One-sided difference schemes and transonic flow

(conversion law/numerical approximation)

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ABSTRACT Two one-sided conservation form difference approximations to a scalar one-dimensional convex conservation law are introduced. These are respectively of first- and second-order accuracy and each has the minimum possible bandwidth. They are nonlinearly stable, they converge only to solutions satisfying the entropy condition, and they have sharp monotone profiles. No such stable approximation of order higher than two is possible. Dimensional splitting algorithms are constructed and used to approximate the small-disturbance equation of transonic flow. These approximations are also nonlinearly stable and without nonphysical limit solutions.

In this paper we shall introduce two one-sided conservation form difference approximations to scalar one-dimensional convex (and more general) conservation laws. These are, respectively, of first- and second-order accuracy and each has the minimum possible bandwidth. We claim that the schemes are nonlinearly stable, they converge only to solutions satisfying the entropy condition, and they have sharp monotone profiles. We also claim that no such stable approximation of order higher than two is possible. We then construct dimensional splitting algorithms and use them to approximate the small disturbance equation of transonic flow and claim that the resulting approximations have the desirable properties of stability and no nonphysical limit solutions. Proofs of these claims will appear in forthcoming papers along with positive numerical evidence.

Nonlinear hyperbolic systems of conservation laws are well known to develop singularities after a finite time has elapsed, even when their initial data are very smooth. These systems are of the form

$$u_t + div f(u) = 0, \quad i = 1, \ldots, n, \quad [1]$$

in which $f^i$ is a function of the variables $u^i, \ldots, u^n$.

Another equation that has physically and mathematically meaningful discontinuous solutions is the low-frequency, time-dependent, small-disturbance equation of transonic flow

$$2\Phi_{xx} = (K\Phi_x - \frac{1}{2}(\gamma + 1)\Phi_x^2)_x + \Phi_{yy} \quad [2]$$

and the time-independent version

$$0 = (K\Phi_x - \frac{1}{2}(\gamma + 1)\Phi_x^2)_x + \Phi_{yy}, \quad [3]$$

in which $\Phi$ is the velocity potential, $t$ is time, and $K$ and $\gamma$ are positive constants. Eqs. 2 and 3 are common models for describing subsonic and supersonic flow close to the local speed of sound (see ref. 1). The flow is assumed to be that of an inviscid perfect gas.

The most successful methods for calculating solutions with discontinuities involve shock capturing, in which the discontinuity appears merely as a rapid transition region. It was observed in ref. 2 that to satisfy the integral form of the conservation laws it suffices to approximate them by difference equations in conservation form. This requirement may be necessary as well. For example, the useful difference approximation to Eqs. 2 and 3 of Cole and Murman (3) gave incorrect shocks for limit solutions until it was put in conservation form (4). Another problem even for commonly used schemes such as the conservation form version of Cole and Murman and the Lax–Wendroff approximation to 1 is convergence to nonphysical solutions—e.g., solutions with expansion shocks (4, 5). It was proven in ref. 6 that the addition of a certain amount of numerical viscosity rules out these nonphysical solutions for the Lax–Wendroff scheme, and the numerical evidence is that any amount will do. Experiments also indicate that the same is true for the Cole–Murman scheme, with the help of more complicated local viscosities (4). Moreover, nonlinear instabilities for both schemes can be removed in this fashion (6, 7). For the scalar version of 1, monotone schemes are known to converge to the correct physical solution (5, 8). However, these schemes are at most first-order accurate.

A last common difficulty arising in achieving good shock resolution. High-order accurate schemes tend to have overshoot—i.e., numerical oscillation—whereas monotone schemes tend to smear the shock over a large number of points. The addition of numerical viscosities increases the spreading. Several approaches have been suggested to prevent overshoot and spreading (9–11).

The method we propose here involves upwind differencing. This is not a new idea; see, e.g., refs. 12 and 13. In particular, the above-mentioned Cole–Murman scheme and its variants have been quite successful modulo a few difficulties involving the appearance of expansion shocks and nonlinear instabilities. Moreover, its accuracy is limited to first order. To some extent these problems are caused by the switching mechanism—the differencing of the $x$ derivatives in Eqs. 2 and 3 goes from upwind to downwind as the velocity $\Phi_x$ goes from supersonic to subsonic.

