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Towards the Ultimate Conservative Difference Scheme. II. Monotonicity and Conservation Combined in a Second-Order Scheme

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Fromm's second-order scheme for integrating the linear convection equation is made monotonic through the inclusion of nonlinear feedback terms. Care is taken to keep the scheme in conservation form. When applied to a quadratic conservation law, the scheme notably yields a monotonic shock profile, with a width of only $1\frac{1}{2}$ mesh.

I. INTRODUCTION

This paper is a sequel to Van Leer [1]. Likewise, it deals with the design of monotonic difference schemes, of second-order accuracy, for integrating the nonlinear conservation law

$$\frac{\partial w}{\partial t} + \frac{\partial f(w)}{\partial x} = 0. \tag{1}$$

In [1] it was shown that the scheme of Lax and Wendroff [2] can be made monotonic only at the expense of the conservation form. There is not enough play in the Lax–Wendroff scheme to achieve monotonicity and conservation together. The simplest scheme that does offer enough play is the "zero-average-phase-error method" of Fromm [3]. This scheme will be the present subject.

Fromm's scheme can be regarded as the average of two differently centered second-order schemes, one of which is the usual Lax–Wendroff scheme. When each of the composing schemes is made monotonic, in the way of [1], the average scheme will become monotonic too. If due care is taken, the average scheme may even be conservative, although the composing schemes no longer are. This is demonstrated in Section 2.

Section 3 describes a comparative numerical experiment, in which a monotonic version of Fromm's scheme competes with the original version and with the monotonic first-order scheme of Godunov [4].

As in [1], the monotonicity analysis of Section 2 is based on the linear convection equation

$$\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = 0, \tag{2}$$

where a is a positive constant. For the sake of brevity, an algebraic line of reasoning is followed, rather than the geometric line followed in [1]. The notation, summarized in Table I, is essentially the same as in [1]. The only change is in the choice of the so-called "smoothness monitor", a quantity that, in some way, measures the rate of change of Δw across a nodal point. The expression

$$\zeta_i = \frac{2\Delta_{i-1/2}w}{\Delta_{i+1/2}w - \Delta_{i-1/2}w}, \tag{3}$$

chosen as the monitor for the particular purpose of [1], has been replaced by the simpler expression

$$\vartheta_i = \frac{\Delta_{i+1/2}w}{\Delta_{i-1/2}w}. \tag{4}$$

If $\Delta_{i-1/2}w$ and $\Delta_{i+1/2}w$ both vanish, ϑ_i is set equal to one.

TABLE I

Notation Used in the Grid

Symbol	Definition
x_0	abcissa where the time difference of w is evaluated
x_i	$x_0 + i\Delta x$
t^0	initial time level
t^1	$t^0 + \Delta t$, final time level
w_i	$w(t^0, x_i)$, initial value of w in x_i
w^0	$w(t^1, x_0)$, final value of w in x_0
$\Delta^t w$	$w^0 - w_0$
$\Delta_{i+1/2}w$	$w_{i+1} - w_i$
$w_{i+1/2}$	$\frac{1}{2}(w_i + w_{i+1})$
ϑ_i	$\Delta_{i+1/2}w/\Delta_{i-1/2}w$, smoothness monitor
λ	$\Delta t/\Delta x$, mesh ratio
σ	λa, Courant number

2. Fromm's Scheme Made Monotonic

Fromm's scheme for Eq. (2) is the simplest upstream-centered scheme of second-order accuracy. The upstream centering shows best when the scheme is written as follows:

$$\Delta_F^t w = -\sigma \Delta_{-1/2} w - \frac{\sigma}{4}(1 - \sigma)(\Delta_{1/2} w - \Delta_{-3/2} w); \tag{5}$$

the subscript F stands for "Fromm". Consider further only those values of σ for which this scheme is stable, namely

$$0 \leqslant \sigma \leqslant 1. \tag{6}$$

Note that both members of (5) are perfect differences, hence the scheme is conservative.

