Affordable, entropy-consistent, Euler flux functions

(with application to the carbuncle phenomenon)

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Entropy pairs (U, F)

The one-dimensional Euler equations are

$$\partial_t \mathbf{u} + \partial_t \mathbf{f} = 0$$

$$\mathbf{u} = (\rho, m, E)^T, \quad \mathbf{f} = (m, p + m^2/\rho, m(E+p)/\rho)^T$$

For an ideal gas $p = (\gamma - 1)(E - \frac{1}{2}m^2/\rho)$. This is the only case for which we show results, but the non-ideal case is not much harder.

The physical entropy is then

$$S = \ln p - \gamma \ln \rho$$

with the *entropy density* $U = -\rho S/(\gamma - 1)$ and *entropy flux* $F = -mS/(\gamma - 1)$ satisfying

$$\partial_t U + \partial_x F \leq 0$$

Many important physical systems share this structure, by possessing one or more *entropy pairs*, such as (u, F)

The entropy variables

The vector $\mathbf{v} = \partial_{\mathbf{u}} U$ is given by

$$\mathbf{v} = \left(\frac{\gamma - S}{\gamma - 1} - \frac{\rho u^2}{2p}, \frac{m}{p}, -\frac{\rho}{p} \right)^T$$

and maps $1 \to 1$ onto $\mathbf{u}$, providing an alternative description of the flow.

These *entropy variables* satisfy many useful identities, including the inner product

$$\mathbf{v} \cdot \mathbf{u} = U + \rho$$

and the Jacobian matrix

$$\partial_{\mathbf{v}} \mathbf{u} = \mathbf{R}\mathbf{R}^T$$

where $\mathbf{R}$ is a suitably normalized set of right eigenvectors (Barth '99)

Generalization to 3D is trivial, including numerics of FV schemes.

Finite volume schemes

The entropy production at the interface between two finite volumes is (Tadmor '87)

$$[\mathbf{v}] \cdot \mathbf{f}^* - [m]$$

where $\mathbf{f}^*$ is the numerical flux between the cells and [ ] denotes the difference between the two cells.

For the central difference flux $\mathbf{f}^* = \bar{\mathbf{f}}$, it can be shown that

$$[\mathbf{v}] \cdot \bar{\mathbf{f}} = \mathcal{O}(\delta^3)$$

which is small in smooth regions, but large (and essentially correct) across shocks, and wrong (it should vanish) across rarefactions.

How much entropy?

Take a discrete IVP in 1D, with initial data and boundary values corresponding to a stationary shock. We will have $m_L = m_R$ but $S_L \neq S_R$ and so $F_L \neq F_R$. To attain a steady state, entropy must be *produced* within the domain.

The entropy inside the domain is

$$-(\gamma - 1) \sum_j U_j = (\gamma - 1) \sum_j \rho_j - \sum_j \mathbf{v}_j \cdot \mathbf{u}_j$$

For perturbations that preserve the shock position, the first term is constant; the second can be written, introducing mean values $\bar{\mathbf{v}}, \bar{\mathbf{u}}$

$$-\sum_j \mathbf{v}_j \cdot \mathbf{u}_j = -\sum_j (\mathbf{v}_j - \bar{\mathbf{v}} + \bar{\mathbf{v}}) \cdot (\mathbf{u}_j - \bar{\mathbf{u}} + \bar{\mathbf{u}})$$

$$= -\sum_j (\mathbf{v}_j - \bar{\mathbf{v}}) \cdot (\mathbf{u}_j - \bar{\mathbf{u}}) - \sum_j \bar{\mathbf{v}}\bar{\mathbf{u}}$$

Moving values closer to the mean smears the shock and increases the entropy.

Therefore we want to create *enough* entropy but not *too much*.

Conserving entropy

For a flux to create no entropy, we need

$$[\mathbf{v}] \cdot \mathbf{f}^* = [\rho u]$$

which defines a plane in $\mathbf{f}$-space, but to find even one point in this plane is not easy.