In ref. 14 we showed how to implement a simple switch so that expansion shocks and nonlinear instabilities are ruled out. We now have devised a second-order method having the same properties. Moreover, both of our schemes (even the second-order ones) in the one-dimensional case have sharp shock profiles with no overshoot. Finally, we have proven that this is the best possible accuracy by showing that no scheme approximating even a linear, one-dimensional, scalar problem with constant coefficients can have accuracy greater than second order if it is fully one sided and stable.

Our procedure for solving Eq. 2 numerically is via dimensional splitting:

$$2\Phi_{xx} = (K\Phi_x - \frac{1}{2}(\gamma + 1)\Phi_x^2)_x \quad \text{(Step 1)} \quad [4]$$

$$2\Phi_{yy} = \Phi_{yy} \quad \text{(Step 2)} \quad [5]$$

Step 1 involves an equation of type 1:

$$u_t + f(u)_x = 0,$$
in which \( f(u) = -\frac{1}{2}p(Ku - \frac{1}{2}b \gamma + 1)u^2 \) and \( u = \Phi_x \). This is a single scalar convecton conservation law.

We set up a grid \( x_i = i\Delta x \), \( t^n = \frac{n\Delta t}{\gamma + 1} \) with \( u^n_j \) approximating \( u(x_i, t^n) \) and define the difference operators \( \Delta_t u_j = u_{j+1} - u_j \), \( \Delta x u_j = u_j - u_{j-1} \). The conservative Cole–Murman scheme is based on the first-order space differencing

\[
(f(u))_x \to \frac{1}{\Delta x} (\Delta_x f(u_{j+1}) - \Delta_x f(u_{j-1})) \tag{6}
\]

for

\[
\mathcal{O}_j = \begin{cases} 
1 & \text{if } u_j + u_{j+1} \geq 2\bar{u}, \\
0 & \text{if } u_j + u_{j+1} < 2\bar{u},
\end{cases}
\]

in which \( \bar{u} \) is the sonic point—i.e., \( f'(\bar{u}) = 0 \) and \( f \) takes on its minimum value there. This differencing admits expansion or shocks. For example, the following piecewise constant function is annihilated by this difference operator. Moreover, both of

\[
\text{Expansion shock}
\]

\[
\begin{array}{c}
\text{Subsonic} \\
\text{Supersonic}
\end{array}
\]

these discontinuities are numerically stable (14).

Our first-order scheme is based on the switch:

\[
(f(u))_x \to \frac{1}{\Delta x} (\Delta_x f(u_{j+1}) + \Delta_x f(u_{j})) \tag{7}
\]

Here and for any convex \( f \) we define:

\[
f_+(u) = f(\max(u, \bar{u}))
\]

\[
f_-(u) = f(\min(u, \bar{u}))
\]

For general \( f(u) \) we first let \( \chi(u) = 1 \) if \( f'(u) \geq 0 \), \( \chi(u) = 0 \) if \( f'(u) < 0 \), and then define:

\[
f_+(u) = \sum_0^u \chi(s)f'(s)ds
\]

\[
f_-(u) = \sum_0^u (1 - \chi(s))f'(s)ds.
\]

For the time differencing we let

\[
u_i \to \frac{u_i^{n+1} - u_i^n}{\Delta t^n}
\]

and define \( \lambda^n = \Delta t^n/\Delta x \).

The resulting scheme is:

\[
u_i^{n+1} = u_i^n - \lambda^n[\Delta_x f_-(u_i^n) + \Delta_x f_+(u_i^n)]
\]

\[
= G(u_i^n, u_j^n, u_{j+1}^n).
\]

Then for \( f(u) \) a \( C^1 \) and piecewise \( C^2 \) function, Eq. 9 is first-order accurate and monotone—\( G \) is a nondecreasing function of its arguments—if the Courant–Friedrichs–Lewy (CFL) condition \( |f'(u)| \leq 1 \) is valid. Thus by the results of refs. 5 and 8, it follows that for initial data \( u \) in \( L(1) \cap L_\infty \) and of bounded variation, the approximate solution converges to the physically correct solution of \( \Delta x, \Delta t^n \to 0 \).