Fromm's scheme may be regarded as the average of the following schemes:

$$\Delta_r^t w = -\sigma \Delta_{-1/2} w - \frac{\sigma}{2}(1 - \sigma)(\Delta_{1/2} w - \Delta_{-1/2} w), \tag{7}$$

$$\Delta_l^t w = -\sigma \Delta_{-1/2} w - \frac{\sigma}{2}(1 - \sigma)(\Delta_{-1/2} w - \Delta_{-3/2} w). \tag{8}$$

Both are stable when (5) is stable. Scheme (7) is the scheme of Lax and Wendroff, giving $\Delta^t w$ in terms of $\Delta_{1/2} w$ and $\Delta_{-1/2} w$ with second-order accurancy. Scheme (8) also gives $\Delta^t w$ with second-order accuracy, but in terms of $\Delta_{-1/2} w$ and $\Delta_{-3/2} w$. The subscripts r and l stand for "right" and "left" and refer to the choice of the spatial differences in these schemes.

In the present context, a scheme is called monotonic if it yields a value of w^0 that lies between w_0 and w_{-1}. In formula:

$$0 \leqslant -\frac{\Delta^t w}{\Delta_{-1/2} w} \leqslant 1. \tag{9}$$

If both schemes (7) and (8) are modified so that they satisfy condition (9), their average will also satisfy (9). In other words, making both (7) and (8) monotonic is one way to make scheme (5) monotonic. As shown below, it is also the only way in which the conservation form may be maintained.

In making scheme (7) monotonic, the quantity that matters is the ratio of $\Delta_{1/2} w$ and $\Delta_{-1/2} w$. This ratio is the local value of the smoothness monitor ϑ_i defined in

Eq. (4). In order to achieve monotonicity, it must be fed back into the coefficients of the scheme. The monotonic version of (7), derived in [1], has the form

$$\Delta^t_{rm} w = -\sigma \Delta_{-1/2} w - \frac{\sigma}{2}(1-\sigma)\{1 - Q(\vartheta_0)\}(\Delta_{1/2} w - \Delta_{-1/2} w); \tag{10}$$

the subscript m stands for "monotonic". The function $Q(\vartheta_0)$ must lie between certain limits in order to make scheme (10) satisfy condition (9) for any value of ϑ_0, and for any value of σ in the stability range (6). To keep scheme (10) quadratic in σ, Q is assumed to be independent of σ.

Scheme (8) is modified in the same way as scheme (7). The monotonic version reads

$$\Delta^t_{lm} w = -\sigma \Delta_{-1/2} w - \frac{\sigma}{2}(1-\sigma)\{1 - R(\vartheta_{-1})\}(\Delta_{-1/2} w - \Delta_{-3/2} w). \tag{11}$$

Condition (9) is satisfied by properly choosing the function $R(\vartheta_{-1})$; assume that R, too, is independent of σ.

It is seen that the schemes (10) and (11) are not conservative: the nonlinear terms needed for monotonicity are no perfect differences. However, the average of (10) and (11) may again be conservative, if only we can find a function $S(\vartheta)$ with the following property:

inserting $Q(\vartheta_0) = S(\vartheta{=}\vartheta_0)$ makes scheme (10) monotonic, while

inserting $R(\vartheta_{-1}) = -S(\vartheta{=}\vartheta_{-1})$ makes scheme (11) monotonic.

Using such a function, the average scheme becomes

$$\begin{aligned}\Delta^t_{Fm} w = &-\sigma \Delta_{-1/2} w - \frac{\sigma}{4}(1-\sigma)(\Delta_{1/2} w - \Delta_{-3/2} w)\\ &+ \frac{\sigma}{4}(1-\sigma)\{S(\vartheta_0)(\Delta_{1/2} w - \Delta_{-1/2} w) - S(\vartheta_{-1})(\Delta_{-1/2} w - \Delta_{-3/2} w)\}.\end{aligned} \tag{12}$$

As desired, the terms between curly brackets form a perfect difference. This difference is of the third order, hence does not disturb the second-order accuracy achieved in the linear terms of scheme (12).

