A Second-Order Finite Volume Method that Reduces Numerical Shockwave Anomalies in One Dimension

Daniel W. Zaide[†] and Philip L. Roe[*]

[†]Department of Mechanical Engineering, University of British Columbia

[*]Department of Aerospace Engineering, University of Michigan

cfd@mech.ubc.ca, philroe@umich.edu

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Five very short words to express why I'm so grateful.

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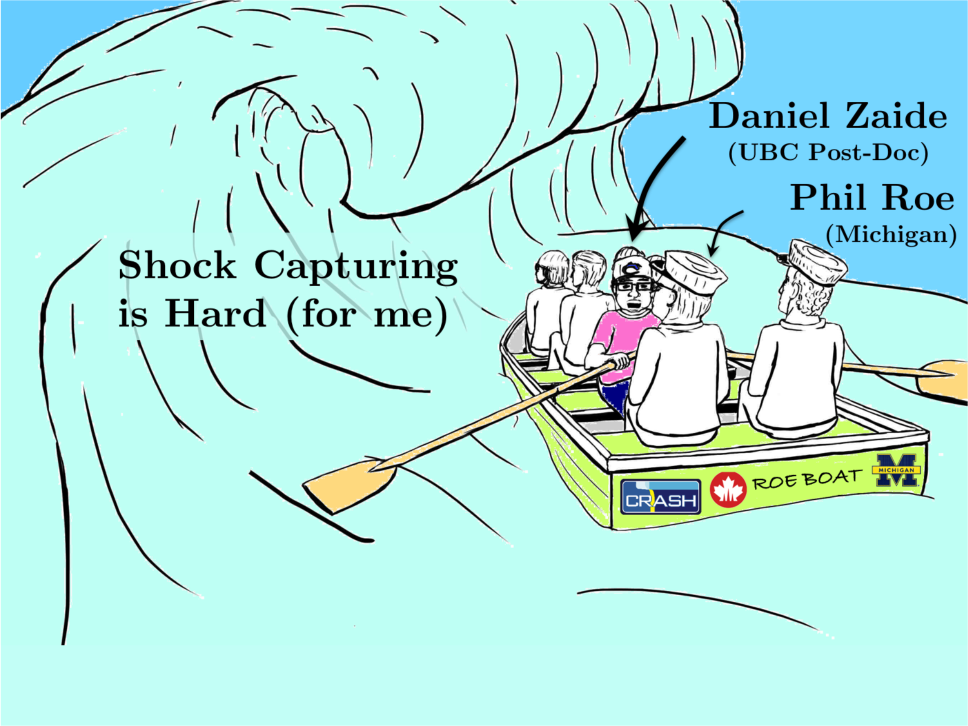
He let me, be me.

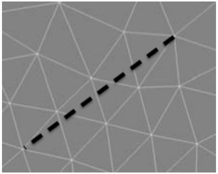

Shock Capturing
is Hard (for me)
Daniel Zaide
(UBC Post-Doc)
Phil Roe
(Michigan)
CRASH
ROE BOAT
MICHIGAN

My Beginning - Summer 2006

"My First CFD Research"

A Local Shock Alignment Method for the 2D Euler Equations on Unstructured Meshes.

By Daniel Zaide, Supervised by Dr. Carl Ollivier-Gooch.



Before

After

[redacted] with regards to shock alignment, [redacted] since the majority of shocks are not linear (at least in interesting problems), shock capturing schemes will never completely result in alignment. True "alignment" or capturing [redacted] is clearly impractical. [redacted]

Current Post-Doc research is similar, but applied to simulation of semi-conductor manufacturing process.

The Euler Equations

To model shockwaves, we examine the Euler Equations for compressible fluid flow,

$$\frac{\partial}{\partial t}\left[\begin{array}{c}\rho\\ \rho u\\ E\end{array}\right]+\frac{\partial}{\partial x}\left[\begin{array}{c}\rho u\\ \rho u^2+p\\ \rho u H\end{array}\right]=\mathbf{0},$$

with $H=\frac{E+p}{\rho}$ and closure from the ideal gas law,

$$p=(\gamma-1)\left(E-\frac{1}{2}\rho u^2\right).$$

While the ideal gas law is often used to solve problems with shockwaves, it does not apply within a shock, but rather outside the shock.

