

High Order, Non-linear Finite Difference Schemes

Thesis Research - Overview

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

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

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

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

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.

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

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

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

- 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

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

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

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

- 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)
- $\Gamma_1 = \frac{1}{\gamma-1}$
- $\Gamma_2 = \frac{\gamma\Pi}{\gamma-1}$

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

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

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

where

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

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

taking $j = 1$, we have

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

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

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

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 $2^{nd}, 3^{rd}, 4^{th} \dots$ order terms cancel.

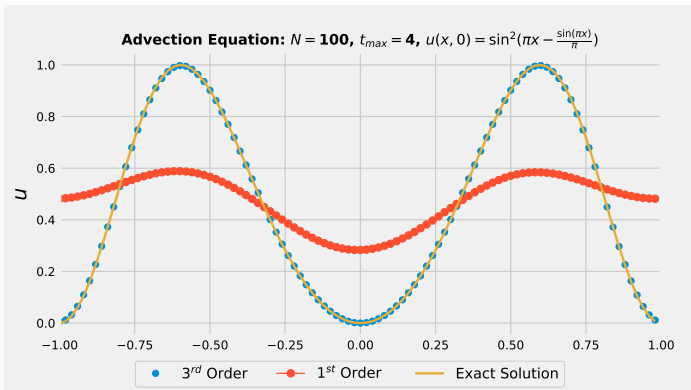


Figure 1: Comparison of First and Third Order solutions for advection equation with smooth initial condition

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.

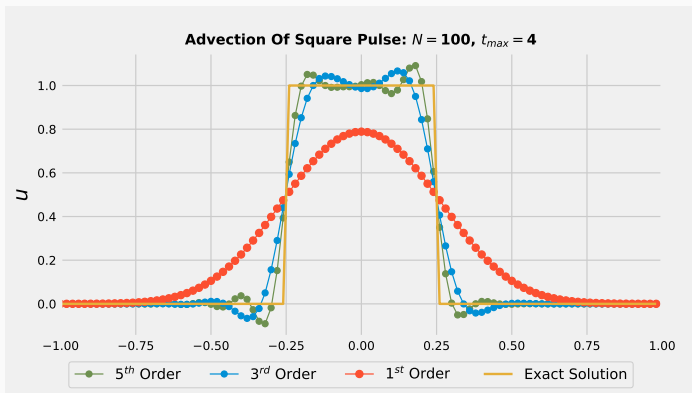


Figure 2: Comparison of First and Third Order solutions for advection equation with discontinuous initial condition

Considering, the

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

The Weighted Essentially Non-Oscillatory (WENO) method is a non-linear scheme designed to achieve non-oscillatory behavior near discontinuities while preserving high-order accuracy in smooth regions [1]. The method involves forming r Lagrange polynomial reconstructions on $k_s \in [0, r - 1]$ stencils surrounding a point x_i .

$$P_{r,k_s}(x_{i+\frac{1}{2}}) = \sum_{q=0}^{q=r-1} a_{r,k_s,q} u_{i-k_s+q} \quad (11)$$

These r^{th} order polynomial approximations are then summed as a convex combination

$$P_{WENO,2r-1}(x_{i+\frac{1}{2}}) = \sum_{k_s=0}^{k_s=r-1} \omega_{r,k_s,i+\frac{1}{2}} P_{r,k_s}(x_{i+\frac{1}{2}}) \quad (12)$$

where the non-linear weights $\omega_{r,k_s,i+\frac{1}{2}}$ are calculated using a smoothness indicator function such that any smooth sub-stencil is assigned an optimal weight while the contribution of any oscillatory sub-stencil goes to zero. Thus, when all sub-stencils contain smooth approximations, the overall reconstruction will be of order $2r - 1$.

