Numerical Shockwave Anomalies

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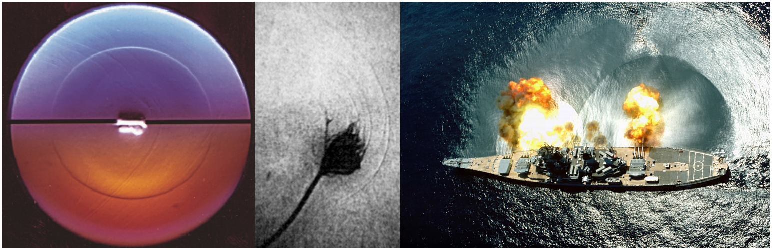
Numerical **Shockwave** Anomalies

Shockwaves

"A shockwave is a surface of discontinuity propagating in a gas at which density and velocity experience abrupt changes."

- Zemplén, 1905



Images - Krehl, Bernstein, Wikipedia

Shockwaves

"Natura non facit saltus."

(Nature does not make jumps.)

Wave equation studied by d'Alembert, Euler, Lagrange, Monge (1700s)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

which has the solution

$$u(x,t) = f(x - ct) + g(x + ct)$$

Compressible flows studied by Hugoniot, Poisson, Rankine, Rayleigh, Stokes (1800s)

Shockwaves

The Euler Equations

The compressible flows they studied were similar to the Euler equations,

$$\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = 0$$

or, expanded as

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \end{bmatrix} = \mathbf{0},$$

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

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

Though initial attempts were wrong, their work would result in the conditions for a the jump across a shock, $\Delta \mathbf{f} = S \Delta \mathbf{u}$

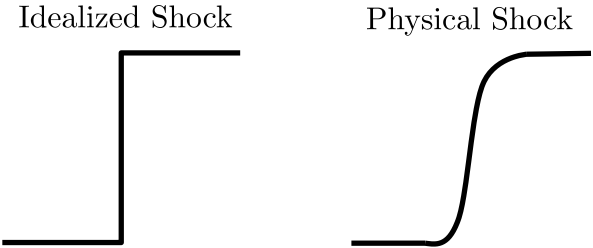
Given the left preshock state $\mathbf{u}_L$ and the postshock density, ρ_R, the right pressure and velocity can be computed from

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

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.

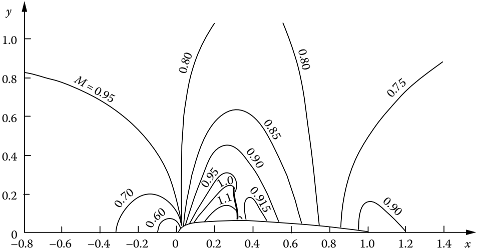


Physically, a shock has a finite width, coming from the physical viscosity not present in the governing equations.

Numerical Shockwave Anomalies

Numerical Shockwaves

The Beginning



The first computations were hand calculations of the flow around a transonic airfoil (Emmons, 1940s).

He assumed the idealized shock, representing it as an explicit discontinuity (underestimating the width).

This was the start of **shock-fitting**.

Image - Salas

Numerical Shockwaves

The Beginning

A Method for the Numerical Calculation of Hydrodynamic Shocks

J. VonNeumann and R. D. Richtmyer
Institute for Advanced Study, Princeton, New Jersey

(Received September 26, 1949)

Around the same time as Emmons, the numerical simulations of shocks were carried out at Los Alamos during the Manhattan Project.

Artificial viscosity was introduced to create entropy and tuned to give computed shocks an internal structure whose length scale was that of the grid size (overestimating the width).

This was the start of **shock-capturing**.