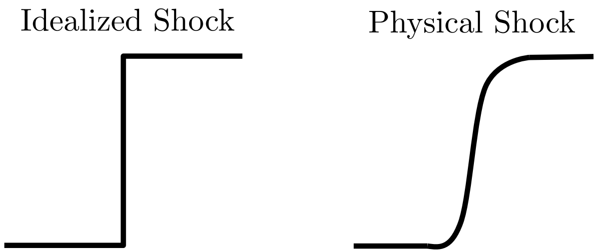
For the Euler Equations, given the left preshock state $\mathbf{u}_L$ and the postshock density, ρ_R, the right pressure and velocity can be computed from

$$
\begin{aligned}
\frac{p_R}{p_L} &= \frac{(\gamma+1)\rho_R - (\gamma-1)\rho_L}{(\gamma+1)\rho_L - (\gamma-1)\rho_R} \\
u_R - u_L &= (p_L - p_R)\sqrt{\frac{2}{\rho_L\left((\gamma-1)p_L + (\gamma+1)p_R\right)}}
\end{aligned}
$$

Taking $\rho_R > \rho_L$ results in the physical Hugoniot curve, and $\rho_R < \rho_L$ results in the nonphysical Hugoniot curve.

Shockwaves

Even with the jump conditions, the picture is not complete.



Physically, a shock has a finite width, coming from the physical viscosity not present in the governing equations.

This leads to two main classes of methods:

- Shock Fitting - *Underestimate* the width of the shock.
- Shock Capturing - *Overestimate* the width of the shock.

Issues in Shock-Capturing

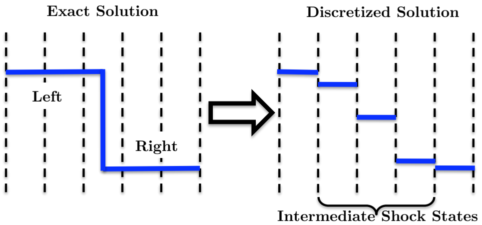
Early attempts to capture shocks led to shocks that were badly smeared or oscillatory. Since then, there are many anomalies that have been identified, such as

- Oscillations behind slowly-moving shocks,
- Start-up errors,
- Wall heating,
- Unstable equilibria,
- Slow convergence to steady state,
- First-order errors in "high-order" schemes,
- "Carbuncles"

Once created, shock capturing methods cannot distinguish between this anomalous behavior and physical waves.

2$^{\text{nd}}$-order methods do not alleviate shock anomalies; they instead preserve errors for much longer than 1$^{\text{st}}$-order methods.

Intermediate Shock States



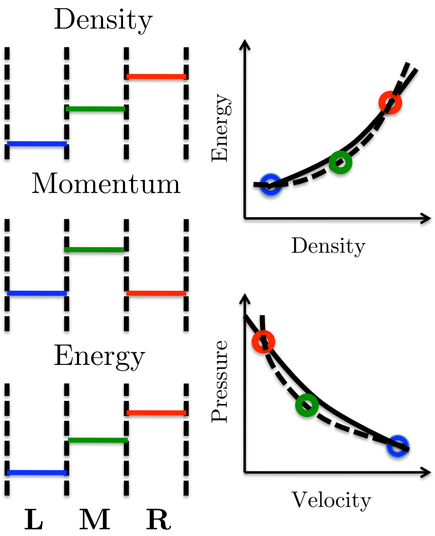
For a single captured shock to be located anywhere on a 1D grid, at least one intermediate state is needed.

Shock-capturing methods treat these intermediate states with value that they should not have, immediately treating them as if they satisfies the governing equations.

However, inside a shock, local thermodynamic equilibrium is not satisfied.

