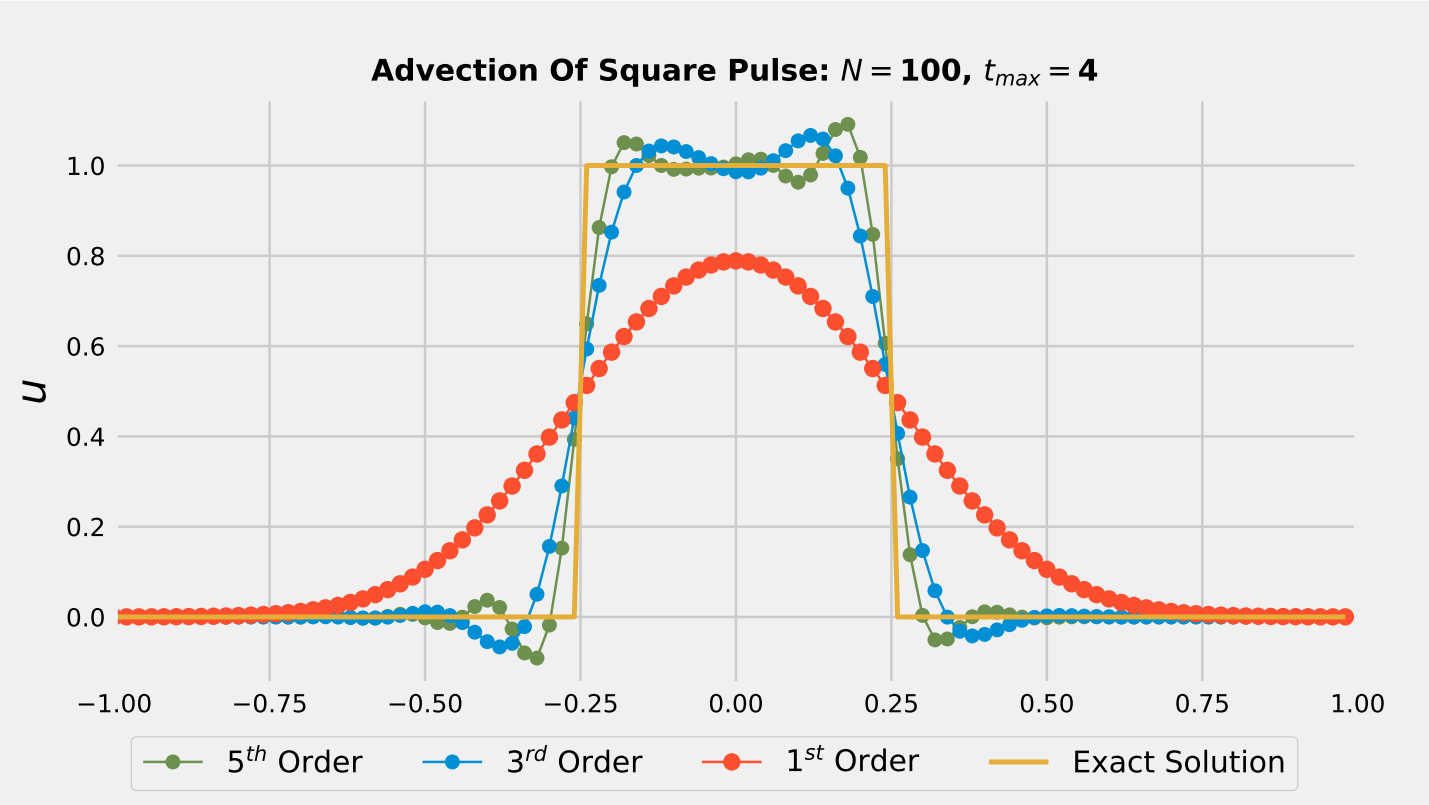

Figure 2: Comparison of First and Third Order solutions for advection equation with discontinuous initial condition

Why Non-Linear Schemes?

- High order Finite Difference schemes suffer from spurious oscillations near discontinuities
- Non-linear methods attenuate oscillations by utilizing a feedback loop to adjust the solution scheme near discontinuities
  - High order solution is retained in smooth regions
  - First order, non-oscillatory solution is obtained in discontinuous regions

WENO Method

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

$$\frac{\partial}{\partial x}[f(u_i)] = \frac{\bar{f}_{i+1/2} - \bar{f}_{i-1/2}}{h} \tag{11}$$

where

$$f(u_i) = \frac{1}{h}\int_{x-h/2}^{x+h/2} \bar{f}(\xi)d\xi \tag{12}$$

- Thus, the goal of the WENO scheme is to develop high order, non-oscillatory approximations for the numerical flux function $\hat{f}_{i\pm1/2}$
- The numerical flux function can be computed from the known flux $f(u_i)$
- Technically, WENO is not, in itself, a finite difference scheme; rather it is a method of flux reconstruction. [2, 1]

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:

$$u(x_i + \tfrac{1}{2}h) \approx P_{r,k_s,i+\frac{1}{2}} = \sum_{q=0}^{q=r-1} a_{r,k_s,q}\, u_{i-k_s+q} \tag{13}$$