A linear stability analysis of scheme (12) yields the same stability condition as for scheme (5), provided that

$$S^2(\vartheta) \leqslant 1 + O(\Delta x). \tag{13}$$

This restriction is too weak to be useful in determining $S(\vartheta)$. A stronger restriction can be obtained as follows. Assume, for a moment, that $\Delta_{-3/2}w = \Delta_{1/2}w$, or

$$\vartheta_{-1} = 1/\vartheta_0 . \tag{14}$$

Fromm's original scheme (5) then reduces to the scheme of Godunov:

$$\Delta_G^t w = -\sigma\Delta_{-1/2}w, \tag{15}$$

which is monotonic. In this case, the S-terms in Eq. (12) serve no purpose, and their net contribution therefore must vanish. It follows that

$$S(\vartheta_{-1}) = -S(\vartheta_0) \qquad \text{for} \quad \vartheta_{-1} = 1/\vartheta_0 , \tag{16}$$

or, in general,

$$S(1/\vartheta) = -S(\vartheta). \tag{17}$$

This kind of anti-symmetry immediately fixes the following function-values:

$$S(1) = S(-1) = 0. \tag{18}$$

Eq. (18) can be further interpreted. From the definition of ϑ it follows that, in general,

$$\vartheta = 1 + O(\Delta x). \tag{19}$$

In those points where, in the exact solution of Eq. (2), w reaches a local extremum, (19) makes way for

$$\vartheta = -1 + O(\Delta x). \tag{20}$$

Thus, Eq. (18) essentially says that

$$S(\vartheta) = O(\Delta x), \tag{21}$$

which, by a large margin, renders stability to scheme (12).

Further information on $S(\vartheta)$ follows from applying condition (9) to both schemes (10) and (11), with $Q(\vartheta_0)$ and $R(\vartheta_{-1})$ replaced by $S(\vartheta_0)$ and $-S(\vartheta_{-1})$. When σ runs from 0 to 1, the key quantity $-\Delta^t w/\Delta_{-1/2}w$ runs from 0 to 1 in all schemes considered. It will not go beyond these bounds provided that

$$\frac{\partial}{\partial\sigma}\left(-\frac{\Delta^t w}{\Delta_{-1/2}w}\right) \geqslant 0 \qquad \text{for} \quad \sigma = 0, 1. \tag{22}$$

Imposing condition (22) on schemes (10) and (11), for arbitrary values of ϑ_0 and ϑ_{-1}, yields the following restrictions on the choice of $S(\vartheta)$:

$$|\{1 - S(\vartheta)\}(\vartheta - 1)| \leqslant 2, \tag{23}$$

$$\left|\{1 + S(\vartheta)\}\left(1 - \frac{1}{\vartheta}\right)\right| \leqslant 2. \tag{24}$$

Imposing condition (22) merely on scheme (12) leads to

$$\left|\{1 - S(\vartheta_0)\}(\vartheta_0 - 1) + \{1 + S(\vartheta_{-1})\}\left(1 - \frac{1}{\vartheta_{-1}}\right)\right| \leqslant 4. \tag{25}$$

This, however, splits into (23) and (24), since it must hold for any combination of values of ϑ_0 and ϑ_{-1}. In order words: the monotonicity of both scheme (10) and scheme (11) indeed is necessary for the monotonicity of scheme (12).

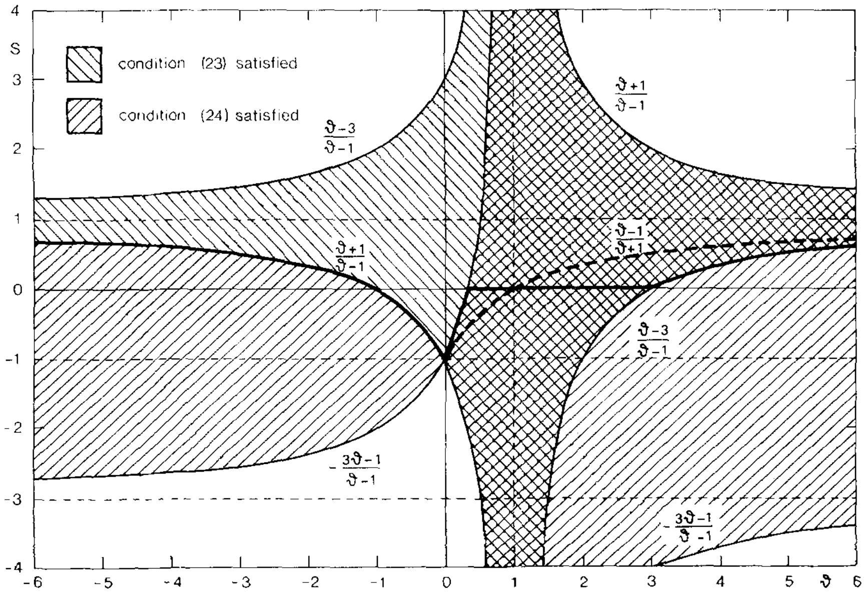

FIG. 1. Graphic representation of the conditions on $S(\vartheta)$.

