Flux Functions for Reducing Numerical Shockwave Anomalies

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The Issue of Shock Capturing

Although schemes in conservation form are guaranteed to converge to weak solutions of the governing equations, they are subject on practical grids to a number of anomalies:

- 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”

We speculate that all of these are related to another, very basic, anomaly, which is ambiguity in shock location. This in turn is related to curvature of the Hugoniot locus.

Shockwaves

The Euler Equations

The Euler equations in one dimension are,

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

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 enthalpy $H = \frac{E+p}{\rho}$. For an ideal gas in thermodynamic equilibrium, the equation of state is

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

Shock-Capturing

Godunov-Type Finite Volume Methods

We use an explicit Forward Euler in space and time with

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

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

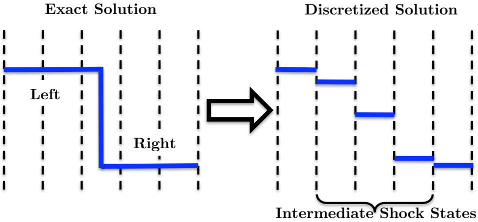
Godunov's method introduces a "viscosity" for numerical reasons.

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

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.

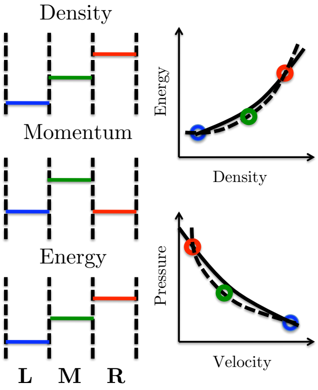
However, inside a shock, local thermodynamic equilibrium is not satisfied.

Numerical Shockwaves

Stationary (Steady) Shocks

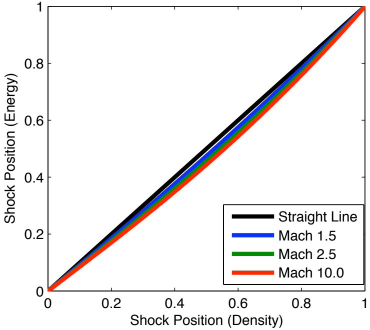
Creating a one-point stationary shock.

- 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

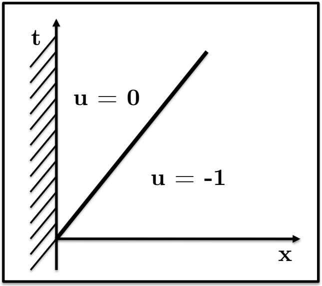
Where is a Captured Shock?

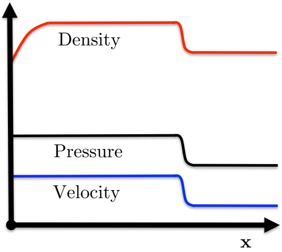


Because the Hugoniot is not linear, the shock positions calculated from the conserved variables do not agree.

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

Wall Heating

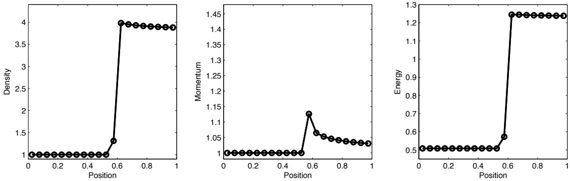




Virtually all shock-capturing methods provide quite good solutions for pressure and velocity, but predict too small a density in a small region at the origin.

Because the shock does not gather density and total energy at the same rate, the shock has a density excess - by conservation there must be a density defect somewhere.

Slowly Moving Shocks



$S = 1/100$

A slowly moving shock is almost stationary and as it moves across the grid, the intermediate shock state follows closely the set of steady intermediate states, and therefore remains close to the Hugoniot.

Because the Hugoniot is curved, the various conserved variables cannot all increase in the same proportions, resulting in the shedding of nonphysical waves.

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 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

Intermediate states have no physical meaning but are book-keeping devices to ensure conservation, thus the values of the conserved quantities must be accepted.

In this artificial situation, any interpretation of them is legitimate. Why should $\mathbf{f}(\mathbf{u}_M) = \mathbf{f}_M$?

Instead of using the equilibrium equation of state to compute the flux, use neighboring information to interpolate its value.

No pseudo-physical arguments will be invoked to evaluate $\mathbf{f}_M$. It is motivated solely by the desired numerical behavior.

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

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.

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

Flux Function A

With interpolated fluxes defined, a new flux function can be described similar to the original Roe framework. A rather conventional scheme might take the form

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

but this does not preserve the desired shock structure. A scheme that does is

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

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

However this flux is not C^0 continuous.