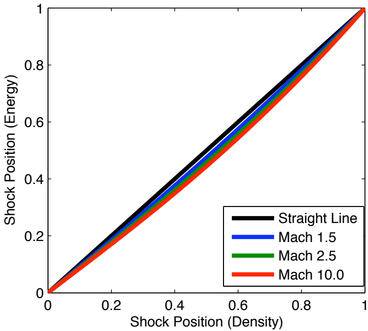
Stationary Shocks

- The intermediate state lies on the nonphysical branch of the Hugoniot.
- This is an exact result for the Godunov, Roe, and CUSP Riemann solvers, and approximately true for many others.
- Stationary shocks with more than one intermediate state still have intermediate states clustered around the nonphysical Hugoniot.
- $\mathbf{f}_L = \mathbf{f}_R \neq \mathbf{f}_M$.



Where is a Captured Shock?

So what's anomalous about the stationary shock? Lets compute shock position.



Because the Hugoniot is not linear, the shock positions calculated from the conserved variables do not agree.

This is an error in an $\mathcal{O}(1)$ quantity, introducing an $\mathcal{O}(\Delta x)$ error into even a nominally high-order scheme.

A Tribute to H.T. Huynh

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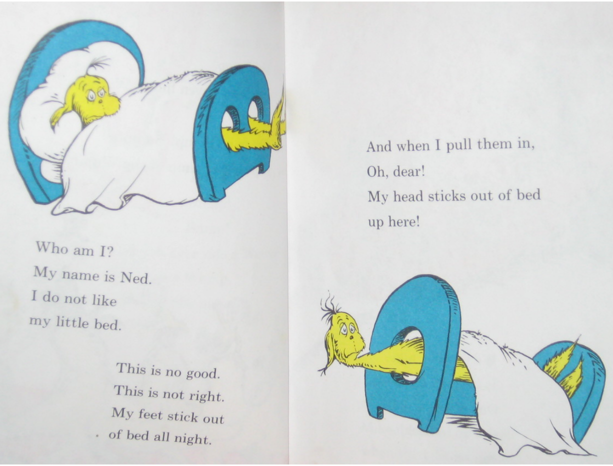
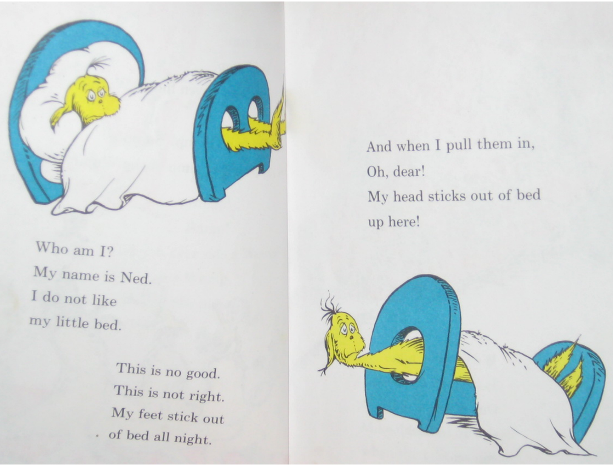


Excerpt from One Fish, Two Fish, Red Fish, Blue Fish by Dr. Seuss.

A Tribute to H.T. Huynh



Excerpt from One Fish, Two Fish, Red Fish, Blue Fish by Dr. Seuss.

It is time for a new bed!

New Flux Functions

Ideas:

- Inside the shock, the assumption of local thermodynamic equilibrium is invalid - why should we use the equation of state inside for these intermediate states?
- Straight-line (Temple) systems do not suffer from these anomalies. Define a modified flux that allows for intermediate shock states to be only on a straight line in state space.
- Most shockwave anomalies occur around slowly moving shocks - focus on getting the stationary case exactly.

Goal: construct a flux function with one-point stationary shocks and no positional ambiguity.

