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Note

High Order "ZIP" Differencing of Convective Terms

The ZIP flux form for differencing the term $(wv)_x$, where w is a convected quantity and v is a convective velocity, is observed to be equivalent to differencing the alternative expression $wv_x + w_x v$ using centered second order finite differences. The advantage of this form is that one class of nonlinear computational instabilities is eliminated. Based on this observation, the extension of the ZIP flux concept to arbitrarily high order accuracy is given. Computational examples show the advantage both of the ZIP flux concept itself and of its higher order forms within the context of flux-corrected transport (FCT) algorithms.

I. Introduction

Consider equations of the form

$$w_t + f_x = 0, \tag{1}$$

where

$$f = wv + f' \tag{2}$$

and hence

$$w_t + (wv)_x + f'_x = 0. \tag{3}$$

Here w, f and v are functions of the independent variables x and t.

The second term in Eq. (3) is called a convective term and is the subject of this paper. We shall say that a finite difference approximation to Eq. (3) is in conservation or "flux" form when the approximation can be written

$$w_i^{n+1} = w_i^n - \Delta t\, \Delta x_i^{-1}[F_{i+1/2} - F_{i-1/2}]. \tag{4}$$

Here the subscripts refer to the spatial grid points x_i, the superscripts to the temporal grid points t^n, $\Delta t \equiv t^{n+1} - t^n$, and $\Delta x_i \equiv \frac{1}{2}(x_{i+1} - x_{i-1})$. We shall assume henceforth that Δx_i is independent of i, and denote the quantity simply by Δx. In this author's opinion, nonuniform meshes are best handled by coordinate transformation or mapping techniques [3, 4, 13]. The $F_{i+1/2}$ are called transportive fluxes, and are functions of the f_i at one or more of the time levels t^n. For a given time level, the functional dependence of F on f can be written to achieve any desired order of spatial accuracy (see [1, Appendix]). For instance, centered second order differences require

$$F_{i+1/2} = \tfrac{1}{2}(f_{i+1} + f_i) \tag{5}$$

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while centered fourth order differences give

$$F_{i+1/2} = (7/12)(f_{i+1} + f_i) - (1/12)(f_{i+2} + f_{i-1}). \tag{6}$$

For the purposes of this paper we wish to divide the net transportive flux $F_{i+1/2}$ into two components: $F^c_{i+1/2}$, the convective component, and $F'_{i+1/2}$, the non-convective component:

$$F_{i+1/2} \equiv F^c_{i+1/2} + F'_{i+1/2}. \tag{7}$$

Thus $F^c_{i+1/2}$ and $F'_{i+1/2}$ are the fluxes corresponding to the second and third terms respectively of Eq. (3). We shall consider only $F^c_{i+1/2}$ here.

II. Second Order ZIP Fluxes

A straightforward implementation of Eq. (5) for the convective flux would yield

$$F^c_{i+1/2} = \tfrac{1}{2}[w_{i+1} v_{i+1} + w_i v_i]. \tag{8}$$

However, as is pointed out in the classic 1968 paper by Hirt [2], a better form for this convective flux is

$$F^c_{i+1/2} = \tfrac{1}{2}[v_{i+1} w_i + w_{i+1} v_i]. \tag{9}$$

Hirt refers to this form as "ZIP" differencing, a convention we shall keep here. Hirt's "heuristic" stability analysis of difference equations entails expanding each term in the difference equation in a Taylor series to obtain the differential equation one is actually solving. Examination of the properties of this new differential equation sheds much light on the stability and error characteristics of the difference equation. Expanding our flux form representation for the second term in (3) we find

$$\left(\frac{\partial wv}{\partial x}\right)^{\mathrm{FD}} \equiv \Delta x^{-1}[F^c_{i+1/2} - F^c_{i-1/2}] = \left(\frac{\partial wv}{\partial x}\right)_i + \mathrm{TE}, \tag{10}$$

where the superscript refers to the finite difference approximation and TE represents the truncation error terms.