Non-linear Schemes are awesome

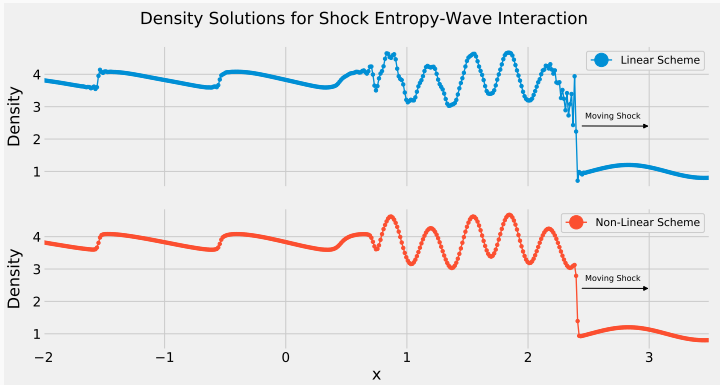


Figure 3: Comparison of linear and non-linear schemes for shock-entropy wave interaction problem

Explain positivity (show graphic?)

math

Positivity is good for Burgers equation

show several plots - demos to illustrate this.

Non-linear Scheme Comparison

The figure below shows two high-order solutions to a moving shock problem. The linear scheme gives un-physical oscillations near the shock and other sharp features in the solution; these issues are remedied by the non-linear scheme.

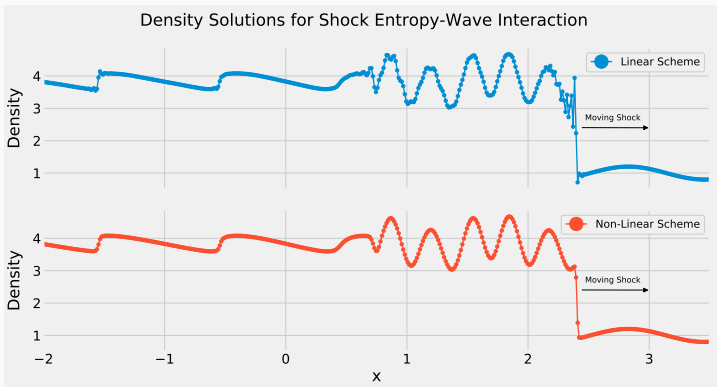


Figure 4: Comparison of linear and non-linear schemes for shock-entropy wave interaction problem

The overall goals of this project are as follows:

- Implement Dr. Shahbazi's proposed primitive variable based WENO scheme [2] for 9th order and higher
- Enforce positivity preservation for density and pressure
 - Generalize methods of Xiong et al [3] 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

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

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

$$\frac{\partial}{\partial t} [\rho v_i] + \frac{\partial}{\partial x_j} [\rho v_i v_j + p \delta_{ij}] = 0 \quad (14)$$

$$\frac{\partial}{\partial t} [\rho (e + \frac{v_j v_j}{2})] + \frac{\partial}{\partial x_i} [(\rho e + \frac{\rho v_j v_j}{2} + p) v_i] = 0 \quad (15)$$

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:

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}[f(u)] \quad (16)$$

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:

$$\mathbf{f} = [\rho v, \rho v^2 + p, (\rho e + \frac{\rho v^2}{2} + p)v]^T \quad (17)$$

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

$$\mathbf{u}_p = [\rho, v, p]^T \quad (18)$$

Traditional Flux Based Approach

Traditionally, the WENO reconstruction process has been performed on the flux functions (17). This allows for the right hand side of a conservation law to be expressed exactly as:

$$\left. \frac{\partial}{\partial x} [f(u)] \right|_{x_i} = \frac{h(u_{i+1/2}) - h(u_{i-1/2})}{\Delta x} \quad (19)$$

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:

$$f(u(x)) = \frac{1}{\Delta x} \int_{x-\frac{1}{2}\Delta x}^{x+\frac{1}{2}\Delta x} h(u(\xi)) d\xi \quad (20)$$

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.

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:

$$h \left. \frac{\partial f}{\partial x} \right|_{x_i} \approx (\hat{f}_{i+1/2} - \hat{f}_{i-1/2}) = \sum_{q=0}^{q=r} d_q (f_{i+q-1/2}^{WENO} - f_{i-q-1/2}^{WENO}) \quad (21)$$

With Equation 21 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



G.-S. Jiang and C.-W. Shu.

Efficient implementation of weighted eno schemes.

Journal of Computational Physics, 126:202–228, 1996.



K. Shahbazi.

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

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



T. Xiong, J.-M. Qiu, and Z. Xu.

Parametrized positivity preserving flux limiters for high order finite difference weno scheme solving compressible euler equations.

J Sci Comput, 67:1066–1088, 2016.