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

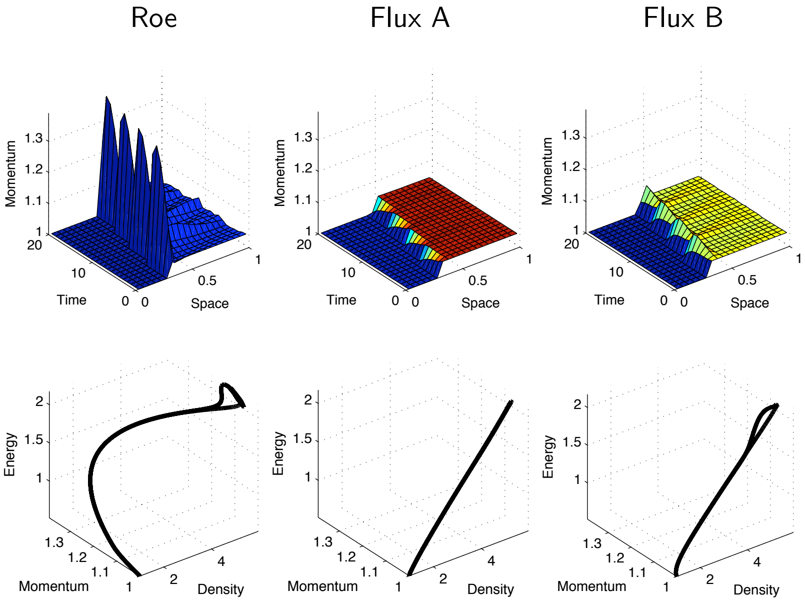
$$\mathbf{f}^B_{i+\frac{1}{2}} = \frac{1}{2}(\mathbf{f}^*_i + \mathbf{f}^*_{i+1}) - \frac{1}{2}|\overline{\mathbf{A}}_{i+\frac{1}{2}}|(\mathbf{u}_{i+1} - \mathbf{u}_i)$$

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

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

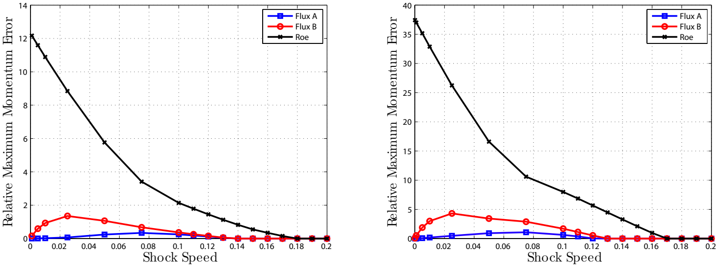
The matrix $\overline{\mathbf{A}}_{i+\frac{1}{2}}$ looks at the big picture, around the shock.

Slowly Moving Shocks



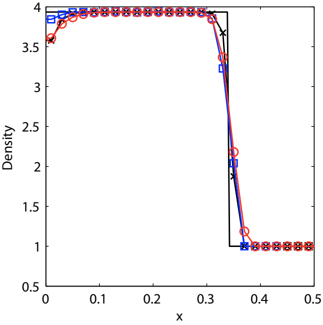
Slowly Moving Shocks

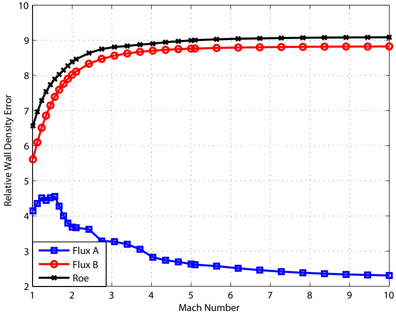
Maximum Momentum Error vs Shock Speed for Mach 2 (left) and Mach 10 (right)



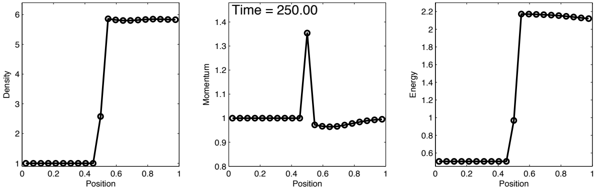
Wall Heating

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.





The Carbuncle

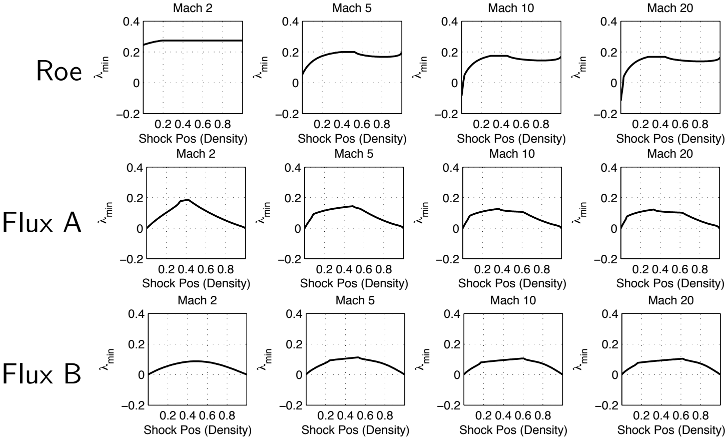


1D Carbuncle

The 1D carbuncle is an initially stationary one-point shock that does not remain stationary for some choice of intermediate state.

Results-unstable equilibria

A numerical eigenvector analysis, in the manner of Barth (1992) reveals that all one-point equilibrium shock solutions are stable for both versions. There are no "one-dimensional carbuncles".



Further Observations

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

Both new flux functions are one-dimensional carbuncle-free

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

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 (continued)

The new schemes are constructed to eliminate any ambiguity in the location of stationary shocks.

Stationary shocks are now always stable in any location.

There is negligable loss of resolution.

Slowly-moving shocks are much improved; with version A the momentum spike is virtually eliminated.

Wall heating is reduced by about 60% with version A.

Startup errors are reduced.

A criterion for multidimensional shocks can be defined but has yet to be made practical.

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

Acknowledgements

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Questions?

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A few common questions:

- Aren't you just avoiding the problem, ignoring the small scales inside the shockwave?

  Yes, Exactly.

- Isn't this just a form of artificial viscosity?

  Mathematically, yes, although ours is proportional to $\mathbf{A}_x|\mathbf{u}_x|$ *rather than* $\mathbf{u}_x|\mathbf{u}_x|$*, such as that of Von Neumann - Richtmyer.*

Two Dimensional Approach