NASA Contractor Report 172478

ICASE REPORT NO. 84-53

ICASE

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(NASA-CR-172478) GENERALIZED FORMULATION OF TVD LAX-WENDROFF SCHEMES Final Report (NASA) 16 p HC A02/MF A01 CSCL 12A

N85-13528

Unclas

G3/64 24518

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Contract No. NAS1-17070

October 1984

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Operated by the Universities Space Research Association

National Aeronautics and
Space Administration

Langley Research Center
Hampton, Virginia 23665

GENERALIZED FORMULATION OF TVD LAX-WENDROFF SCHEMES

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Abstract

The work of Davis [1], which imports the concept of total-variation-diminution (TVD) into non-upwinded, Lax-Wendroff type schemes, is reformulated in a way which is easier to analyze. The analysis reveals a class of TVD schemes not observed by Davis.

Research was supported by the National Aeronautics and Space Administration under NASA Contract No. NAS1-17070 while the author was in residence at the Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, Hampton, VA 23665.

Introduction

Davis [1] has recently sought to show that concepts developed in the context of upwind-differencing schemes, such as flux limitation and total variation diminution, can be applied to more traditional, Lax-Wendroff-like algorithms, to provide a rational artificial viscosity. His technique was to take a particular class of upwind TVD schemes in a form analyzed by Sweby [2], and then to modify them in such a way as to make them independent of the wave direction.

Our aim in this note is to show that results similar to, but somewhat stronger than, those of Davis can be obtained more simply and directly. Only the case of one-dimensional linear advection will be treated. An extension to two-dimensional nonlinear systems is given in [1].

Analysis

To solve the equation

$$u_t + au_x = 0 \tag{1}$$

on a regular rectangular mesh $x = i\Delta x$, $t = n\Delta t$ with mesh proportions given by the Courant number $\nu = a\Delta t/\Delta x$, consider schemes of the form below, in which $\Delta u_{i+1/2} = u^n_{i+1} - u^n_i$

$$u_i^{n+1} - u_i^n = -\tfrac{1}{2}\nu(1+\nu)\Delta u_{i-1/2} - \tfrac{1}{2}\nu(1-\nu)\Delta u_{i+1/2}$$

$$-\tfrac{1}{2}|\nu|(1-|\nu|)(1-Q_{i-1/2})\Delta u_{i-1/2}$$

$$+\tfrac{1}{2}|\nu|(1-|\nu|)(1-Q_{i+1/2})\Delta u_{i+1/2}. \qquad (2)$$

Here the first line represents the usual Lax-Wendroff scheme, and the other terms represent a conservative dissipation, in which $Q_{i+1/2}$ depends on three consecutive gradients, $\Delta u_{i-1/2}$, $\Delta u_{i+1/2}$, $\Delta u_{i+3/2}$. In fact, since $Q_{i+1/2}$ is dimensionless, it can only depend on the ratios of those gradients, and so we write it as

$$Q_{i+1/2} = Q\left(\frac{\Delta u_{i-1/2}}{\Delta u_{i+1/2}}, \quad \frac{\Delta u_{i+3/2}}{\Delta u_{i+1/2}}\right) \qquad (3)$$

or, more concisely

$$Q_{i+1/2} = Q(r^-_{i+1/2}, \ r^+_{i+1/2}). \qquad (4)$$

The particular form chosen for the scheme will justify itself when it turns out to be very simple to analyze. The factors $|\nu|(1-|\nu|)$ multiplying the dissipative terms can be motivated by noting that the basic Lax-Wendroff scheme is exact and needs no modification if $|\nu| = 0$ or 1. We shall show that Q can be chosen in such a way as to ensure that (2) total-variation diminishing, in the sense of Harten [3]. For this purpose, Davis made use of the Harten-Sweby lemma which requires the scheme to assume the form

$$u_i^{u+1} = u_i^n - C_{i-1/2}\ \Delta u_{i-1/2} + D_{i+1/2}\ \Delta u_{i+1/2}, \qquad (5)$$

which can be rewritten

$$u_i^{n+1} = Cu_{i-1}^n + (1 - C - D)u_i^n + Du_{i+1}^n. \tag{6}$$

Evidently, if the weights C, D, $1 - C - D$ in (6) are all positive, u_i^{n+1} will be bounded by the greatest and least of u_{i-1}^n, u_i^n, u_{i+1}^n; and this is sufficient to ensure that the total variation of u^{n+1} is less than that of u^n. A somewhat stronger constraint, which we shall employ here, is to require, when $\nu > 0$, that $D = 0$ and $0 < C < 1$ (and when $\nu < 0$, that $C = 0$ and $0 < D < 1$). This condition specifies that u_i^{n+1} must be bounded by the data in the ´upwind´ interval. It is rather surprising that this upwind constraint can be met by a non-upwind scheme.