Shock-Capturing

Godunov-Type Finite Volume Methods

Begin by dividing the physical domain into cells x_i with constant width Δx and integrate the conserved quantities in space to get cell-averaged quantities as

$$\overline{\mathbf{u}} = \frac{1}{\Delta x} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} \mathbf{u} \, \mathrm{d}x$$

Integrating the full equations in space then gives

$$\Delta x \overline{\mathbf{u}}_t + \mathbf{f}(\mathbf{u}(x_{i+\frac{1}{2}})) - \mathbf{f}(\mathbf{u}(x_{i-\frac{1}{2}})) = \mathbf{0}$$

Discretizing the temporal derivative in time t^n to t^{n+1} leads to

$$\overline{\mathbf{u}}_t = \frac{\overline{\mathbf{u}}^{n+1} - \overline{\mathbf{u}}^n}{\Delta t}$$

Shock-Capturing

Godunov-Type Finite Volume Methods

The final scheme, explicit Forward Euler in space and time with $(\bar{\ })$ dropped for simplicity, is then

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

with the flux $\mathbf{f}_{i+\frac{1}{2}}^n(\mathbf{u}_i^n, \mathbf{u}_{i+1}^n)$ coming from a Riemann solver.

Godunov's method introduces a "viscosity" for numerical reasons.

Godunov's method looks perfect; simple reasoning based on exact solutions of the governing equations.

However, early attempts to capture shocks led to shocks that were badly smeared or oscillatory.

Numerical Shockwaves

> ... all codes derived from the "conservation" equations are clumsier, slower and less efficient than codes based on Riemann's characteristic equations; therefore, if the formers are also incapable to capture shock properly, there is no reason for using them. What is the alternative? Fitting, of course.

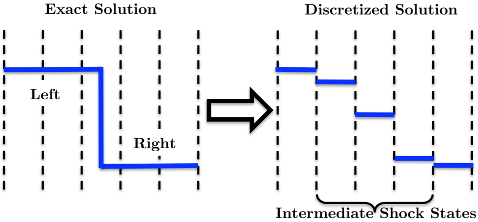
Moretti (1974) also argued that shock capturing was an attempt to differentiate the nondifferentiable.

In practice, due to implementation challenges, shock-capturing makes up the majority of codes for simulating shockwaves.

Moretti (2002) - Note: not actually Moretti pictured.

Numerical Shockwaves

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.

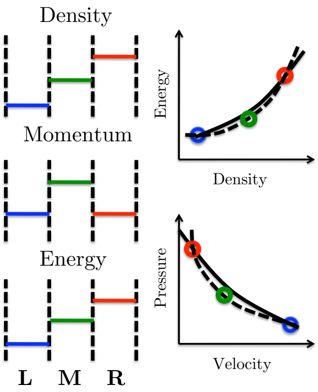
However, inside a shock, local thermodynamic equilibrium is not satisfied.

Numerical Shockwaves

Stationary (Steady) Shocks

Creating a one-point stationary shock.

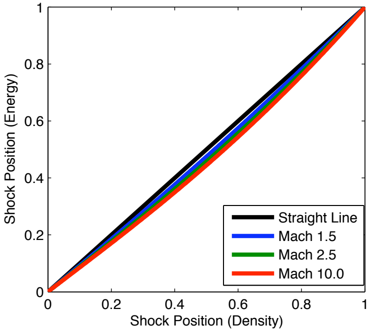
- 1. Define a supersonic left state $\mathbf{u}_L$.
- 2. Compute the subsonic right state $\mathbf{u}_R$ from $\Delta\mathbf{f} = \mathbf{0}$ (Hugoniot Curve).
- 3. Find the set of intermediate states $\mathbf{u}_M$ such that $\mathbf{f}_L = \mathbf{f}_{LM} = \mathbf{f}_{MR} = \mathbf{f}_R$.
- The intermediate state lies on the nonphysical branch of the Hugoniot.
- $\mathbf{f}_L = \mathbf{f}_R \neq \mathbf{f}_M$.



Stationary Shocks

Where is a Captured Shock?