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

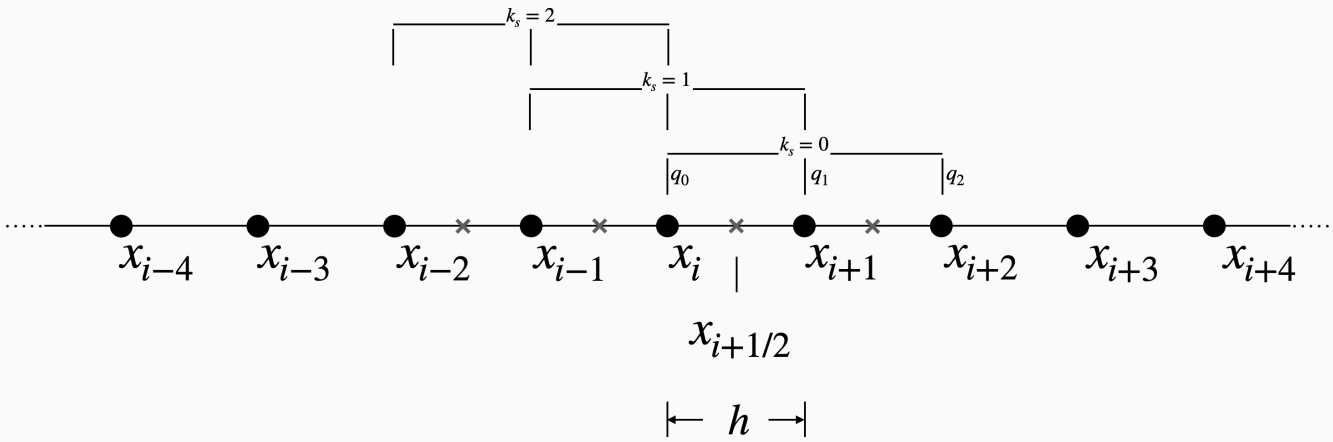

Figure 3: Illustration of candidate stencils for forming $P_{r,k_s,i+1/2}$

WENO Framework Continued

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

$$P^*_{r,i+\frac{1}{2}} = \sum_{k_s=0}^{k_s=r-1} b_{r,k_s} P_{r,k_s,i+\frac{1}{2}} \tag{14}$$

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

- The goal of WENO is to modify 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 Continued

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

$$P^{WENO}_{r,i+\frac{1}{2}} = \sum_{k_s=0}^{k_s=r-1} \omega_{r,k_s,i+\frac{1}{2}} P_{r,k_s,i+\frac{1}{2}} \tag{15}$$

where

$$\omega_{r,k_s} = \frac{\alpha_{r,k_s}}{\sum_{j=0}^{R} \alpha_{r,j}} \tag{16}$$

$$\alpha_{r,k_s} = \frac{b_{r,k_s}}{(\beta_{r,k_s,i} + 10^{-40})^r} \tag{17}$$

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.

$$\beta_{r,k_s,i} = \sum_{l=0}^{r-1} h^{2m-1} \int_{-\frac{1}{2}h}^{\frac{1}{2}h} \left[\frac{d^m}{d\xi} P_{r,k_s,i+1/2}(\xi) \right]^2 d(\xi - x_i) \tag{18}$$

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.

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

- Performing the reconstruction on the known fluxes supplies the high order derivative approximation as:

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

- Alternately, the WENO reconstruction can be performed *directly* on 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[3]:

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

Non-linear Schemes are awesome

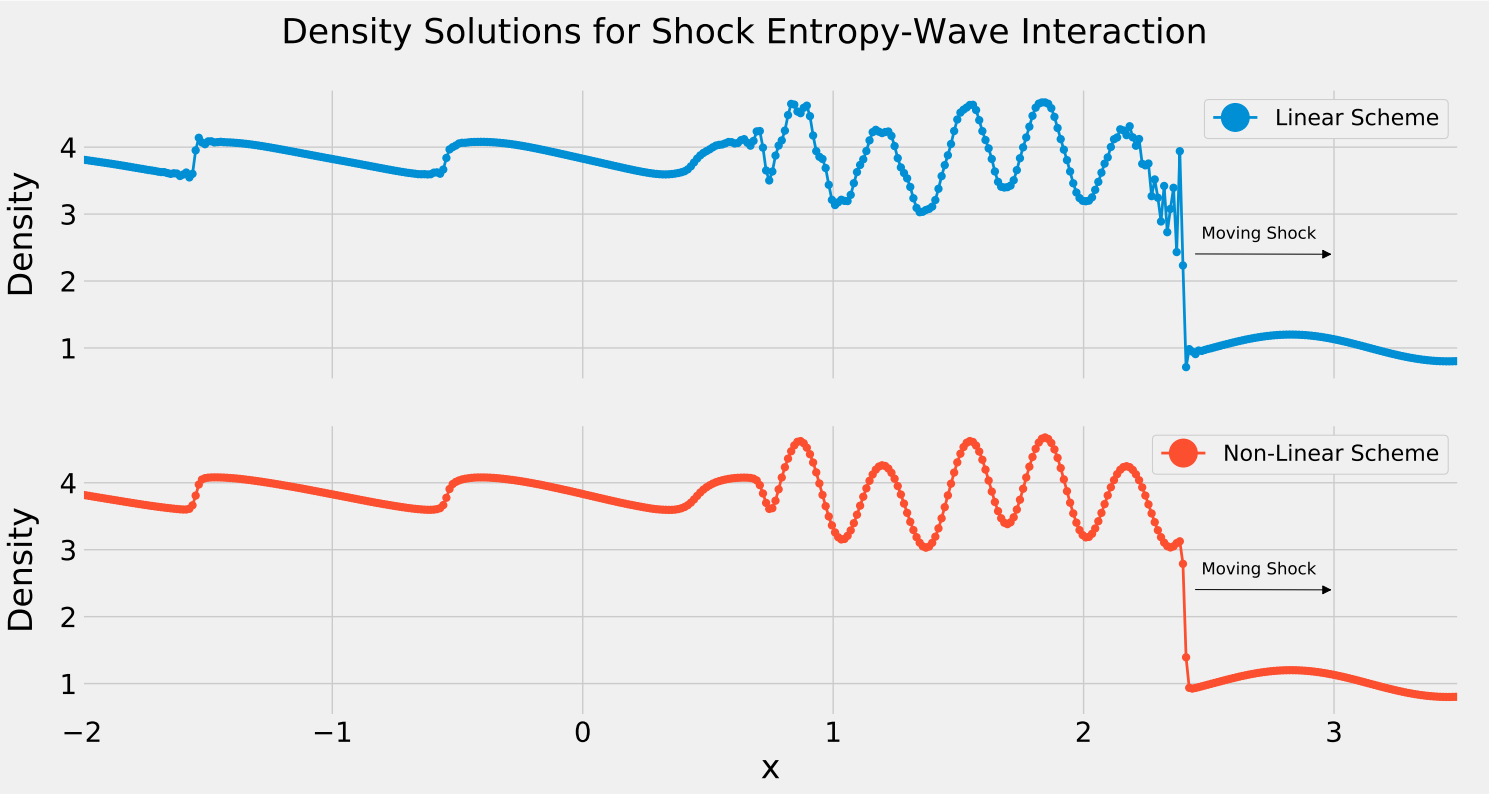

Figure 4: Comparison of linear and non-linear schemes for shock-entropy wave interaction problem

Non-linear schemes also have issues

- 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 remedy this, a positivity preserving scheme needs to be developed.

Parameterized Flux Limiting Positivity Preservation Scheme

$$u_i^{n+1} = u_i^n - \frac{\tau}{h}\{H_{i,+}^{RK} - H_{i,-}^{RK}\}$$

Positivity is good for Burgers equation

Positivity is even better for Euler

show several plots - demos to illustrate this.

Research Goals

The overall goals of this project are as follows:

- Implement Dr. Shahbazi's proposed primitive variable based WENO scheme [3] for 9^{th} order and higher
- Enforce positivity preservation for density and pressure
  - Generalize methods of Xiong et al [4] to primitive variable based WENO scheme.
- Extend to multi-phase model
  - Four equation model of Saurel et al [**?**]
  - Five equation model [**?**]
- Extend to 2D

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:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}[\rho v_j] = 0 \tag{19}$$

$$\frac{\partial}{\partial t}[\rho v_i] + \frac{\partial}{\partial x_j}[\rho v_i v_j + p\delta_{ij}] = 0 \tag{20}$$

$$\frac{\partial}{\partial t}[\rho(e + \tfrac{v_j v_j}{2})] + \frac{\partial}{\partial x_i}[(\rho e + \tfrac{\rho v_j v_j}{2} + p)v_i] = 0 \tag{21}$$

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:

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}[f(u)] \tag{22}$$

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:

$$\mathbf{f} = [\rho v, \rho v^2 + p, (\rho e + \frac{\rho v^2}{2} + p)v]^T \tag{23}$$

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

$$\mathbf{u}_p = [\rho, v, p]^T \tag{24}$$

Traditional Flux Based Approach

Traditionally, the WENO reconstruction process has been performed on the flux functions (23). This allows for the right hand side of a conservation law to be expressed exactly as:

$$\frac{\partial}{\partial x}[f(u)]\bigg|_{x_i} = \frac{h(u_{i+1/2}) - h(u_{i-1/2})}{\Delta x} \tag{25}$$

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:

$$f(u(x)) = \frac{1}{\Delta x}\int_{x-\frac{1}{2}\Delta x}^{x+\frac{1}{2}\Delta x} h(u(\xi))d\xi \tag{26}$$

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 [3], 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 [3] 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:

$$h\frac{\partial f}{\partial x}\bigg|_{x_i} \approx (\hat{f}_{i+1/2} - \hat{f}_{i-1/2}) = \sum_{q=0}^{q=r} d_q (f^{WENO}_{i+q-1/2} - f^{WENO}_{i-q-1/2}) \tag{27}$$

With Equation 27 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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