For Eq. (8) we find that

$$\mathrm{TE} = \frac{1}{6}\left(\frac{\partial^3 wv}{\partial x^3}\right)_i \Delta x^2 + \frac{1}{120}\left(\frac{\partial^5 wv}{\partial x^5}\right)_i \Delta x^4 + O(\Delta x^6) \tag{11}$$

while for the ZIP flux (9) we find

$$\mathrm{TE} = \frac{1}{6}\left[w\frac{\partial^3 v}{\partial x^3} + v\frac{\partial^3 w}{\partial x^3}\right]_i \Delta x^2 + \frac{1}{120}\left[w\frac{\partial^5 v}{\partial x^5} + v\frac{\partial^5 w}{\partial x^5}\right]_i \Delta x^4 + O(\Delta x^6). \tag{12}$$

In Hirt's heuristic stability analysis one looks for truncation error terms of the form $\partial^2 w/\partial x^2$ on the right-hand side of (3), since each terms will destabilize numerical solutions to Eq. (1) if they are negative and artificially damp the solutions if they are positive. (It should be noted that for certain schemes, terms of this form are destabilizing regardless of their sign. For the leapfrog scheme in particular, this result follows directly from the unconditional instability of the scheme when applied to the heat or diffusion equation [3, p. 61].) A look at (12) shows that terms of this form are simply not present. One can extend Hirt's argument and look for terms involving *any* even derivatives of w with respect to x, since any such terms could potentially be destabilizing, but these too are absent when ZIP fluxes are used. The odd order derivatives in the truncation error terms *will* give rise to error, but these will be of a dispersive rather than of a dissipative or antidissipative nature.

By contrast, if we examine the truncation errors given by (11), we find that the leading term is

$$\frac{1}{6}\frac{\partial^3 wv}{\partial x^3}\Delta x^2 = \left[\frac{1}{2}\frac{\partial^2 w}{\partial x^2}\frac{\partial v}{\partial x} + \frac{1}{2}\frac{\partial^2 v}{\partial x^2}\frac{\partial w}{\partial x} + \frac{1}{6}w\frac{\partial^3 v}{\partial x^3} + \frac{1}{6}v\frac{\partial^3 w}{\partial x^3}\right]\Delta x^2, \tag{13}$$

which will contribute a destabilizing or dissipative term except in the trivial case $\partial v/\partial x = 0$. Thus although both forms for the convective flux have the same formal order of accuracy in terms of Δx, we find the ZIP form preferable from stability considerations.

We wish to emphasize here that the kinds of numerical instability being addressed by ZIP differencing are nonlinear in nature since the instability vanishes when either w or v is constant; indeed, fluxes (8) and (9) are identical in this limit.

III. High Order "ZIP" Fluxes

The extension of the ZIP concept to higher order can be seen by expanding $(wv)_x^{\mathrm{FD}}$ for the second order ZIP flux (9)

$$\begin{aligned}
\left(\frac{\partial wv}{\partial x}\right)_i^{\mathrm{FD}} &= \Delta x^{-1}[F^c_{i+1/2} - F^c_{i-1/2}] \\
&= \tfrac{1}{2}\Delta x^{-1}[w_{i+1}v_i + w_i v_{i+1} - w_i v_{i-1} - w_{i-1}v_i] \\
&= \tfrac{1}{2}\Delta x^{-1}[w_{i+1} - w_{i-1}]\, v_i + \tfrac{1}{2}\Delta x^{-1}[v_{i+1} - v_{i-1}]\, w_i \\
&= v_i\left(\frac{\partial w}{\partial x}\right)_i^{\mathrm{FD}} + w_i\left(\frac{\partial v}{\partial x}\right)_i^{\mathrm{FD}}.
\end{aligned} \tag{14}$$

So we see that ZIP differencing of the convective flux is equivalent to taking a central second order finite difference approximation to the term $wv_x + vw_x$ rather than $(wv)_x$. We point out that Cheng and Shubin [5] have also noted that second order central differencing of the term $wv_x + vw_x$ leads to a conservative scheme, something we have proven here by showing the ZIP form to be the equivalent convective flux. It would seem, then, that higher order forms for ZIP fluxes, if they exist at all, are equivalent to higher order central difference approximations to the form $wv_x + vw_x$. In fact, it is now quite clear why the ZIP fluxes work as they do: For central differences of all orders of accuracy, the truncation error of approximations to first derivatives involve only odd order derivatives of the function. Hence, the form $wv_x + vw_x$ can never produce terms involving even order derivatives of w, as long as centered finite differences are used. By way of contrast "straightforward" central differencing of the form $(wv)_x$ will still produce only odd order derivatives, but those derivatives will operate on the *quantity* wv, and can always be expanded to show that terms involving the undesirable even order derivatives of w are present. For example, the "straightforward" fourth order convective flux

$$F^c_{i+1/2} = (7/12)(w_i v_i + w_{i+1} v_{i+1}) - (1/12)(w_{i-1} v_{i-1} + w_{i+2} v_{i+2}) \tag{15}$$

gives the truncation error

$$\text{TE} = -\frac{1}{90}\frac{\partial^5 wv}{\partial x^5}\Delta x^4 + O(\Delta x^6). \tag{16}$$

Expansion of the leading term shows components involving both $\partial^2 w/\partial x^2$ and $\partial^4 w/\partial x^4$.