From (23) it follows that the graph of $S(\vartheta)$ must lie in the domain enclosed by the graphs of the functions $(\vartheta - 3)/(\vartheta - 1)$ and $(\vartheta + 1)/(\vartheta - 1)$, while (24) implies that the graph of $S(\vartheta)$ must lie in the domain enclosed by the graphs of the functions $-(3\vartheta - 1)/(\vartheta - 1)$ and $(\vartheta + 1)/(\vartheta - 1)$. These domains and their cross-section are depicted in Fig. 1. For $\vartheta \leqslant 0$, $S(\vartheta)$ appears to be uniquely determined:

$$S(\vartheta) = \frac{\vartheta + 1}{\vartheta - 1} \quad \text{for} \quad \vartheta \leqslant 0. \tag{26}$$

These values are indicated in Fig. 1 by a heavy solid line; note that they agree with (17). For $\vartheta > 0$, the heavy solid line is continued by minimizing $|S(\vartheta)|$:

$$\begin{aligned} S(\vartheta) &= -\frac{3\vartheta - 1}{\vartheta - 1} && \text{for} \quad 0 < \vartheta < \tfrac{1}{3}, \\ S(\vartheta) &= 0 && \text{for} \quad \tfrac{1}{3} \leqslant \vartheta \leqslant 3, \\ S(\vartheta) &= \frac{\vartheta - 3}{\vartheta - 1} && \text{for} \quad \vartheta > 3, \end{aligned} \tag{27}$$

again in agreement with (17). The S-values in (26) and (27) are the same as the Q-values derived for scheme (10) in [1], at least for $|\vartheta| \geqslant 1$. For $|\vartheta| < 1$, Q could be set equal to zero since condition (17) did not arise.

A not-so-tight choice of $S(\vartheta)$, permitted by (17), is

$$S(\vartheta) = \frac{\vartheta - 1}{\vartheta + 1} \quad \text{for} \quad \vartheta > 0, \tag{28}$$

indicated by the heavy broken line in Fig. 1. Combining it with (26) yields the simple expression

$$S(\vartheta) = \frac{|\vartheta| - 1}{|\vartheta| + 1} \quad \text{for any value of } \vartheta. \tag{29}$$

This choice of S may be the safer one to be used in a scheme for a nonlinear conservation law. From a computational viewpoint, expression (29) certainly is the most convenient choice, since it does not really require the evaluation of ϑ. In practice, S will be evaluated as

$$S(\vartheta_i) = \frac{|\Delta_{i+1/2}w| - |\Delta_{i-1/2}w|}{|\Delta_{i+1/2}w| + |\Delta_{i-1/2}w|}. \tag{30}$$

The denominator is calculated first; if it vanishes, S is set equal to zero.

3. A Numerical Experiment

For the nonlinear conservation law (1), a is defined as

$$a(w) = \frac{df(w)}{dw}; \tag{31}$$

assume that $a(w)$ is positive. In reformulating scheme (12) for Eq. (1), $\sigma \Delta_{i+1/2} w$ is replaced by $\lambda \Delta_{i+1/2} f$, and $\sigma(1 - \sigma) \Delta_{i+1/2} w$ by $\lambda(1 - \lambda a_{i+1/2}) \Delta_{i+1/2} f$. Scheme (12) then changes into

$$\begin{aligned} \Delta^t w = {} & - \lambda \Delta_{-1/2} f \\ & \quad \underline{G}| \\ & - \frac{\lambda}{4} \{(1 - \lambda a_{1/2}) \Delta_{1/2} f - (1 - \lambda a_{-3/2}) \Delta_{-3/2} f\} \\ & \qquad\qquad\qquad\qquad\qquad\qquad \underline{F}| \\ & + \frac{\lambda}{4} [S(\vartheta_0)\{(1 - \lambda a_{1/2}) \Delta_{1/2} f - (1 - \lambda a_{-1/2}) \Delta_{-1/2} f\} \\ & - S(\vartheta_{-1})\{(1 - \lambda a_{-1/2}) \Delta_{-1/2} f - (1 - \lambda a_{-3/2}) \Delta_{-3/2} f\}]. \qquad (32) \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad \underline{Fm}| \end{aligned}$$

As indicated, in this formula are also embedded the nonlinear versions of Fromm's original scheme (5) and Godunov's scheme (15).