To show that it can, consider first the case $\nu > 0$, and rewrite (1) as

$$\begin{aligned}
u_i^{n+1} - u_i^n &= -\nu\Delta u_{i-\frac{1}{2}} + \tfrac{1}{2}\nu(1 - \nu)\Delta u_{i-\frac{1}{2}} - \tfrac{1}{2}\nu(1 - \nu)\Delta u_{i+\frac{1}{2}} \\
&\quad - \tfrac{1}{2}\nu(1 - \nu)(1 - Q_{i-\frac{1}{2}})\Delta u_{i-\frac{1}{2}} + \tfrac{1}{2}\nu(1 - \nu)(1 - Q_{i+\frac{1}{2}})\Delta u_{i+\frac{1}{2}} \\
&= -\nu\Delta u_{i-\frac{1}{2}} + \tfrac{1}{2}\nu(1 - \nu)Q_{i-\frac{1}{2}}\Delta u_{i-\frac{1}{2}} - \tfrac{1}{2}\nu(1 - \nu)Q_{i+\frac{1}{2}}\Delta u_{i+\frac{1}{2}} \\
&= -\nu\left[1 - \tfrac{1}{2}(1 - \nu)Q_{i-\frac{1}{2}} + \tfrac{1}{2}(1 - \nu)Q_{i+\frac{1}{2}}/r_{i+\frac{1}{2}}^-\right]\Delta u_{i-\frac{1}{2}}
\end{aligned} \tag{7}$$

which is of the form (5) with $D = 0$, and

$$C = \nu\left[1 - \tfrac{1}{2}(1 - \nu)Q_{i-\frac{1}{2}} + \tfrac{1}{2}(1 - \nu)Q_{i+\frac{1}{2}}/r_{i+\frac{1}{2}}^-\right]. \tag{8}$$

The condition that C is positive yields

$$Q_{i-1/2} - Q_{i+1/2}/r^{-}_{i+1/2} < \frac{2}{1-\nu} \tag{9}$$

and the condition that C is less than one is

$$Q_{i+1/2}/r^{-}_{i+1/2} - Q_{i-1/2} < \frac{2}{\nu} . \tag{10}$$

The case $\nu < 0$ follows a similar pattern, which is most clearly revealed by writing $|\nu| = -\nu$, so that

$$u_i^{n+1} - u_i^n = |\nu|\Delta u_{i+1/2} - 1/2\,|\nu|(1 - |\nu|)\Delta u_{i+1/2} + 1/2\,|\nu|(1 - |\nu|)\Delta u_{i-1/2}$$

$$- 1/2\,|\nu|(1 - |\nu|)(1 - Q_{i-1/2})\Delta u_{i-1/2}$$

$$+ 1/2\,|\nu|(1 - |\nu|)(1 - Q_{i+1/2})\Delta u_{i+1/2}$$

$$= |\nu|\Delta u_{i+1/2} - 1/2\,|\nu|(1 - |\nu|)Q_{i+1/2}\,\Delta u_{i+1/2}$$

$$+ 1/2\,|\nu|(1 - |\nu|)Q_{i-1/2}\,\Delta u_{i-1/2}$$

$$= |\nu|[1 - 1/2(1 - |\nu|)Q_{i+1/2} + 1/2(1 - |\nu|)Q_{i-1/2}/r^{+}_{i-1/2}]\Delta u_{i+1/2} \tag{11}$$

which is of the form (5) with $C = 0$ and

$$D = |\nu|[1 - 1/2(1 - |\nu|)Q_{i+1/2} + 1/2(1 - |\nu|)Q_{i-1/2}/r^{+}_{i-1/2}]. \tag{12}$$

The similarity between (12) and (8) reveals that to ensure $0 < D < 1$ the conditions are

$$Q_{i+1/2} - Q_{i-1/2}/r^{+}_{i-1/2} < \frac{2}{1-|\nu|} \tag{13}$$

$$Q_{i-1/2}/r^{+}_{i-1/2} - Q_{i+1/2} < \frac{2}{|\nu|}\,. \tag{14}$$

The task of devising a function Q which meets the conditions (9), (10) (13), (14) is greatly simplified if it is assumed that both Q and Q/r are always positive. In that case we have

$$Q_{i+1/2} < \frac{2}{1-|\nu|} \tag{15}$$

$$Q_{i+1/2}/r^{-}_{i+1/2} < \frac{2}{|\nu|} \tag{16}$$

$$Q_{i+1/2}/r^{+}_{i+1/2} < \frac{2}{|\nu|}\,. \tag{17}$$

These inequalities are precisely those which appear in the theory of flux-limited upwind schemes using 'B-functions' [4] which depend only on r^- when $\nu > 0$, and only on r^+ when $\nu < 0$. $B(r)$ is bounded as in (15), and $B(r)/r$ as in (16) or (17). Here Q must bear a bounded ratio to each of its arguments.