Without further ado, we give here the appropriate ZIP fluxes for the indicated spatial order of accuracy:

Second Order:

$$F^c_{i+1/2} = \tfrac{1}{2}[w_{i+1} v_i + w_i v_{i+1}]. \tag{17}$$

Fourth Order:

$$\begin{aligned} F^c_{i+1/2} = &\tfrac{2}{3}[w_{i+1} v_i + w_i v_{i+1}] \\ &- \tfrac{1}{12}[w_{i+2} v_i + w_i v_{i+2} + w_{i+1} v_{i-1} + w_{i-1} v_{i+1}]. \end{aligned} \tag{18}$$

Sixth Order:

$$\begin{aligned} F^c_{i+1/2} = &(3/4)[w_{i+1} v_i + w_i v_{i+1}] \\ &-(3/20)[w_{i+2} v_i + w_i v_{i+2} + w_{i+1} v_{i-1} + w_{i-1} v_{i+1}] \\ &+(1/60)[w_{i+3} v_i + w_i v_{i+3} + w_{i+2} v_{i-1} + w_{i-1} v_{i+2} + w_{i+1} v_{i-2} + w_{i-2} v_{i+1}]. \end{aligned} \tag{19}$$

In general

$$F^c_{i+1/2} = \sum_{k=1}^{N} \frac{1}{k} C^N_k P_{ki}, \tag{20}$$

where $N =$ order of approximation (even) $\div 2$

$$C_1^N = \frac{N}{N+1}, \tag{21}$$

$$C_k^N = -C_{k-1}^N \cdot \frac{N-k+1}{N+k}, \tag{22}$$

$$P_{ki} = \sum_{j=0}^{k-1} (w_{i-j+k} v_{i-j} + w_{i-j} v_{i-j+k}). \tag{23}$$

The reader can verify easily that the quantity $[F^c_{i+1/2} - F^c_{i-1/2}]\, \Delta x^{-1}$ does in fact reproduce the appropriate order finite difference approximation to the quantity $(wv_x + w_x v)_i$ when the above expressions are used.

IV. Numerical Example

We choose as our computational example the exploding diaphragm or Riemann problem for the one-dimensional equations of ideal inviscid compressible fluid flow:

$$\begin{bmatrix} \rho \\ \rho v \\ \rho E \end{bmatrix}_t + \begin{bmatrix} \rho v \\ \rho v^2 \\ \rho E v \end{bmatrix}_x + \begin{bmatrix} 0 \\ P \\ Pv \end{bmatrix}_x = 0, \tag{24}$$

where ρ, v, P and E are the fluid density, velocity, pressure and specific total energy, respectively. Also,

$$P = (\gamma - 1)(\rho E - \tfrac{1}{2}\rho v^2), \tag{25}$$

where we will choose $\gamma = 1.4$. Our initial condition consists of two constant states, one to the left and one to the right, separated by a discontinuity which is assumed to lie midway between two grid points, in this case points 50 and 51. For these calculations $\rho_{\text{left}} = P_{\text{left}} = 1.0$, $\rho_{\text{right}} = 10.0$, and $P_{\text{right}} = 100.0$. All calculations were done on a uniform mesh of 100 grid points using a Courant number of 0.1, and utilizing the second and fourth order leapfrog–trapezoidal flux-corrected transport (FCT) algorithms described in [1]. For simplicity the Boris–Book flux limiter [1, 6] was used. Briefly, FCT algorithms solve Eq. (1) by forming a point by point weighted average of two transportive fluxes, one chosen to give monotone results (free of spurious oscillations) for the problem at hand, and the other to give formally high order accuracy. The high order fluxes are weighted as heavily as possible without violating monotonicity constraints, a process referred to as "flux limiting." In this example our monotone flux is given by the first order Rusanov scheme [7], while our high order fluxes are given by the aforementioned second and fourth order leapfrog–trapezoidal schemes. The tests we will make of ZIP versus non-ZIP differencing of convective terms refer only to the high order portion of the FCT algorithm. FCT algorithms are extremely effective in suppressing the numerical oscillations and instabilities which would otherwise occur with the high order scheme. Because of this, there may be a tendency on the part of the user to believe that great care is not required in choosing the higher order portion of the total FCT scheme since the flux limiting will "save" him. We shall show that this is not always the case.