Interpolated Fluxes

To begin, suppose the flux is extrapolated from one side as

$$\mathbf{f}_M^* = \mathbf{f}_L + \tilde{\mathbf{A}}_M(\mathbf{u}_M - \mathbf{u}_L)$$

and extrapolated from the other side as

$$\mathbf{f}_M^* = \mathbf{f}_R - \tilde{\mathbf{A}}_M(\mathbf{u}_R - \mathbf{u}_M).$$

where $\mathbf{A} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}}$. These two equations are consistent if

$$\mathbf{f}_R - \mathbf{f}_L = \tilde{\mathbf{A}}_M(\mathbf{u}_R - \mathbf{u}_L).$$

The simplest flux Jacobian having this property is the cell-centered Roe matrix $\tilde{\mathbf{A}}(\mathbf{u}_L, \mathbf{u}_R)$. The flux can be interpolated from both sides as

$$\mathbf{f}_M^* = \frac{1}{2}(\mathbf{f}_L + \mathbf{f}_R) - \frac{1}{2}\tilde{\mathbf{A}}_{L,R}(\mathbf{u}_R - 2\mathbf{u}_M + \mathbf{u}_L).$$

Interpolated Fluxes

1. If the problem is linear so that the Jacobian matrix $\mathbf{A}(\mathbf{u})$ is constant, then $\mathbf{f}_i^* = \mathbf{f}_i$.
2. For nonlinear systems with smooth data,

$$\mathbf{f}^* \simeq \mathbf{f} + \frac{(\Delta x)^2}{2}\mathbf{A}_x\mathbf{u}_x \simeq \mathbf{f} + \frac{1}{2}\Delta\mathbf{A}\Delta\mathbf{u}$$

3. Near a discontinuity, the effect is $\mathcal{O}(1)$.
4. For data corresponding to a one-point stationary shock, then $\mathbf{f}_i^*$ is constant, not only on each side of the shock, but also in the intermediate cell.

$$\mathbf{f}_L = \mathbf{f}_L^* = \mathbf{f}_M^* = \mathbf{f}_R^* = \mathbf{f}_R$$

Interpolated Fluxes

For the Euler Equations, the interpolated mass flux remains unchanged (conservative quantities are trusted),

$$\textbf{interpolated mass flux} = \rho_i u_i$$

The interpolated momentum flux takes a more interesting form

$$\textbf{interpolated momentum flux} =$$
$$\underbrace{\left(p_i + \rho_i u_i^2\right)}_{\text{equilibrium flux}} + \underbrace{\frac{3-\gamma}{2}\left(\frac{\rho_{i-1}\rho_{i+1}(u_{i-1}-u_{i+1})^2}{(\sqrt{\rho_{i-1}}+\sqrt{\rho_{i+1}})^2} - \rho_i\left(\tilde{u}_i - u_i\right)^2\right)}_{\text{equation of state `correction'}}$$

effectively correcting the equation of state within a shock.

The interpolated energy flux is much more complex...

New Flux Functions

We first begin with **Flux A**, inspired by Roe's Riemann Solver,

$$\boxed{\mathbf{f}^A_{i+\frac{1}{2}} = \frac{1}{2}(\mathbf{f}^*_i + \mathbf{f}^*_{i+1}) - \frac{1}{2}\mathrm{sign}(\tilde{\mathbf{A}}_{i+\frac{1}{2}})(\mathbf{f}^*_{i+1} - \mathbf{f}^*_i)}$$

where $\mathrm{sign}(\mathbf{A}) = \mathbf{R}\mathrm{sign}(\Lambda)\mathbf{L}$.

However this flux is not C^0 continuous, so we introduce **Flux B**

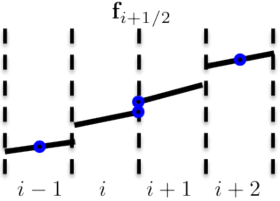
$$\boxed{\mathbf{f}^B_{i+\frac{1}{2}} = \frac{1}{2}(\mathbf{f}^*_i + \mathbf{f}^*_{i+1}) - \frac{1}{2}|\overline{\mathbf{A}}_{i+\frac{1}{2}}|(\mathbf{u}_{i+1} - \mathbf{u}_i)}$$

where $\overline{\mathbf{A}}_{i+\frac{1}{2}}$ is the Roe matrix across cells $i-1$ and $i+2$,

$$\overline{\mathbf{A}}_{i+\frac{1}{2}}(\mathbf{u}_{i+2} - \mathbf{u}_{i-1}) = \mathbf{f}_{i+2} - \mathbf{f}_{i-1}$$

The matrix $\overline{\mathbf{A}}_{i+\frac{1}{2}}$ looks at the big picture, around the shock.

