Entropy Traces In Lagrangian and Eulerian Calculations

Philip L. Roe and Daniel W. Zaide

1 Introduction

The decision to capture rather than fit shockwaves and other discontinuities probably compromises some aspects of a computation, although exactly how has never been completely clarified. One issue that has long been identified is that of the propagating errors called *entropy traces* by Rodzhestvenskii and Yanenko [6]. These are regions of spurious entropy or temperature that propagate along particle paths or solid boundaries. They are sometimes associated especially with Lagrangian methods, although we have found that nearly identical behavior can occur in Eulerian codes. For example, Figure 1 compares Eulerian and Lagrangian computations of the Sod test problem. The Eulerian computation is done in a moving frame that makes the contact discontinuity stationary. Based on this and other experiments we have concluded that the mechanisms that create such traces are essentially the same for both types of code. Merely, Lagrangian methods suffer the faults of their virtues. By using a mesh that follows the flow, diffusion across material pathlines can be reduced or eliminated. Then the good news is that physical changes to the entropy are conserved; the bad news is that errors in the calculated entropy are also conserved. These considerations apply to any method, even in Eulerian coordinates, in which successful measures are taken to combat numerical diffusion. Where flow features are fully resolved at the Navier-Stokes scale, there is usually no problem. The difficulty arises because we wish to avoid anomalies that are associated with unresolved features.

The simplest way consists of re-introducing diffusion, hopefully in a selective manner [5, 4]. When a Riemann solver is used to evaluate the flux, the (local) use of a more diffusive flux can be successful [2]. However, if methods are local in time, it is impossible for the code to determine, at any one timestep, whether the entropy changes being propagated are physically meaningful or due to numerical error. It follows that any method that avoids the pitfalls must either avoid making the error in the first place, or must be equipped with some kind of memory. The method of Roe and Zaide [8] seems

Philip L. Roe
University of Michigan, Ann Arbor, MI, USA, e-mail: philroe@umich.edu

Daniel W. Zaide
University of Michigan, Ann Arbor, MI, USA, e-mail: zaidedan@umich.edu

to remove about half the error by comparing conservative and nonconservative pressure calculations (See also [3]).

In this paper, we concentrate on identifying the causes of the error. We have identified two main causes, and believe that there are no other important ones. However, we do not yet have any practical cures to propose.

2 The Noh Problem

A canonical example is the Noh problem [5], a seemingly trivial Riemann problem with initial data corresponding to the collision of two equal shocks, or equivalently the reflection of a single shock from a solid wall. In Eulerian variables the data is $\mathbf{u}_L = (\rho_0, \rho_0 u_0, E_0)^T$, $\mathbf{u}_R = (\rho_0, -\rho_0 u_0, E_0)^T$ or in Lagrangian variables $\mathbf{v}_L = (V_0, u_0, i_0)^T$, $\mathbf{v}_R = (V_0, -u_0, i_0)^T$. We take $\gamma = 5/3, \rho_0 = 1, u_0 = 1$, and p_0 left to set shock speed. Virtually all shock-capturing methods of either type 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*. In the more than 20 years since Noh proposed the problem, no satisfactory solution has been exhibited that would carry over to other settings, nor is there even any generally accepted explanation of the mechanism. Here we demonstrate that one driving mechanism is the one put forward by Xu and Hu [9] for anomalies associated with general shock collisions, and that the Noh problem is merely the simplest instance of a pervasive difficulty, arising from the convexity of the pressure as a function of the conserved variables.

Analysis of the first time step (which is effectively identical in both methods) is instructive. For example, any consistent finite-volume method that avoids explicit diffusion will place identical fluxes on all interfaces except for the one at $x = 0$, where the only non-zero flux is the interface pressure in the momentum equation. Solutions therefore depend on just two parameters, one being this pressure p, and the other being the Courant number ν, defined here as $\nu = S\Delta t/\Delta x$ with S being the speed of the reflected shock. Whatever pressure P is used, the conserved variables will change in proportion to ν. Then the pressure in the cells next to the origin will be updated using the equation of state. For example, using the exact Riemann solution for an ideal gas, this results in the following expression for the pressure in the first cells as a function of Courant number;

$$p(\nu) = \nu p_1 + (1-\nu)p_0 + \left(\frac{\gamma-1}{2}\right)\frac{\nu(1-\nu)\rho_0\rho_1 u_0^2}{(\nu\rho_1 + (1-\nu)\rho_0)}. \tag{1}$$