Tadmor ('87) found the solution by quadrature

$$\mathbf{f}^* = \int_0^1 \mathbf{f}(\mathbf{v}(\xi)) \, d\xi$$

with $\mathbf{v}(\xi) = \xi \mathbf{v}_R + (1 - \xi)\mathbf{v}_L$ and in ('03) found the explicit solution

$$\mathbf{f}^* = \sum_k \frac{[\rho u]_{k+\frac{1}{2}}}{[\mathbf{v}] \cdot \delta \mathbf{u}_{k+\frac{1}{2}}} \delta \mathbf{u}_{k+\frac{1}{2}}$$

The sums are over subpaths of an approximate Riemann solution in $\mathbf{u}$-space.

Another entropy-conservative flux

Define the *parameter vector*

$$\mathbf{z} = \sqrt{\frac{\rho}{p}}(1, u, p)$$

in terms of which

$$\mathbf{v} = \left(\frac{\gamma}{\gamma - 1} + \frac{\gamma + 1}{\gamma - 1} \ln z_1 + \ln z_3 - \frac{1}{2} z_2^2, z_1 z_2, -z_1^2 \right)^T$$

This allows the explicit solution

$$
\begin{aligned}
f_1^* &= \bar{z}_1 z_3^{\ln} \\
f_2^* &= \frac{\bar{z}_3 + \bar{z}_2 f_1^*}{\bar{z}_1} \\
f_3^* &= \frac{1}{2\bar{z}_1} \left(\frac{\gamma + 1}{\gamma - 1} \frac{f_1^*}{z_1^{\ln}} + \bar{z}_2 f_2^* \right)
\end{aligned}
$$

where $(\bar{\cdot})$ denotes an arithmetic mean and $(\cdot)^{\ln}$ a "logarithmic" mean.

This flux *exactly preserves* contact discontinuities.

The "logarithmic mean"

Given two real numbers x_1 and x_2, we define their logarithmic mean as

$$L(x_1, x_2) = \frac{x_1 - x_2}{\ln x_1 - \ln x_2} \qquad (1)$$

If x_1, x_2 both approach x, this reduces to x. Otherwise it defines a symmetric average of the two numbers. This average enables us to replace $[\ln p]$, for example, with $[p]/p^{\ln}$ where $p^{\ln} = L(p_L, p_R)$.

In most of the cases that arise in a computation, x_1 and x_2 will be fairly similar. Then, an accurate approximation is

$$L(x_1, x_2) = \overline{x}\left(1 + \frac{1}{12}\left(\frac{[x]}{\overline{x}}\right)^2 + \frac{1}{80}\left(\frac{[x]}{\overline{x}}\right)^4 + \cdots\right)^{-1} \qquad (2)$$

Only seldom will it be necessary to employ (1).

Entropy due to upwinding

A typical first-order upwind flux is written

$$\mathbf{f}^* = \bar{\mathbf{f}} - \frac{1}{2}|\mathbf{A}|[\mathbf{u}]$$

where $|\mathbf{A}| = \mathbf{R}|\Lambda|\mathbf{L}$ is the absolute value of the interface Jacobian, evaluated for example at the Roe-averaged state. The entropy produced by this term is

$$-\frac{1}{2}[\mathbf{v}]\mathbf{R}|\Lambda|\mathbf{L}[\mathbf{u}]$$

and may not be of the required sign for very strong shocks (Barth '99) This can be fixed using the reformulation

$$
\begin{aligned}
\frac{1}{2}[\mathbf{v}]\mathbf{R}|\Lambda|\mathbf{L}[\mathbf{u}] \;&\simeq\; \frac{1}{2}[\mathbf{v}]\mathbf{R}|\Lambda|\mathbf{L}(\partial_{\mathbf{v}}\mathbf{u})[\mathbf{v}] \\
&\simeq\; \frac{1}{2}[\mathbf{v}]\mathbf{R}|\Lambda|\mathbf{L}(\mathbf{R}\mathbf{R}^T)[\mathbf{v}] \\
&=\; \frac{1}{2}[\mathbf{v}]\mathbf{R}|\Lambda|\mathbf{R}^T[\mathbf{v}]
\end{aligned}
$$

which is a positive definite quadratic form.