Second-Order Framework



For the four point flux functions, the interface fluxes can be computed using reconstructed data at the edges, with

$$\mathbf{f}_{i+\frac{1}{2}} = \mathbf{f}(\mathbf{u}_{i-1}, \mathbf{u}_i^+, \mathbf{u}_{i+1}^-, \mathbf{u}_{i+2}).$$

This is equivalent to reconstructing the interpolated flux within a cell, *but* using a different slope at each edge of a cell.

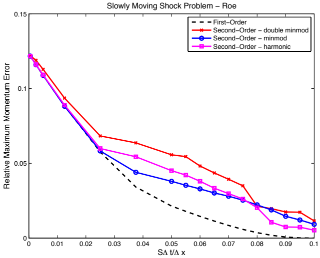
The accuracy of these reconstructions can be analytically verified by noting that for smooth data, $\mathbf{f}^{*,+} = \mathbf{f}^*(\mathbf{u}_{i-1}, \mathbf{u}_i^+, \mathbf{u}_{i+1}^-) \approx \mathbf{f}(\mathbf{u}_i^+)$, the classical result for a second-order finite volume scheme.

Around shockwaves, limiters are still needed to prevent oscillations from the reconstruction, which are a different kind of discontinuity error.

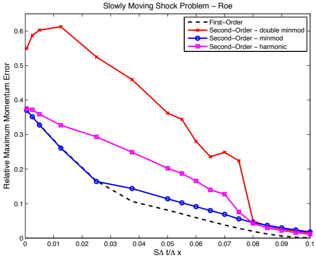
Slowly Moving Shockwaves

Momentum Error vs Shock Speed

$$\text{Relative Maximum Momentum Error } = \max_{x,t}(\rho u)/\rho_R u_R - 1$$



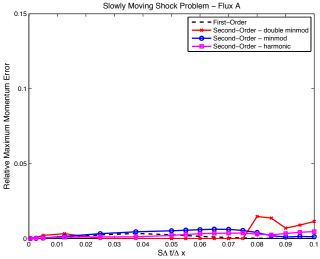
Roe, Mach 2



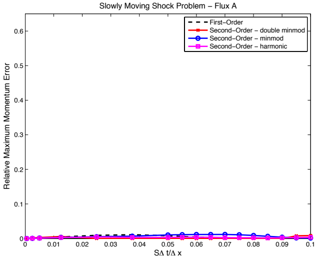
Roe, Mach 10

Slowly Moving Shockwaves

Momentum Error vs Shock Speed



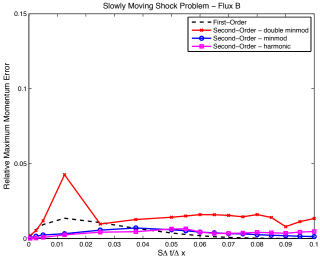
Flux A, Mach 2



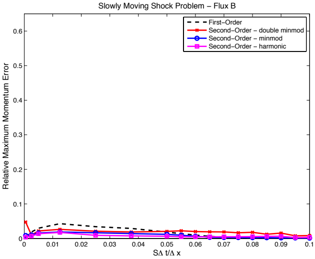
Flux A, Mach 10

Slowly Moving Shockwaves

Momentum Error vs Shock Speed



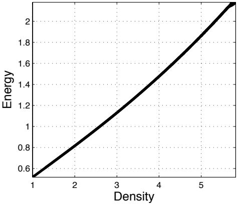
Flux B, Mach 2



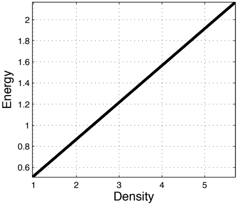
Flux B, Mach 10

Slowly Moving Shockwaves

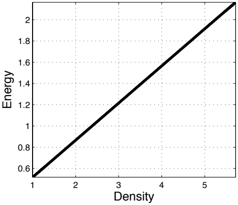
Density-Energy State Plots



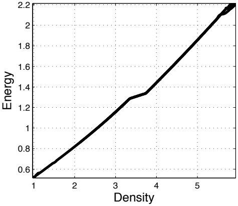