The leading terms represent the exact evolution of the pressure. The remaining term, which is always positive, reflecting the convexity of the pressure law, is an error arising from the evaluation of internal energy as the difference in total and kinetic energies. Although the error vanishes for ν equal to 0 or 1.0, it cannot be removed by choosing $\nu = 0$ (no progress) or $\nu = 1.0$ (unstable). At the second and subsequent time steps, this excessive pressure expels mass from the central region. The pressure and velocity reach constant values by emitting acoustic waves, but the density is left too low. This density (temperature) anomaly is traceable to initial errors in pressure, or, equivalently, entropy. This error persists until late times because there is no diffusion mechanism to remove it. Similar effects occur in methods employing artificial viscosity, since this is also a form of mixing.

3 Isolating Pressure Convexity

If the explanation given above is both correct and complete, then no phenomenon analogous to wall heating should result if the pressure were to depend linearly on the conserved variables. There is no physically meaningful closure of the gasdynamic equations with this property, and the only nonphysical possibility that is dimensionally consistent is to take the pressure as proportional to the total energy rather than the internal energy. In this way the pressure itself becomes a conserved variable. Therefore we set

$$p = (\gamma - 1)E. \tag{2}$$

Under this assumption, the gasdynamic equations remain hyperbolic, with regular shocks, rarefactions, and contacts. We want to see if initial data analogous to the Noh problem results in an error being deposited on the wall.

In Figure 2, we plot the evolution of pressure and density in the cell next to the wall, as the solution there evolves to its steady state. In the left picture we see that with the true equation of state, either the pressure is overpredicted, or the density underpredicted, depending on the point of view. In either case the temperature is overpredicted. On the right (having contrived the data so that the final densities are the same) we see that eliminating the need for nonlinear pressure evaluation indeed eliminates the temperature error, but only for small times. This compels the conclusion that there is at least one other driving mechanism.

4 Shock Motion

A clue to this comes from modifying the Noh problem by specifying the initial condition at $t < 0$. This is, we set up initial conditions corresponding to two shocks that will collide in the future, but have not yet done so. To our surprise, the amount of wall heating turned out to depend on the initial distance of the shock from the wall. We realised that this was related to the well-known way [7, 1] in which a propagating shock changes its structure depending on its phase relative to the grid. The shock reflects from the wall in a way that depends on its phase at the moment of impact. In some cases the outcome can even be wall cooling, but in many cases the most pronounced error was not actually at the wall. The location was at a point that can be simply predicted by accounting for the fact that a shock that is initially prescribed with too narrow an initial structure will suffer "start-up errors". These cause spurious waves to propagate along the other families of characteristics. This is often referred to as the "slowly-moving shock" problem, although it can, and does, occur for strong shocks propagating at any speed. In this case, a spurious contact discontinuity propagates inward with speed $-u_0$. This is eventually intercepted by the reflected shock, and brought to rest. This spurious, stationary, contact is the location of the worst temperature error as seen in Figure 3.

Again, we examined the validity of this explanation by constructing an artificial system. Arora and Roe [1] conjectured that the spurious waves would not be produced in any system for which the Hugoniot curve is a straight line in the phase space of conserved variables. They noted, but did not show, an example using a 2x2 model system. Here we study a 3x3 model system, to introduce the possibility of a contact discontinuity.

$$\begin{bmatrix} u \\ a \\ b \end{bmatrix}_t + \begin{bmatrix} \frac{1}{2}\left(u^2 + a^2 + b^2\right) \\ ua \\ ub \end{bmatrix}_x = \mathbf{0} \tag{3}$$

This hyperbolic system has a propagation speed $c = \sqrt{a^2 + b^2}$, eigenvalues of $u, u \pm c$. It is simple to show that the Hugoniot curves are actually straight lines. Because there is no explicit equation of state, there is no nonlinear mixing involved. Tests on this system with left and right states of $\mathbf{u}_L = (1, 1, 1)^T$, $\mathbf{u}_R = (-1, 1, 1)^T$ in Figure 4 shows no spurious waves, and no trace of problems like wall heating.