To establish a connection between the present analysis and that of Davis [1], equation (1) of this note should be compared with equations (3-16) and (3-18) of [1]. Using the present notation of r^-, r^+, which is slightly different from the notation used by Davis, it will be found that the algorithm are identical if

$$Q(r^-_{i+1/2}, r^+_{i+1/2}) = \phi(r^-_{i+1/2}) + \phi(r^+_{i+1/2}) - 1, \tag{18}$$

where $\phi(r)$ is Davis' limiting function. This shows that Davis has in effect considered the special case of Q-functions which are 'separable' in the sense that they are the sum of two functions each depending on one of the variables. For such functions Davis establishes the TVD property (not the stronger property proved here) provided

$$0 < \phi(r) < 1 \tag{19}$$

$$0 < \phi(r)/r < 2. \tag{20}$$

These "separable Q-functions" do not necessarily obey conditions (15) - (17), (Q may go down to -1.0, and Q/r may not be bounded). Thus the Q-functions studied here are more general, in the sense of having no special functional form, but more restricted, in the sense of meeting a stronger condition.

To show examples of each type, define "minmod" to be the function which returns the smallest number from a list of positive arguments, but equals zero if any argument is negative. Then a common, though not particularly good limiter for upwind schemes is $\phi(r) = \text{minmod}(1,r)$. Based on this, we could define the separable Q-function

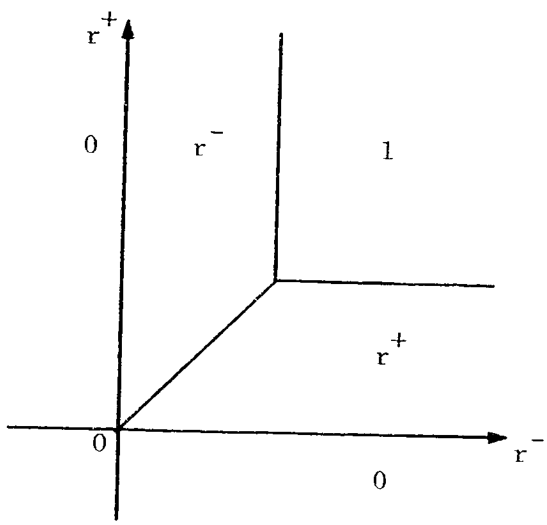
$$Q(r^-,r^+) = \text{minmod}(1,r^-) + \text{minmod}(1,r^+) - 1, \tag{21}$$

or the non-separable Q-function

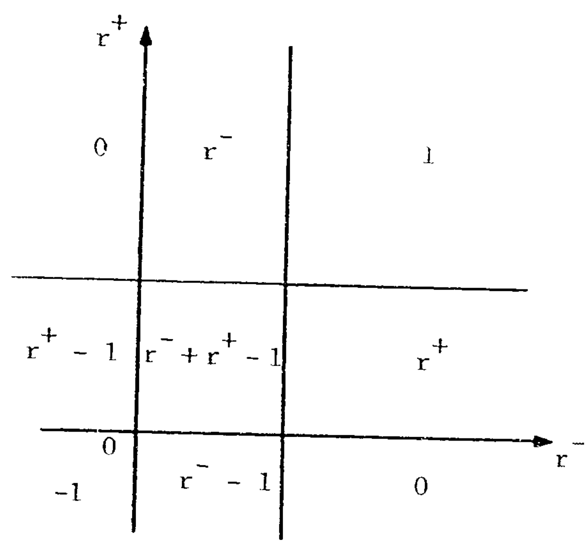
$$Q(r^-,r^+) = \text{minmod}\ (1,r^-,r^+), \tag{22}$$

both of which are sketched below.