Roe, 1^{st}-order



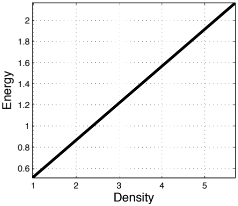
Flux A, 1^{st}-order



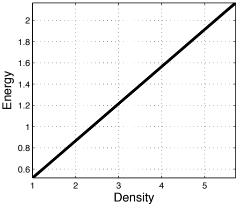
Flux B, 1^{st}-order



Roe, 2^{nd}-order



Flux A, 2^{nd}-order



Flux B, 2^{nd}-order

The Carbuncle

In one dimension, the carbuncle manifests itself as an initially stationary shock that does not remain stationary.

This problem can be set up exactly as a stationary shock problem, with the intermediate state varied as

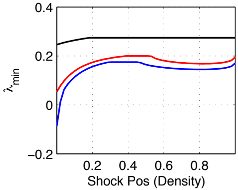
$$\rho_M = x_S \rho_L + (1 - x_S) \rho_R$$

and the remaining variables computed to lie on the nonphysical branch of the Hugoniot curve.

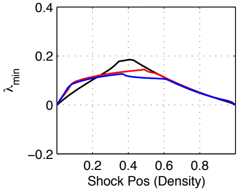
To prevent waves from leaving the domain, a fixed mass outflow boundary condition is used.

The Carbuncle

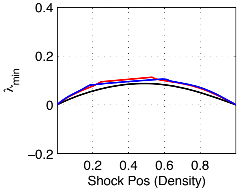
Minimum nonzero eigenvalues for a range of intermediate states for Mach 2 (black), Mach 5 (red) and Mach 10 (blue) are shown



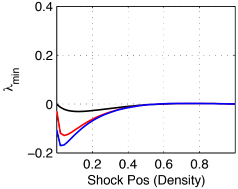
Roe, 1^{st}-order



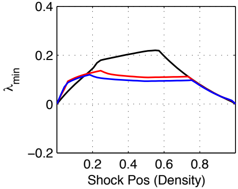
Flux A, 1^{st}-order



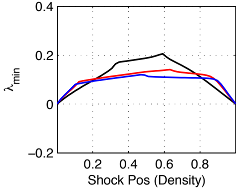
Flux B, 1^{st}-order



Roe, 2^{nd}-order

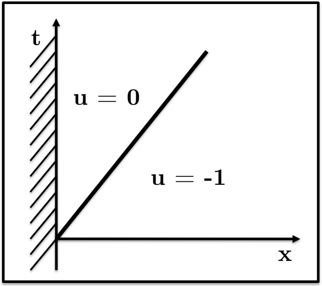


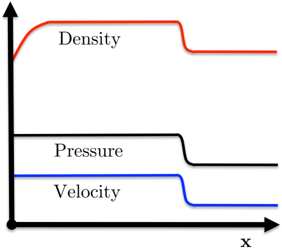
Flux A, 2^{nd}-order



Flux B, 2^{nd}-order

Wall Heating





Virtually all shock-capturing methods provide quite good solutions for pressure and velocity, but predict too small a density in a small region at the origin.

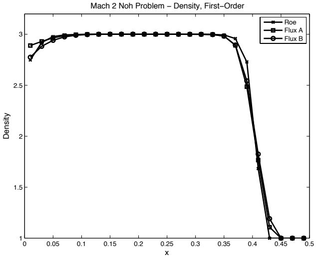
In consequence the temperature there is too high, so that this and related phenomena have been called **wall heating.**