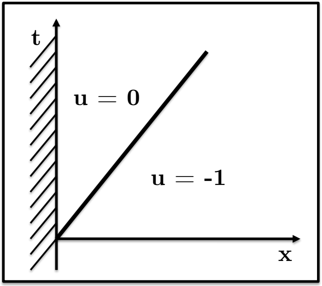
So what's anomalous about the stationary shock? Lets compute shock position.

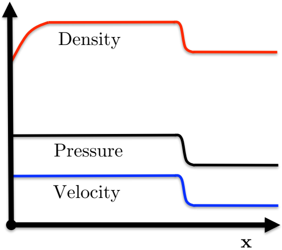


Because the Hugoniot is not linear, the shock positions calculated from the conserved variables do not agree.

Numerical Shockwave Anomalies

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.

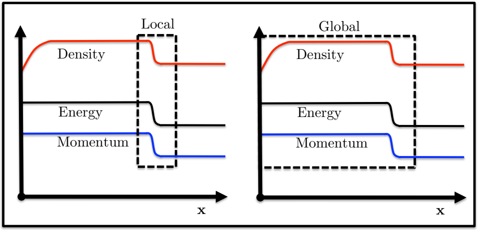
In consequence the temperature there is too high, so that this and related phenomena have been called **wall heating.**

Wall Heating

Shock Position

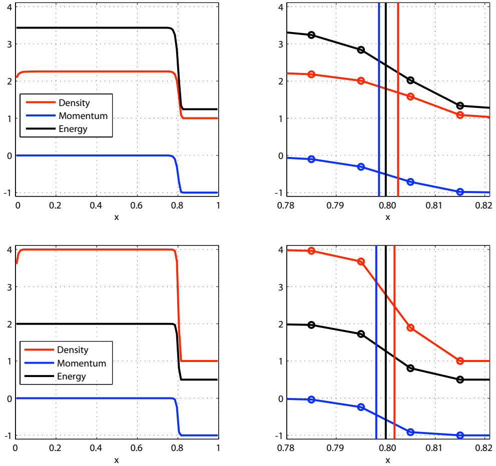
To show how shock position plays a role in wall heating, consider two control volumes:

- **Local** - contains only the region immediately around the shock.
- **Global** - contains the whole domain.



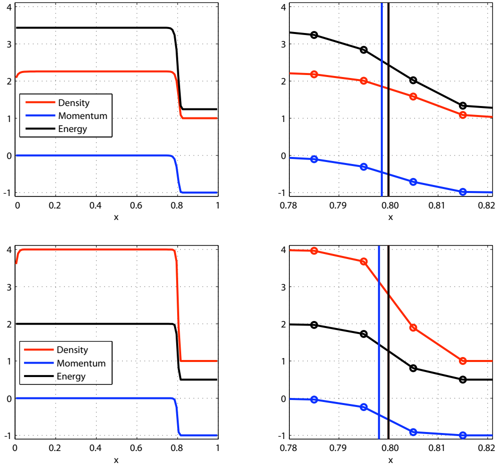
Wall Heating

Mach 1.1 shock (Top) and Mach 10^6 shock (Bottom).
Shock positions for local control volume shown.

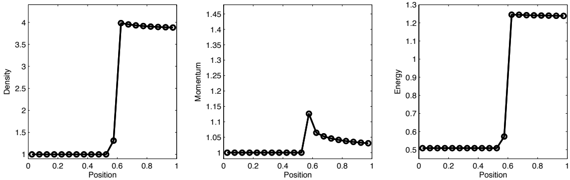


Wall Heating

Mach 1.1 shock (Top) and Mach 10^6 shock (Bottom).
Shock positions for global control volume shown.



Slowly Moving Shockwave Phenomenon

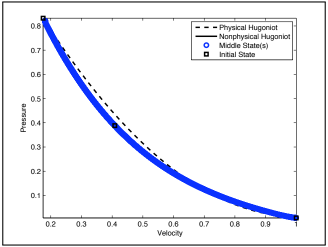


$$S = 1/100$$

Slowly Moving Shockwave Phenomenon

Slowly moving shocks generate spurious waves.