We next turn to the question, whether any special choices of the Q-function will produce algorithms with distinguished properties, such as third-order accuracy. It is easily shown [4]



Equation (22)



Equation (21)

that upwind schemes using a limiting function such that when r is close to unity

$$\phi(r) = \frac{(1 + \nu)}{3}\, r + \frac{(2 - \nu)}{3} \tag{23}$$

are third-order accurate in smooth regions of the flow. Analogously, we may seek a linear Q-function, to be used if r^-, r^+ are both close to unity, of the form

$$Q(r^-,r^+) = ar^- + b + cr^+. \tag{24}$$

Substituting this expression into equation (6) produces the algorithm

$$u_i^{n+1} - u_i^n = -\nu\Delta u_{i-1/2} + \frac{a}{2}\nu(1-\nu)\Delta u_{i-3/2} + \frac{b}{2}\nu(1-\nu)\Delta u_{i-1/2}$$

$$+ \frac{c}{2}\nu(1-\nu)\Delta u_{i+1/2} - \frac{a}{2}\nu(1-\nu)\Delta u_{i-1/2}$$

$$- \frac{b}{2}\nu(1-\nu)\Delta u_{i+1/2} - \frac{c}{2}\nu(1-\nu)\Delta u_{i+3/2}\ . \tag{25}$$

Conditions for the accuracy of algorithms of this form were given by Roe [5], the general case being

$$u_i^{n+1} - u_i^n = -\nu \sum \gamma_k \, \Delta u_{i+1/2-k} \tag{26}$$

with the conditions for first, second, and third-order accuracy being respectively

$$\sum_k \gamma_k = 1 \tag{27a}$$

$$\sum_k k\gamma_k = 1/2\,(1+\nu) \tag{27b}$$

$$\sum_k k^2\,\gamma_k = 1/6(1+\nu)(1+2\nu). \tag{27c}$$

In equation (20) the coefficients are

$$\gamma_{-1} = 1/2\,(1-\nu)c \tag{28a}$$

$$\gamma_0 = 1/2\,(1-\nu)(b-c) \tag{28b}$$

$$\gamma_1 = \tfrac{1}{2}(1 - \nu)(a - b) + 1 \tag{28c}$$

$$\gamma_2 = -\tfrac{1}{2}(1 - \nu)a. \tag{28d}$$

Obviously (27a) is satisfied for any a, b, c, and (27b) is satisfied provided

$$a + b + c = 1. \tag{29}$$

After simplification, (27c) reduces to

$$3a + b - c = (1/3)(2\nu - 5). \tag{30}$$

Clearly, there is no way to specify a, b, c independently of ν so that (30) is satisfied, and our ambition to create a third-order, non-upwind, TVD scheme is frustrated.

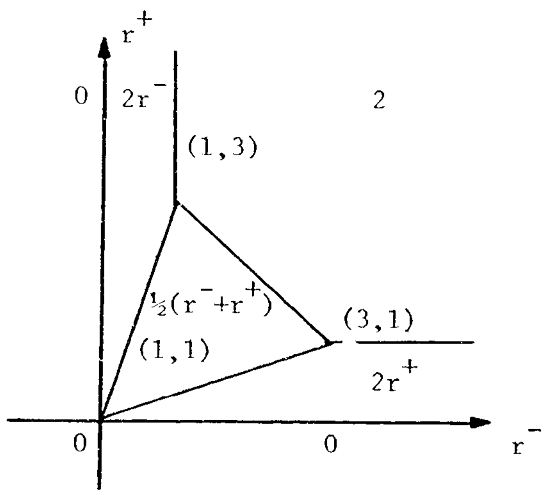
In the absence of a third-order scheme, we may seek special second-order schemes. One possibility is to preserve the property of the basic Lax-Wendroff scheme that it convects exactly any quadratic function of x. For any such function three consecutive differences Δu are in arithmetic progression. Thus the arguments of Q are of the form

$$r^- = 1 - \varepsilon, \qquad r^+ = 1 + \varepsilon \tag{31}$$

and we should seek Q-functions which equal unity for these arguments. The dissipation terms in equation (1) will then vanish. For example, any linear function such as (24) in which $a = c$ and $a + b + c = 1$ will have this property. It is worth remarking that $Q = \frac{1}{2}(r^- + r^+)$ generates a fourth-order dissipation. Of course, linear Q-functions cannot be used for large values of the arguments because they exceed the bounds placed on them by conditions (15) - (17). However, for arguments close to unity, linear Q-functions can be used, although they must be replaced for other arguments. As an example, consider the readily-evaluated function

$$Q = \text{minmod}\left(2,\ 2r^-,\ 2r^+,\ \tfrac{1}{2}(r^- + r^+)\right) \tag{32}$$

whose behavior is displayed in the sketch.