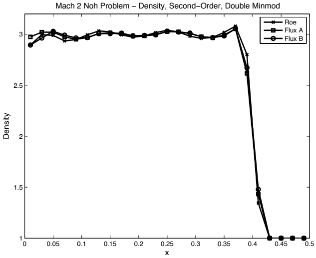
Wall Heating

First-Order

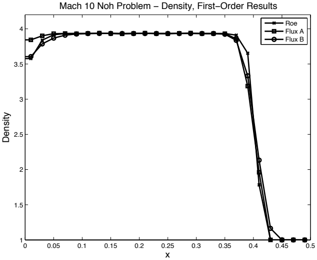
Second-Order

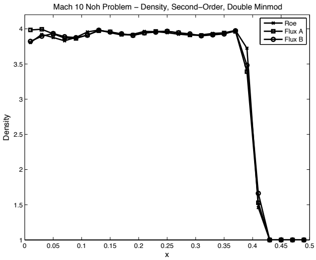
Mach 2





Mach 10

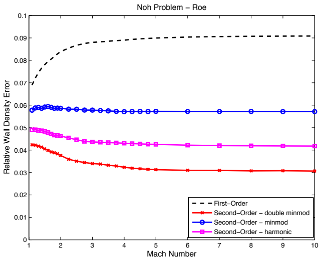




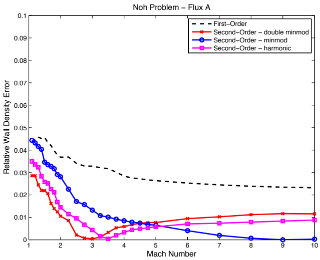
Wall Heating

Wall Density Error

Roe and Flux A shown - Flux B results are comparable to Roe



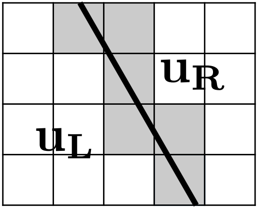
Roe



Flux A

There is a reduction in error at wall, however error is now spread behind shock.

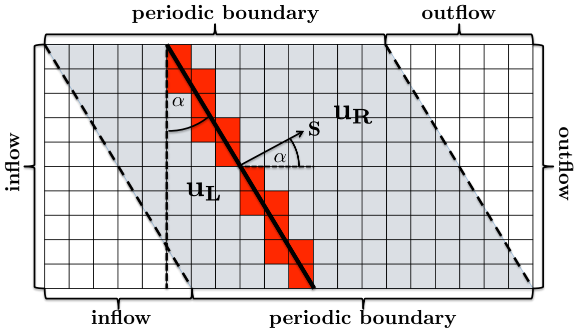
Two Dimensions



Ideally, a definition of the interpolated flux could be chosen such that the flux in each intermediate state equalled that of the flux of the two end states.

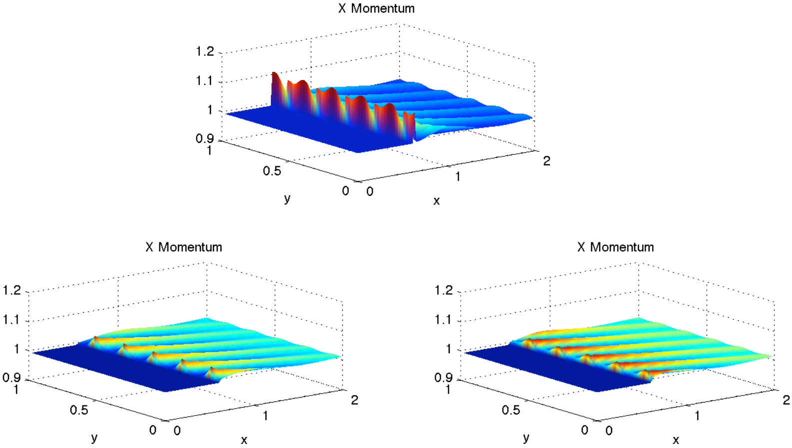
In practice, this is was not trivial, so initially, a simple two-dimensional implementation of both new flux functions was implemented.