The intermediate states of a slowly moving shock remain close to the equilibrium states of a stationary shock.



The 1D Carbuncle

Initial Setup

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

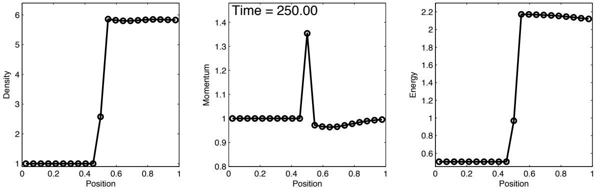
$$\rho_M = x_S \rho_L + (1 - x_S)\rho_R$$

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

Numerical Results

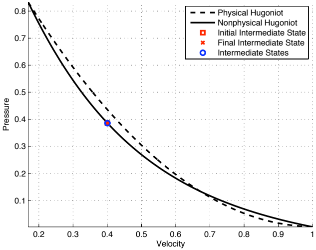


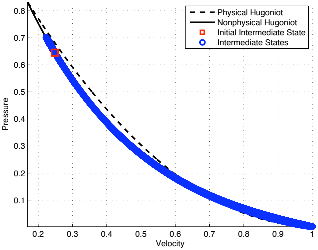
1D Carbuncle

The Carbuncle

Numerical Results

(Left) Stable Equilibrium. (Right) Unstable Equilibrium.





New Flux Functions

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?
- 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

$$\mathbf{f}_i^* = \mathbf{f}_{i-1} + \tilde{\mathbf{A}}_i(\mathbf{u}_i - \mathbf{u}_{i-1})$$

and extrapolated from the other side as

$$\mathbf{f}_i^* = \mathbf{f}_{i+1} - \tilde{\mathbf{A}}_i(\mathbf{u}_{i+1} - \mathbf{u}_i).$$

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

$$\mathbf{f}_{i+1} - \mathbf{f}_{i-1} = \tilde{\mathbf{A}}_i(\mathbf{u}_{i+1} - \mathbf{u}_{i-1}).$$

The simplest flux Jacobian having this property is the cell-centered Roe matrix $\tilde{\mathbf{A}}(\mathbf{u}_{i-1}, \mathbf{u}_{i+1})$. The flux can be interpolated from both sides as

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

Interpolated Fluxes

Interpolated Fluxes: $\mathbf{f}^*$

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. If the problem is nonlinear, but the data is smooth, then

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

3. If the problem is nonlinear and involves 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.

Flux Function A

With interpolated fluxes defined, a new flux function can be described similar to the original Roe framework,

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

The new method recovers Roe's method for linear problems or smooth solutions.

However this flux is not C^0 continuous.

Flux Function B

To overcome the difficulties of new flux function A, another flux function, B, is developed.