We have written Eq. (24) to show explicitly the convective terms as the second terms in the (vector) equation. In Fig. 1 we show the calculated (data points) and analytic (solid line) density profiles after 500 time steps using the second order

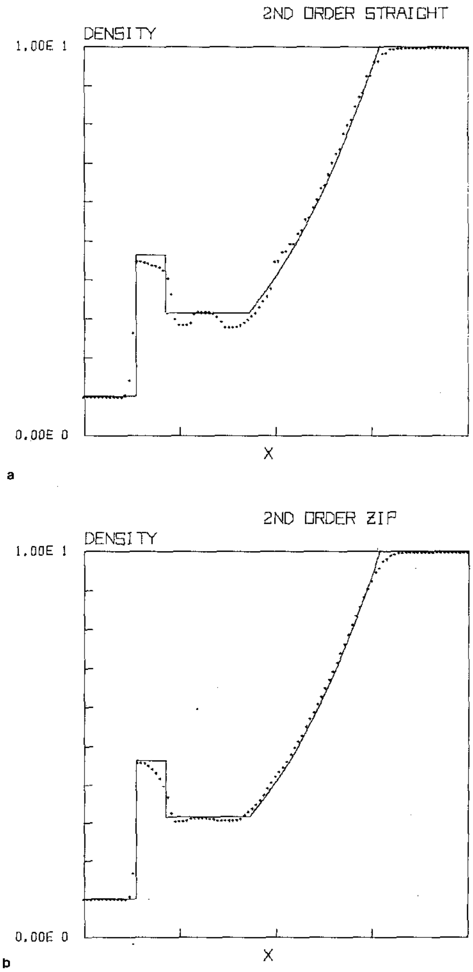

FIG. 1. Comparison of analytic and computed density profiles (solid lines and data points respectively) for the exploding diaphragm problem given in the text for (a) second order straightforward convective fluxes (Eq. (8)), and (b) second order ZIP fluxes (Eq. (17)).

accurate convective fluxes given by the "straightforward" evaluation Eq. (8) and by the ZIP evaluation Eq. (17). We note that analytically we have a shock wave moving to the left, followed by a contact discontinuity, and a rarefaction fan moving to the right. The straightforward calculation is seen to be afflicted by several large scale numerical oscillations while the ZIP calculation yields a reasonably accurate and oscillation-free profile, even though the implementation of FCT has kept both calculations stable. From (3), (10) and (13) we see that straightforward differencing is equivalent to adding a diffusion term with coefficient $-(\partial v/\partial x)/2$ to the right-hand side of (3). When $\partial v/\partial x$ is positive, as in the rarefaction fan, we expect numerical instability; while in the shock $(\partial v/\partial x < 0)$ we expect artificial dissipation. We note

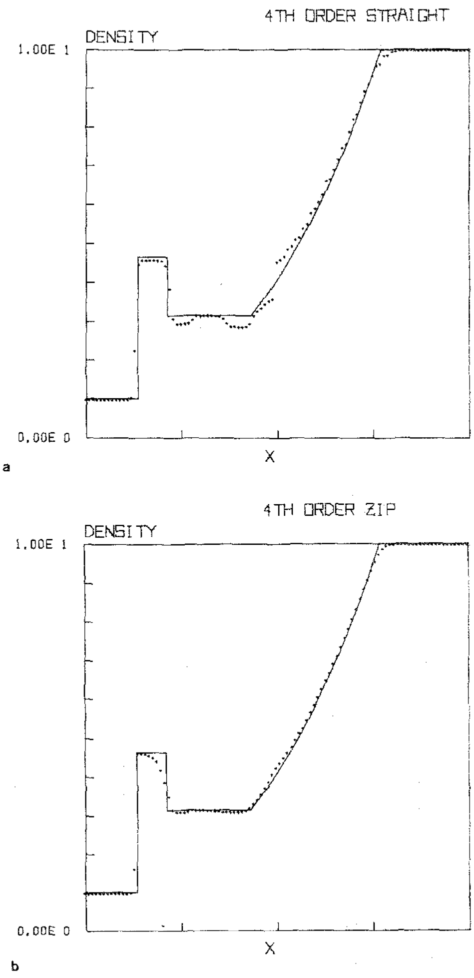

FIG. 2. Same as Fig. 1 but for (a) fourth order straightforward convective fluxes Eq. (15), and (b) fourth order ZIP fluxes Eq. (18).