Two Dimensional Slowly Moving Shock



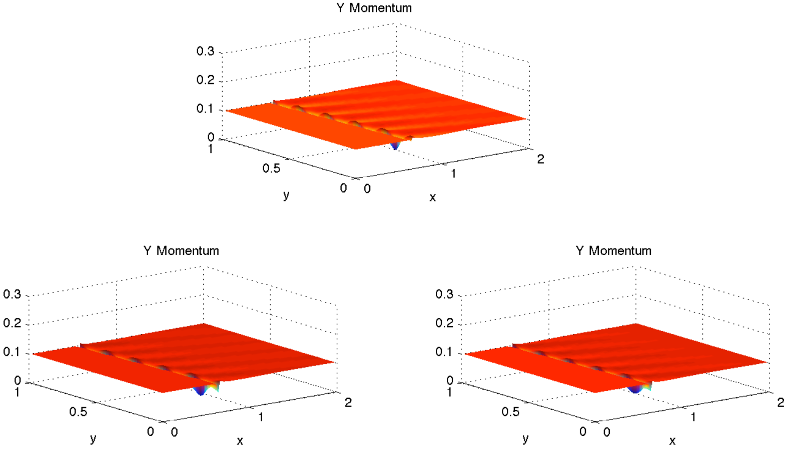
Two Dimensional Slowly Moving Shock

Mach 2 Shock, X momentum, at an angle of 5.7 degrees. Roe (top), Flux A (left), Flux B (right).



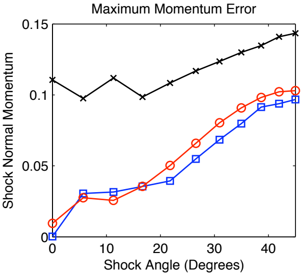
Two Dimensional Slowly Moving Shock

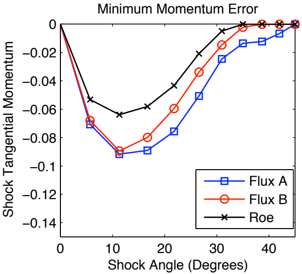
Mach 2 Shock, Y momentum, at an angle of 5.7 degrees. Roe (top), Flux A (left), Flux B (right).



Two Dimensional Slowly Moving Shock

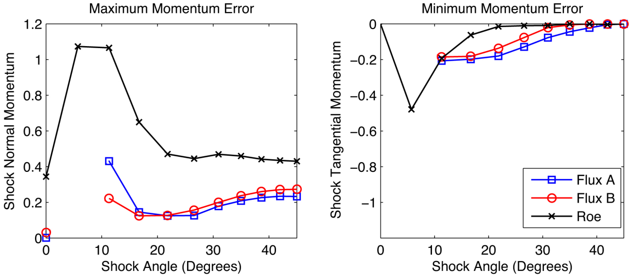
Errors in momentum for both new flux functions and Roe's Riemann solver for the Mach 2 shock with speed 0.01.





Two Dimensional Slowly Moving Shock

Errors in momentum for both new flux functions and Roe's Riemann solver for the Mach 10 shock with speed 0.01.



Further Observations

By construction, both new flux functions show no ambiguity in shock position for the stationary shock.

Away from stationary shocks, both new flux functions perform comparably to Roe's Riemann solver.

Fairly standard MUSCL-type reconstruction is used to obtain second-order accuracy using the extra information already used in the new flux functions.

In two-dimensions, when the method works, it works well. Unfortunately, it tends to be unstable in regions where velocities changed sign, amplifying small oscillations and often resulting in non-physical solutions.

Conclusions

The internal states of a captured shock should not be taken literally; in particular it should not be assumed that they are in thermodynamic equilibrium.

Using the equilibrium equation of state for these internal cells gives rise to ambiguity in the shock location.

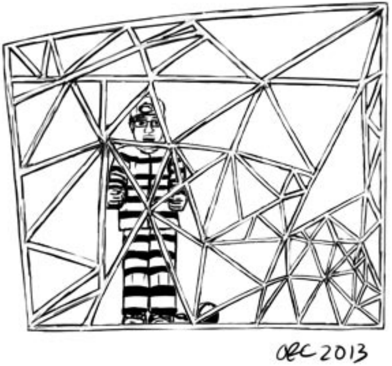
This ambiguity can be linked to many of the anomalies that affect shock-capturing schemes.

It is possible to smooth the fluxes in a way that has no effect on linear systems but which sets the internal fluxes of a stationary shock equal to the external fluxes.

This can be made the basis of schemes that eliminate or greatly reduce anomalous behavior.

By enforcing a shock structure with an unambiguous sub-cell shock position, numerical shockwave anomalies are dramatically reduced.

Questions?



email: cfd@mech.ubc.ca

websites: www.shockcapturing.com, www.unstructuredmesh.com