Inspired by Roe's Riemann solver, it can be written as

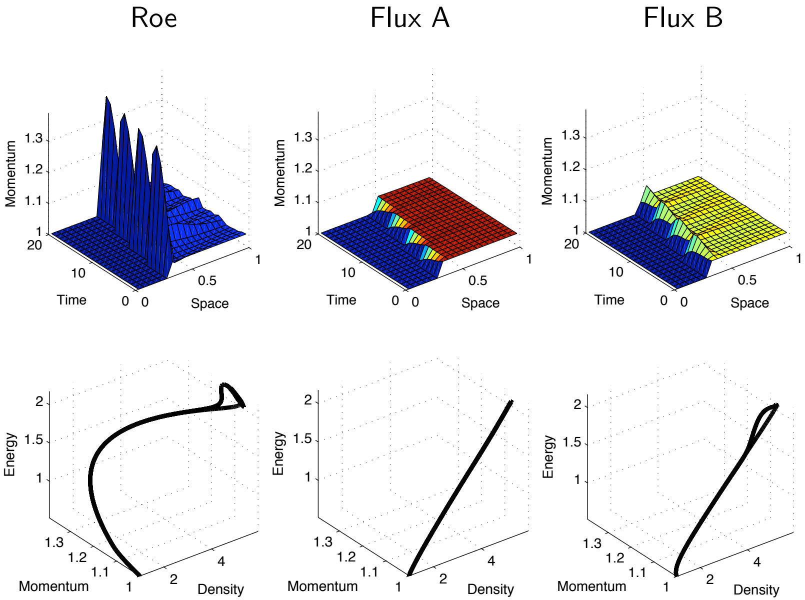
$$\mathbf{f}^B_{i+\frac{1}{2}} = \frac{1}{2}(\mathbf{f}^*_i + \mathbf{f}^*_{i+1}) - \frac{1}{2}|\overline{\mathbf{A}}_{i+\frac{1}{2}}|(\mathbf{u}_{i+1} - \mathbf{u}_i)$$

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

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

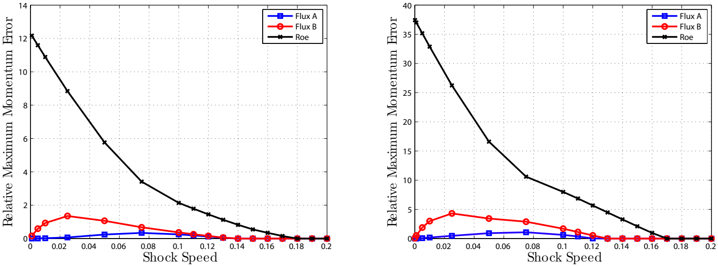
Physically speaking, these new functions trust the values of the conserved quantities, but do not necessarily trust the equilibrium fluxes, and corrects them in the vicinity of a shock.

Slowly Moving Shocks



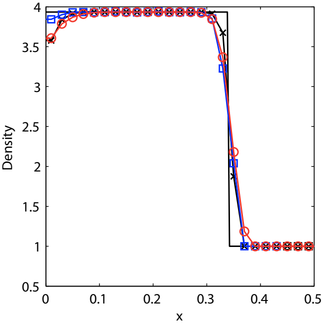
Slowly Moving Shocks

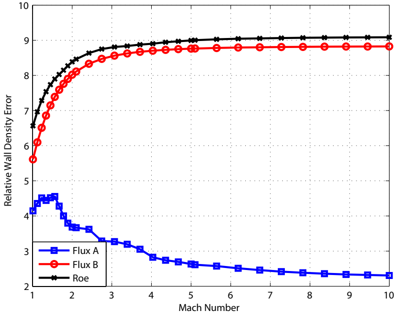
Maximum Momentum Error vs Shock Speed for Mach 2 (left) and Mach 10 (right)



Wall Heating

Wall heating is reduced by at least 60% using version A, and by at most 30% using version B. Density for the Mach 10 shock is shown.





Notes

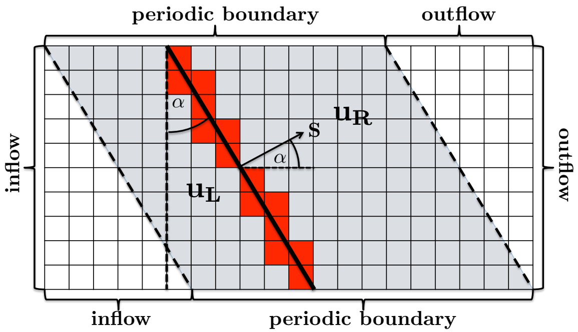
By construction, both new flux functions show no ambiguity in shock position for the stationary shock.

Both new flux functions show can be numerically shown to be carbuncle free in one dimension.

Both new flux functions perform comparably to Roe's Riemann solver on standard test problems (Shu-Osher, Sod, Woodward-Colella double blast wave).