that all of the regions of roughness or oscillations in Fig 1a represent fluid elements that are, or at one time were, in the rarefaction fan; and further that the density jump at the shock is smaller and occupies a greater number of cells than in the corresponding ZIP calculation, Fig 1b. The ZIP calculation is obviously far superior. To be fair, other procedures could have "fixed" the problem. In fact our choice of the virtually non-dissipative leapfrog–trapezoidal scheme is probably not a wise one for a calculation of this type, where discontinuities abound. Nonetheless we do feel this example makes a valid comparison of convective differencing schemes.

In Fig. 2 we show the same comparison as in Fig. 1, but this time for the fourth order "straightforward" flux Eq. (15) and for the fourth order ZIP flux Eq. (18). Again the "straightforward" calculation gives numerical oscillations whereas ZIP differencing experiences no apparent difficulties. Comparing Fig. 1 and 2 we see an improvement in the solution as we go from second to fourth order, a behavior one would expect based on a linear dispersion analysis. Further improvements in the ZIP solutions are seen as the order of the approximation is increased to sixth and higher, but the oscillations associated with the "straightforward" differencing remain intact. In fact the improvement shown here is quite mild compared to what we have seen in other types of calculations as we increase the spatial order of the approximation. It now appears that the "ultimate" FCT scheme will be either a very high order polynomial-based approximation scheme or a pseudospectral scheme (see [8]). Both the second and fourth order calculation smear the contact discontinuity more than is desirable. This is due to the overly conservative assumptions of the flux limiter used (the"clipping" problem—see [1]) at early times, and can be remedied by using a different flux limiter [1] and using monotonicity constraints whose description is beyond the scope of this paper.

Before leaving this section we briefly present several further calculations which may be of some interest to the reader.

Another very popular way of writing a second order convective flux is

$$F^c_{i+1/2} = \tfrac{1}{4}(w_{i+1} + w_i)(v_{i+1} + v_i) \tag{26}$$

In fact MacCormack [14] has also concluded that the straightforward flux (8) is to be avoided in certain regions and is to be replaced by (26) there. Comparison of (8), (9) and (26) shows that (26) is nothing more than an average of second order ZIP and straightforward fluxes. The results for our Riemann test problem using (26) for the convective fluxes are shown in Fig. 3. We note that the results are far superior to those for the straightforward fluxes, Fig. 1a, but not quite as good as those for the ZIP fluxes, Fig. 1b.

We implied earlier that some of the problems associated with straightforward fluxes could be overcome by using a dissipative scheme. In Fig. 4, we show the results of using the fourth order straightforward flux (15) plus a dissipative flux of the form

$$F^D_{i+1/2} = \frac{1}{24}\left(\left|\frac{v_{i+1}+v_i}{2}\right| + \frac{c_{i+1}+c_i}{2}\right)[w_{i+2} - w_{i-1} - 3(w_{i+1} - w_i)], \tag{27}$$

which approximates a fourth order dissipation term involving the fourth derivative of w. Here c_i is the sound speed at grid point i. Note that the results are much improved over Fig 2a. In Fig. 5 we show the results of adding the same dissipative flux (27) to the fourth order ZIP flux (18). The results are degraded only slightly. The idea of using fourth order dissipation with non-dissipative fourth order schemes is originally due to Kreiss and Oliger [15], and the obvious extension to even higher order schemes is the subject of study by the present author.

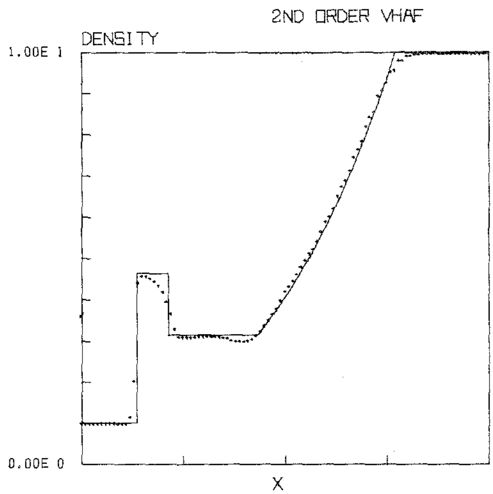

FIG. 3. Same as Fig. 1 but for the second order convectice flux given by Eq. (26).

