How to Capture a Shock Wave?

Daniel W. Zaide

University of Michigan, University of British Columbia

This work supported by the Center for Radiative Shock Hydrodynamics (CRASH) and the Natural Sciences and Engineering Council of Canada

Tuesday, August 7th, 2012

We think we know how to capture a shockwave. Take our governing equations,

$$\mathsf{u}_t + \mathsf{f}(\mathsf{u})_{\mathsf{x}} = \mathbf{0}$$

and integrate them over a discrete cell in space and time,

$$\iint_{x_i,t_i} \phi_i(\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x) \mathrm{d}x \mathrm{d}t = \mathbf{0}$$

using some set of basis functions, ϕ_i , to handle the discontinuous nature of the solution.

From the Lax-Wendroff theorem, we *should* get convergence to a weak solution (shockwave) and things *should* be good...?

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"

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.



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

Current shock-capturing methods assume that these intermediate states obey the regular equation of state.

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

Stationary Shocks

The one-point stationary shock.

- 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.

•
$$\mathbf{f}_L = \mathbf{f}_R \neq \mathbf{f}_M$$
.



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.

This is directly related to the aformentioned anomalies.

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 $\mathbf{f}_M = \mathbf{f}(\mathbf{u}_M)$?

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.

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 $\textbf{A}=\frac{\partial f}{\partial u}.$ 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 $\tilde{A}(\mathbf{u}_{i-1}, \mathbf{u}_{i+1})$. The flux can be interpolated from both sides as

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

- If the problem is linear so that the Jacobian matrix A(u) is constant, then $f_i^* = f_i$.
- Por nonlinear systems with smooth data,

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

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

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

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

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

where sign(\mathbf{A}) = Rsign(Λ)L. However this flux is not C^0 continuous.

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

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

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

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

Slowly Moving Shocks



Daniel W. Zaide How to Capture a Shockwave

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 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.

email: dan.zaide@gmail.com, website: www.danielzaide.com

- 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 it is proportional to $\mathbf{A}_{x}|\mathbf{u}_{x}|$ rather than $\mathbf{u}_{x}|\mathbf{u}_{x}|$, such as that of Von Neumann - Richtmyer.