5 Conclusions and Future Work

Whenever entropy is created by numerical error, it is propagated along particle paths as though it had been created physically. The simplest example of this is wall heating, exemplified by the Noh problem. Two mechanisms behind this phenomenon are examined and isolated. The explanations were validated by constructing examples of artificial conservation laws from which the mechanisms were absent, and then verifying that the phenomenon did not occur. We are currently looking at various shock-broadening mechanisms.

6 Acknowledgements

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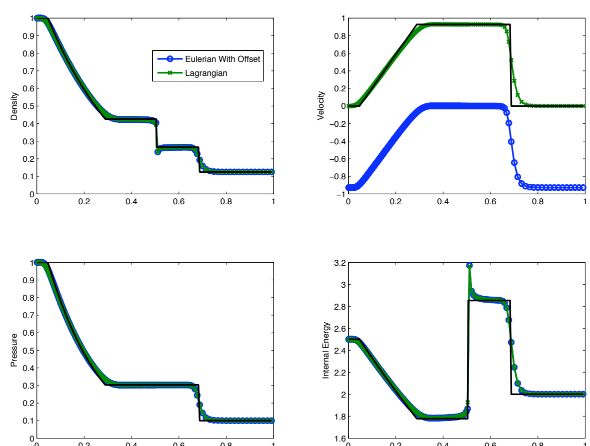

Fig. 1 In Sod's problem, Lagrangian and shifted Eulerian methods behave identically.

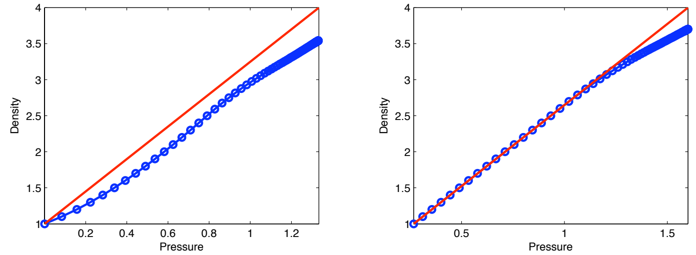

Fig. 2 A $p-\rho$ plot for the Ideal Gas EOS (left) and Linear EOS (right).

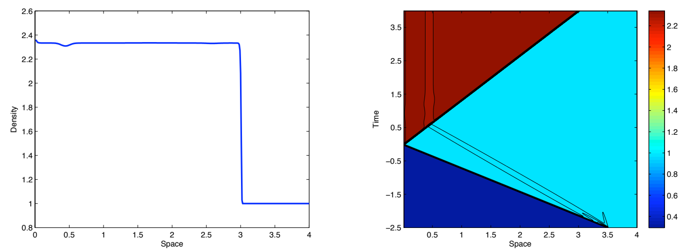

Fig. 3 (Left) Density at final time. Effects at the wall and where the contact has intercepted the reflecting shock are observed. (Right) Density contours. The propagation of the spurious contact is observed, and its residual effect remains.

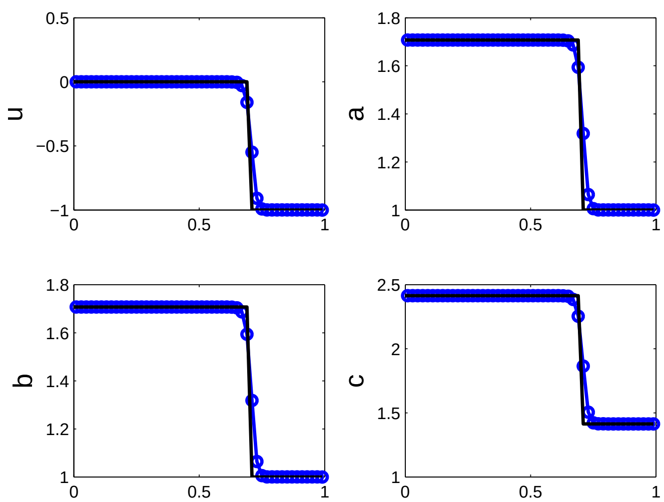

Fig. 4 Conserved variables and propagation speed shown for the Noh problem for the model system of equations described in Section 4.