We also have an \( L_2 \) estimate for this scheme, which we need in order to satisfy the entropy condition and obtain stability for the full problem 2.

**LEMMA 1.** For \( f(u) = -\frac{1}{2}(Ku - \frac{1}{2}b \gamma + 1)u^2 \) and the restricted CFL condition \( |f'(u)| \leq \frac{1}{2} \) the difference scheme \( 9 \) for \( j = 1, \ldots, N-1 \), with boundary data \( u_0^j \) and \( u_N^j \) prescribed satisfies the estimate

\[
\|u^n\|^2 \leq \|u^0\|^2 + \|\text{boundary data}\|^2
\]

**THEOREM 1.** Let \( \Phi_{b0}^k, v_{b0}^k, v_{\Phi}^k \) be defined as above via splitting. Then

\[
\|u^n\|^2 \leq \|u^0\|^2 + \|\text{boundary data}\|^2.
\]

The entropy condition for the small disturbance equation 2 or 3 is supposed to rule out expansion shocks; i.e., we require \( \Phi_{b0} < 0 \iff u_x < 0 \) in the sense of distributions across a shock. This is implied by the more general entropy inequality:

\[
\frac{\partial}{\partial t} \Phi_{b0}^k + \frac{\partial}{\partial x} \left( \frac{1}{2} \Phi_{b0}^k - \frac{1}{2} \Phi_\Phi^k + \gamma \frac{1}{2} \Phi_\Phi^k \right) - \frac{\partial}{\partial y}(x) (\Phi_\Phi^k) \leq 0.
\]

We have

**THEOREM 2.** Suppose \( \Phi_{b0}^k, v_{b0}^k, v_{\Phi}^k \) as defined above converge boundedly almost everywhere as \( \Delta x, \Delta t^n \to 0 \) to \( \Phi, u \), and \( v \). Then \( \Phi \) is a weak solution of 2 satisfying the entropy inequality 11.

We now turn to higher-order approximations of 1. We begin with the above-mentioned saturation result. Consider a method of lines approach to

\[
u_i = au_i
\]

for any constant \( a > 0 \). We let \( u_i(t) \) approximate \( u(x_i, t) = u(f \Delta x, t) \) via the general one-sided differencing-difference equation:

\[
\frac{\partial u_i}{\partial t} = a \frac{\partial}{\partial x} \left( \frac{1}{2} \beta_k \Delta x \right) u_i.
\]

The scheme is of order of accuracy \( q \) if for smooth functions

\[
\psi(x),
\]

\[
\psi(x) \div \frac{1}{\Delta x} \sum_1^\infty \beta_k \Delta x^k \psi(x) = 0(\Delta x^q),
\]

Here \( \| \| \) denotes the usual discrete \( L_2 \) norm and we omit the precise definition of the norm of the boundary term.

If the inflow is subsonic—i.e., \( u_0, u_1 \leq \bar{u} \)—then \( u_0 \) need not be prescribed, and similarly for supersonic outflow. This is an additional advantage of one-sided schemes—a minimal number of nonphysical boundary conditions is required.

The numerical evidence is that the restriction on the CFL number is unnecessarily strong.

The second part of our first-order splitting scheme is linear.

We solve Eq. 5 numerically with \( \Phi_{b0}^k \) approximating \( \Phi(x_k, y_k, t^n) \). Define \( \Delta_t u_{b0} = \Delta_t \Phi_{b0}^k \) and \( \Delta_y v_{b0} = \Delta_t \Phi_\Phi^k \) and construct the linear, implicit, unconditionally stable, and easily invertible scheme:

\[
u_{b0}^{n+1} = \nu_{b0}^n + \frac{\Delta t}{4} \Delta_y \Phi_\Phi^k
\]

to be solved for \( j = 1, \ldots, N-1 \), \( k = 0, 1, \ldots, M \), with \( u_0^j, \Phi_{b0}^i, v_{b0}^k, \Phi_\Phi^k \), and \( v_{b0}^{M+1} \) prescribed. We have:

**LEMMA 2.** The difference scheme 10 satisfies the \( L_2 \) inequality

\[
\|u^n\|^2 \leq \|u^0\|^2 + \|\text{boundary data}\|^2.
\]

Together the computational stencils for \( \Phi \) are:

\[
\text{Subsonic} \quad \text{Supersonic}
\]

By splitting we can combine these lemmas into a stability result for the full algorithm.