This function will convect exactly any quadratic data, provided the gradient ratios, r^-, r^+ do not lie outside the triangular region. That triangular region can be made much larger if advantage is taken of the way the limits in Theorem I depend on ν. For example, if $\nu = \frac{1}{2}$ an acceptable Q-function is

$$Q = \text{minmod}\left(4,\ 4r^-,\ 4r^+,\ \tfrac{1}{2}(r^- + r^+)\right) \tag{33}$$

and the vertices of triangle move to (1,7) and (7,1).

It is this freedom to match the dissipation to a unique Courant number that will be lost when dealing with systems of equations. Davis [1] suggests matching the scheme to the Courant number of the fastest wave. One might also consider matching the scheme to the strongest wave, by some such device as the following. Let $\lambda_1, \lambda_2, \lambda_3$ be the wavespeeds, and $\alpha_1, \alpha_2, \alpha_3$ the amplitudes, of the waves occurring in the interval $i + 1/2$. The values of these quantities for the Euler equations are well known;

$$\lambda_1 = u - a, \qquad \lambda_2 = u, \qquad \lambda_3 = u + a \tag{34}$$

$$\alpha_1 = \frac{1}{2a^2}\left[\Delta p - \rho a \Delta u\right], \quad \alpha_2 = \frac{1}{a^2}\left[a^2 \Delta\rho - \Delta p\right], \quad \alpha_3 = \frac{1}{2a^2}\left[\Delta p + \rho a \Delta u\right]. \tag{35}$$

Define the mean wave speed λ^* to be

$$\lambda^* = \frac{\alpha_1^2 \lambda_1 + \alpha_2^2 \lambda_2 + \alpha_3^2 \lambda_3}{\alpha_1^2 + \alpha_2^2 + \alpha_3^2}. \tag{36}$$

Since λ^* is a convex combination of $u - a$, u, $u + a$, it must lie between $u - a$ and $u + a$. It is actually given by the formula

$$\lambda^* = u + \frac{2\rho\, a^2\, \Delta p\, \Delta u}{(\Delta p)^2 + \rho^2\, a^2 (\Delta u)^2 + 2(\Delta p - a^2\, \Delta\rho)^2}. \tag{37}$$

In the case of two acoustic waves having equal (or opposite) amplitudes equation (31) returns the particle speed, which is not very useful. Perhaps more useful, and more in the spirit of the enterprise (since the dissipative terms only require the absolute value of ν), would be to compute an r.m.s. wavespeed, given by

$$\bar{\lambda}^2 = \frac{\alpha_1^2\lambda_1^2 + \alpha_2^2\lambda_2^2 + \alpha_3^2\lambda_3^2}{\alpha_1^2 + \alpha_2^2 + \alpha_3^2}$$

$$= u^2 + a^2\,\frac{(\Delta p)^2 + 4\rho u \Delta p \Delta u + \rho^2 a^2 (\Delta u)^2}{(\Delta p)^2 + \rho^2 a^2 (\Delta u)^2 + 2[\Delta p - a^2 \Delta\rho]^2} \,. \qquad (38)$$

The term which appears in the denominator of the fractions in (37), (38) measures the total strength of the disturbance in the cell. It is therefore a candidate for the quantity whose ratios in consecutive cells will serve to define r^-, r^+ (see Davis [1], equation (4.13)). All these possibilities however, require extensive numerical testing.

Conclusions

The inspiration of Davis [1] to introduce the TVD concept into non-upwind algorithms has been reformulated in a way which permits more general results to be deduced by rather simpler arguments. A new class of non-separable limiters emerge from the analysis. Preliminary numerical experiments have not shown any striking advantage to these limiters, but the simplified analysis should be of advantage when attempting to extend these ideas to provide viscosities for symmetrical algorithms other than Lax-Wendroff.

References

[1] S. F. Davis, "TVD finite difference schemes and artificial viscosity," ICASE Report No. 84-20, NASA CR No. 172373, 1984.

[2] P. K. Sweby, "High resolution schemes using flux limiters for hyperbolic conservation laws," SIAM J. Numer. Anal., to appear, 1984.

[3] A. Harten, "High-resolution schemes for hyperbolic conservation laws," J/ Comp. Phys., 49, 1983, p. 357.

[4] P. L. Roe, "Some contributions to the modelling of discontinuous flows," Proc. of AMS/SIAM Summer Seminar on Large Scale Computations in Fluid Mechanics, San Diego, 1983, to appear.

[5] P. L. Roe, "Numerical algorithms for the linear wave equation," RAE Technical Report 81047, 1981.