Old and new fluxes

We have

$$\mathbf{f}_{\text{old}}^* = \bar{\mathbf{f}} - \frac{1}{2}\mathbf{R}|\wedge|\mathbf{L}[\mathbf{u}]$$

and

$$\mathbf{f}_{\text{new}}^* = \mathbf{f}_C - \frac{1}{2}\mathbf{R}|\wedge|\mathbf{R}^T[\mathbf{v}]$$

1. $\mathbf{f}_{\text{new}}^* = \mathbf{f}_{\text{old}}^* + \mathcal{O}(\delta^2)$

2. $\mathbf{f}_{\text{new}}^*$ and $\mathbf{f}_{\text{old}}^*$ both exactly preserve stationary discontinuities.

3. $\mathbf{f}_{\text{old}}$ needs to be "fixed" at sonic points; $\mathbf{f}_{\text{new}}^*$ does not.

4. $\mathbf{f}_{\text{old}}^*$ is not entropy stable, but $\mathbf{f}_{\text{new}}^*$ is.

5. $\mathbf{f}_{\text{new}}^*$ is about 20% more expensive.

Instability of strong shocks

Consider again the IVP associated with a stationary shock with nonreflecting downstream BCs. For certain high Mach numbers, the shock computed with $\mathbf{f}^*_{\text{old}}$ (also $\mathbf{f}^*_{\text{God}}$) will spontaneously relocate itself (Barth '89, Bultelle *et al*, '99).
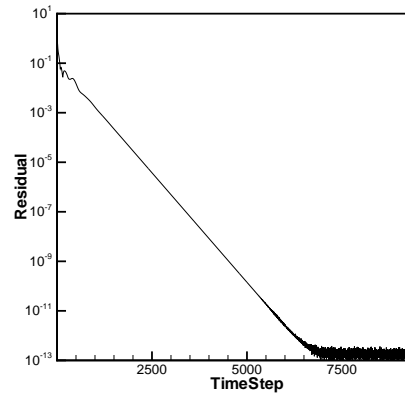
If the downstream BC is taken to be fixed mass flow, which retains the shock in its initial location, both $\mathbf{f}^*_{\text{old}}$ and $\mathbf{f}^*_{\text{God}}$ gives rise to waves that reflect perpetually between the shock and the boundary.

Both problems are removed by using $\mathbf{f}^*_{\text{new}}$.
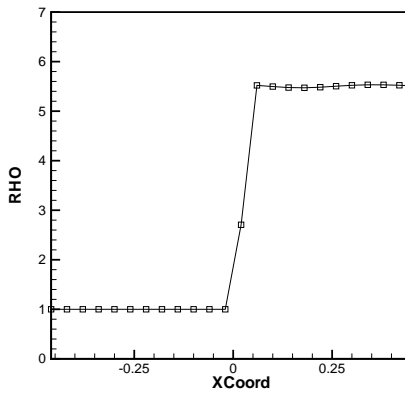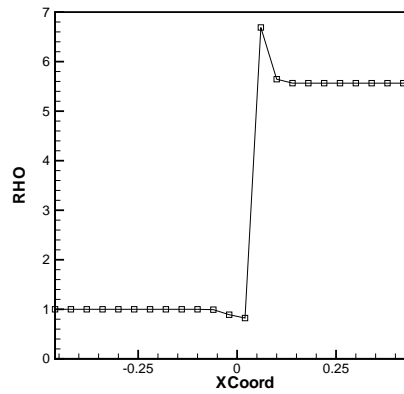
Profiles and histories
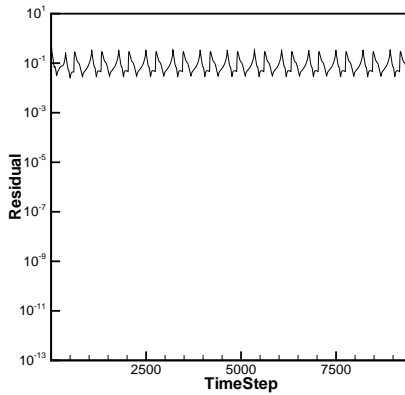
Residual history from $\mathbf{f}^*_{old}$ Residual history from $\mathbf{f}^*_{new}$.