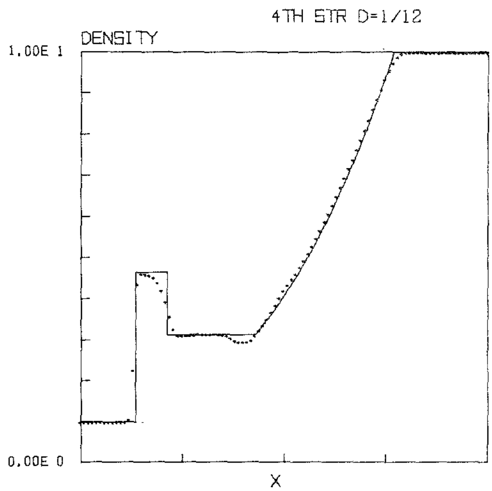

FIG. 4. Same as Fig. 2a but with the addition of a fourth order dissipation term given by Eq. (27).

The reader may note that in the energy component of (24), the Pv term could easily have been treated using the ZIP format. In fact, by (25) P is proportional to one component of ρE and is therefore subject to the same kind of nonlinear instabilities as are the other convective terms. In Fig. 6 we show the results of using the fourth order ZIP flux (18) for both the ρEv and the Pv terms in the energy equation. Although there is very little difference in this case from the straightforward treatment of Pv, the ZIP flux form is recommended on theoretical grounds.

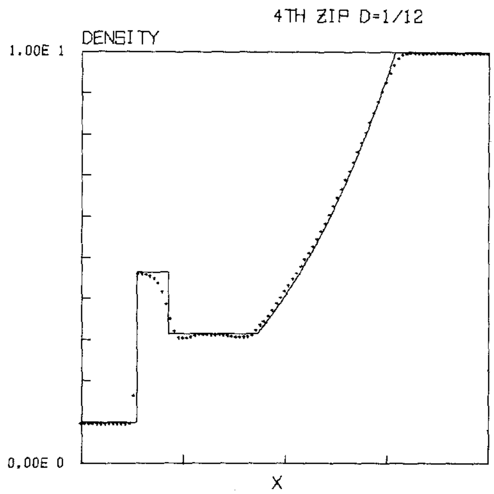

FIG. 5. Same as Fig. 2b but with the addition of a fourth order dissipation term given by Eq. (27).

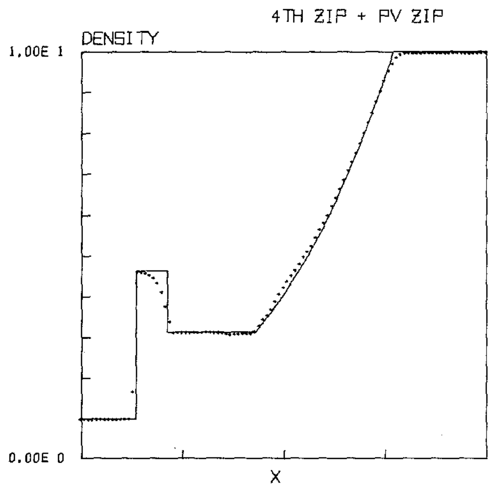

FIG. 6. Same as Fig 2b but using the ZIP format for the term Pv in the energy equation of (24).

V. Conclusions

We have shown that ZIP differencing of the term $(wv)_x$ is the equivalent of a centered differencing of the alternative form $wv_x + w_x v$, both in the second order limit and with regard to the kinds of truncation error terms that are produced for the higher orders. The form of the truncation error terms is such as to eliminate one class of nonlinear computational instabilities. Explicit expressions for the calculation of arbitrarily high order ZIP fluxes have been given, and computational examples have been given to show the advantages of the ZIP flux form over the "straightforward" flux form within the context of FCT algorithms. It seems to us that the "heuristic" stability analysis of Hirt [2] has again proved to be a reliable tool in analyzing numerical schemes. We should point out to the reader that the ZIP flux concept is but one example of a class of numerical techniques based on Hirt's analysis known as truncation error cancellation (TEC) which are now quite highly developed and which have even been automated [9–11]. We also note that while we have limited our discussion here to destabilizing terms due to spatial truncation, TEC considers such terms due to temporal truncation as well. Similar, but not identical, techniques have been given by Warming and Hyett [12], Lerat and Peyret [16], Yanenko and Shokin [17], and by Cheng [18].

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