**THEOREM 1.** Let \( \Phi_{b0}^k, v_{b0}^k, v_{\Phi}^k \) be defined as above via splitting. Then

\[
\|u^n\|^2 \leq \|u^0\|^2 + \|\text{boundary data}\|^2.
\]
We have

THEOREM 3. If 13 is stable, then the scheme has order of accuracy at most 2. Moreover, there do exist stable second-order approximations, and the most compact (smallest p) is given by

\[ \beta_1 = 1, \beta_2 = -\frac{1}{2} \] for \( p = 2 \).

Next we construct a simple second-order one-sided approximation to the scalar one-dimensional version of 1 for our \( f(u) \).

Our first attempt is the simplest second-order analogue of 7

\[ (f(u))_n = \frac{1}{\Delta x} \left[ f(u^-) + \frac{\Delta f(u^-)}{\Delta u} \right] \]

We have been unable to prove nonlinear stability (or instability) for this scheme. However, we can show that all its steady shock solutions have overshoot, which is unpleasant enough.

We proposed instead the following scheme:

\[ \phi(u) = \frac{-1}{\Delta x} \left[ f(u^-) - \frac{1}{2} \Delta f(u^-) \right] \]

in which

\[ z_j = \begin{cases} \max(u_j, u_{j+1}) & \text{if } u_{j-1} < u_j < u_{j+1} \\ u_j & \text{if } u_{j-1} \geq u_j \\ \min(u_j, u_{j-1}) & \text{if } u_{j-1} > u_j \leq u_{j+1} \end{cases} \]

for \( j = 2, \ldots, N-2 \), with \( u_0, u_1, u_{N-1} \), and \( u_N \) prescribed.

This scheme is fully one-sided and uses the minimum number of mesh points (three) away from the sonic point \( u_j \), and it is of second-order accuracy away from \( u_j \) and first-order near \( u_j \).

We have the following stability and entropy results for \( f(u) = -\Delta u/(\Delta u + 2) \).

THEOREM 4. The differential difference approximation 17 enforces the a priori estimate

\[ \|u(T)\| \leq \|u(0)\| + \|\text{boundary data}\| \]

Again the boundary data are redundant in the subsonic-inflow, supersonic-outflow case.

This result is proven for 17 that is not time discretized. However, the numerical evidence is that a second-order explicit Lanczos type of time differencing is stable. Moreover, if we write 17 as:

\[ \frac{\partial u}{\partial t} = -\frac{1}{\Delta x} L \Delta t(u_j) \]

then the implicit difference scheme of Crank-Nicholson type:

\[ \frac{1}{\Delta t} (u^{n+1}_j - u^n_j) = -\frac{1}{\Delta x} L \Delta t \left( \frac{u^{n+1}_j + u^n_j}{2} \right) \]

satisfies the last two theorems unconditionally in \( \lambda^n \). The nonlinear inversion for \( u^{n+1} \) does, however, present some difficulties.

As the second step in the splitting algorithm we use scheme 10, merely replacing \( u \) by \( u^{n+1} \) at time levels \( n + 1 \). Because we use backwards differencing in \( f(u) \) to approximate \( u \), the scheme 17 is second-order accurate with respect to \( \Phi \) at \( x_{j-1/2} = (u_{j-1} + u_j)/2 \), not at \( x_j \). The same is true for 10 modified this way, which we call 10'. Thus, using Strang's procedure (15), the splitting method 18 and 10' gives us a second-order accurate scheme. The stencil of the full scheme for \( \Phi \) in the \( (x,y) \) plane is

We have the stability and entropy results:

THEOREM 5. Let \( \Phi_R, \Phi_A, \Phi_3 \) be defined from 18 and 10' via splitting. Then

\[ \|u^n\| \leq \|u_0\| + \|\text{boundary data}\| \]

Moreover, if \( \Phi_3, \Phi_A, \Phi_2 \) converge boundedly almost everywhere as \( \Delta x, \Delta y, \Delta t \to 0 \) to \( \Phi, u, \) and \( v \), then \( \Phi \) is a weak solution of 2 satisfying the entropy condition 11.