Density profile from $\mathbf{f}^*_{old}$ after 10,000 timesteps.

Density profile from $\mathbf{f}^*_{new}$ after 10,000 timesteps

What does entropy stability do ?

It would be good to have a theorem of the form

$$(\text{Entropy stability}) \Rightarrow (\text{Something nice})$$

such as convergence to some unique and physically relevant weak solution.

This seems to be unlikely at present, since such theorems are lacking in the continuous case.

At first sight, entropy stability rules out limit cycles, but this cannot actually be proved for open systems because of boundary issues. Probably we just have that

$$(\text{Entropy stability}) \Rightarrow (\text{Entropy stability})$$

but it does seem to do something.

Why the overshoots?

The flux $\mathbf{f}^* = \mathbf{f}_C - \frac{1}{2}\mathbf{R}|\Lambda|\mathbf{R}^T[\mathbf{v}]$ generates no entropy from the first term.

The second term provides, in the linear case, the minimal dissipation to remove overshoots, but the entropy generated by it is only $\mathcal{O}(\delta^2)$. However, the entropy generated by a shock is $\mathcal{O}(\delta^3)$. In the old flux, that entropy was generated by the *central* term.

We need another term in the flux, one order higher, that creates the correct entropy in under-resolved shocks. Both it and the upwind term will become negligable for resolved shocks (Tadmor and Zhong '06) and entropy will then be produced entirely by the Navier-Stokes terms.

Entropy production

The rate of entropy production across a shock is given by the formula

$$\dot{U} = \frac{1}{6}(\ell \cdot [\mathbf{u}])^2 [\lambda]$$

in at least two cases

1. Burgers' equation with entropy function $U = ku^2$,

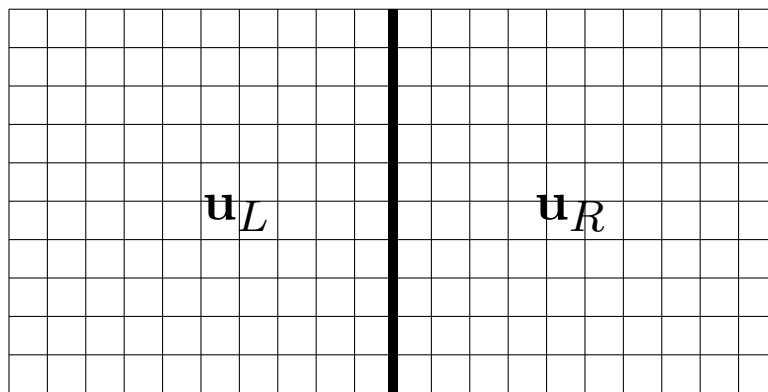2. Euler equations with physical entropy for weak shocks.

Based on this, we have used the flux function

$$\mathbf{f}^* = \mathbf{f}_C - \frac{1}{2}\mathbf{R}\left(|\Lambda| + \alpha|[\Lambda]|\right)\mathbf{R}^T[\mathbf{v}]$$

with $\alpha \simeq 1/3$. This removes the overshoots and also slightly speeds the breakup of under-resolved rarefactions.

The carbuncle

Consider 2D initial data consisting of stacked 1D data

$$\mathbf{u}_L \qquad\qquad \mathbf{u}_R$$

Even slight instability of the layers will create strong vertical gradients close to the shock, leading to two-dimensional behavior.

Carbuncles in practice

Phenomena resembling carbuncles appear in practical calculations and can lead to very erroneous predictions that are not remedied by bigger computers and finer grids. (Perhaps on a fine enough grid one could just use Lax-Friedrichs!)

The code does not converge to the expected solution, but to a second solution that appears to be a genuine weak solution, and can even be realized experimentally under artificial circumstances.

Conclusions

1. A new entropy-conservative flux has been presented.

2. It can be made entropy-stable by upwinding.

3. For under-resolved flows a production term needs to be added.

4. In one dimension, the new flux cures the instability of strong shocks.

5. In two dimensions, there have been no observed anomalies on structured grids.

6. On poor quality unstructured grids, the carbuncle returns.