Fairly standard MUSCL-type reconstruction can be used to obtain second-order accuracy without compromising any properties of the first-order scheme.

Two Dimensions

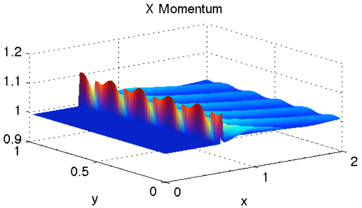


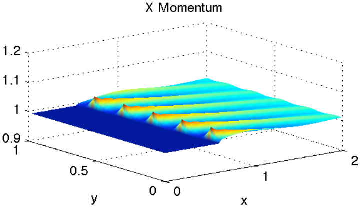
Ideally, a definition of the interpolated flux could be chosen such that the flux in each intermediate state equalled that of the flux of the two end states.

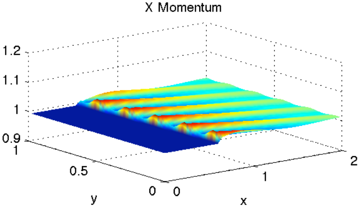
In practice, this is was not trivial, so initially, a simple two-dimensional implementation of both new flux functions was implemented.

Two dimensions

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

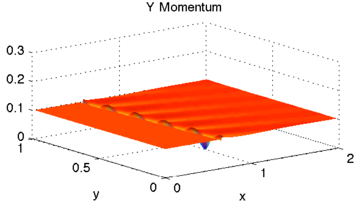


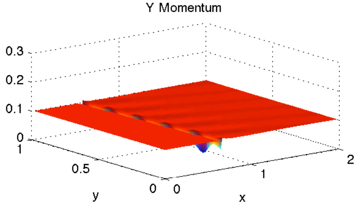


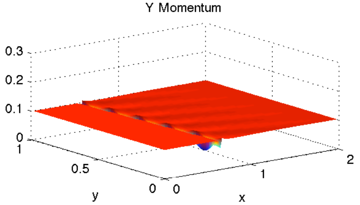


Two dimensions

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

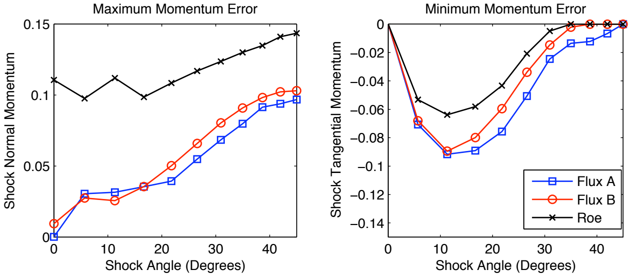






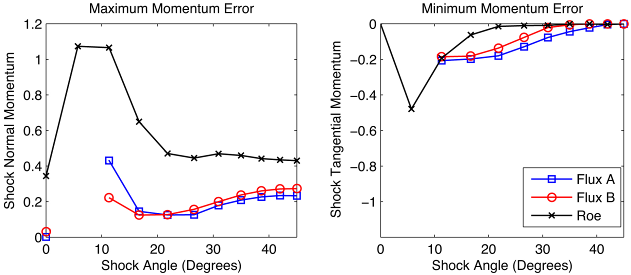
Two Dimensions

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



Two Dimensions

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



Notes

For oblique shocks, both new flux functions reduce errors normal to the shock front.

There are still issues with both new flux functions near oscillations transverse to a shock, which can lead to negative pressures and densities.

Nonetheless, when the new flux functions work, they work very well.

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.

Conclusions

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

Future Work

Pressing Needs

Improved robustness.

Genuinely two-dimensional methods.

Future Visions

Adaptive Riemann solvers.

Improving convergence rates for steady problems with shocks.

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And the CFD Community, the aerospace department staff, my friends, and everyone else.

Questions?

'A Throwback to Christopher Rumsey'