Both of our numerical approximations to the time-dependent equation 2 may be viewed as a relaxation procedures for the steady problem 3. It appears that for time-independent boundary data the approximation to 2 converges to a solution of 3 as \( n \to \infty \). See ref. 5 for numerical and analytic evidence of this.

Next we present analytic evidence that our schemes give excellent shock resolution, at least in the one-dimensional case. For a conservation form approximation to a scalar conservation law

\[ u^{n+1}_j = G(u^{n+1}_{j+k}, \ldots, u^{n+1}_{j-k}) \]

we follow ref. 16 and define a traveling wave solution that moves with speed \( s \) to be a solution of

\[ u_{s\lambda} = G(u_{s\lambda+k}, \ldots, u_{s\lambda-k}) \]

The minimal domain on which 20 makes sense consists of functions defined on the linear span over the integers of \( s \lambda \) and 1. Call the closure of this set \( \mathcal{L}_s \). For \( \eta \) rational \( \mathcal{L}_s \) is discrete. For irrational \( \mathcal{L}_s \) is the real line. Define \( L_1(\mathcal{L}_s) \) in the usual fashion. Let the solution of 20a satisfy

\[ u_{s\lambda} = u_L, u_{s\lambda} = u_R \]

with the Rankine-Hugoniot relation

\[ s(u_R - u_L) = f(u_R) - f(u_L) \]

and Oleinik's strict condition \( E \):

\[ f(u) = f(u_R) - f(u_L) \leq u_R - u_L \]

Then we have the following existence and uniqueness results for solutions of the monotone scheme 9 for general \( f \).

THEOREM 6. If \( |\eta| < 1 \), then for each \( u_0 \in (u_R, u_L) \) there exists a function continuous on \( \mathcal{L}_s \) taking on the value \( u_0 \) at \( j = 0 \) that satisfies 14. The solutions are each monotone functions of \( j \) and they satisfy an ordering principle. If \( u_k > u_0 \) then \( u_j \geq u_k \) for each \( j \).

We also have a result concerning stability of traveling waves.

THEOREM 7. Suppose \( \eta \) is rational and the initial function \( u_0 \) has the following properties:

\[ \sum u_0 - u_L < \infty \]

\[ \sum u_0 - u_R < \infty \]
The sequence

\[ u_j^{n+1} = G(u_{j+1}^n, u_j^n, u_{j-1}^n), \quad n = 0, 1, \ldots \]

converges as \( n \to \infty \) in \( L(L^n) \) to a traveling wave. Next we demonstrate the existence of sharp profiles:

**Theorem 8.**

(i) Let \( s > 0 \) and \( f'(u_R) < 0. \) Then the monotone traveling wave solutions to (9) for \( \eta \) rational each have the property that there exists \( j_0 \) with \( u_j = u_R \) for \( j \geq j_0. \)

(ii) Let \( s < 0 \) and \( f'(u_L) > 0, \) then there exists \( j_0 \) with \( u_j = u_L \) for \( j \leq j_0. \)

(iii) If \( s = 0 \) for convex \( f \) having a single critical point \( \bar{u} \) then there exists \( j_0 \) such that

\[ u_j = u_L \quad j < j_0 \]

\[ u_j = u_R \quad j > j_0 + 1 \]

with \( u_j \in [\bar{u}, u_L], \ u_{j+1} \in [u_R, \bar{u}] \) and

\[ f_-(u_{j+1}) + f_+(u_{j+1}) = f_-(u_L) + f_+(u_L). \]

Finally, we have infinite resolution for steady traveling waves, solutions of the second-order scheme 17 for convex \( f(u). \)

**Theorem 9.** The steady traveling wave solutions to 17 for convex \( f(u) \) having a single critical point \( \bar{u} \) are the same as those for 9 mentioned in part (iii) of Theorem 8.

These waves look like

\[ \text{---} \quad \circ \quad \circ \quad \circ \quad \text{---} \]

It would be desirable to extend these results to systems of conservation laws. This does not seem impossible, because the design principle behind the construction of these schemes is intimately related to the proof of the associated stability and entropy theorems. Moreover, some success with one-sided systems was obtained in ref. 12.

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