In a numerical experiment, the three schemes of Eq. (32) were applied to the nonlinear conservation law

$$\frac{\partial w}{\partial t} + \frac{\partial(\frac{1}{2} w^2)}{\partial x} = 0. \qquad (33)$$

The following initial values were prescribed:

$$\begin{aligned} w_i &= w_- && \text{for} \quad i \leqslant 25, \\ w_i &= \tfrac{1}{2}(w_- + w_+) && \text{for} \quad i = 26, \\ w_i &= w_+ && \text{for} \quad i \geqslant 27, \end{aligned} \qquad (34)$$

where either $w_- = \frac{1}{2}$, $w_+ = 1$, or $w_- = 1$, $w_+ = \frac{1}{2}$. With $w_- < w_+$, these data represent an expansion wave; with $w_- > w_+$, a compression wave. Both waves will move at the speed

$$W = \tfrac{1}{2}(w_- + w_+). \qquad (35)$$

The mesh ratio was chosen according to

$$\lambda W = \tfrac{1}{2}. \qquad (36)$$

Due to this very choice, the waves produced by the schemes considered all moved exactly one space mesh in two time steps, right from the start. Moreover, the form of the waves remained exactly anti-symmetric around the point where $w = W$. These phenomena are related to the fact that the schemes, when applied to the linear Eq. (2), produce no dispersive errors for $\sigma = \frac{1}{2}$.

Figure 2 shows the results of the three schemes for the expansion wave at $t = 24\,\Delta t$, while Fig. 3 shows an overlay of the results for the shock waves at $t = 21\,\Delta t$ and $24\,\Delta t$. The results of the monotonic version of Fromm's scheme were obtained with the S-values of Eq. (28).

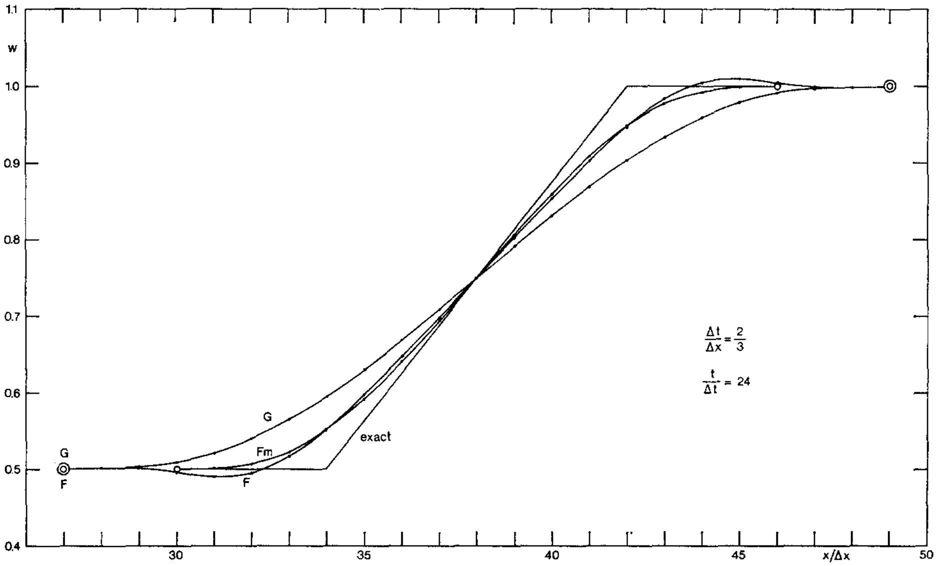

FIG. 2. Numerical representation of an expansion wave by the schemes of Godunov (curve G), Fromm (curve F) and Fromm, monotonic (curve Fm). Beyond the tack marks, the numerical results differ less than 0.0005 from the exact solution.

The figures clearly demonstrate the superiority of the monotonic version of Fromm's scheme. The results of this scheme have the acuity of the results of the original scheme of Fromm, while lacking the ringing generated by the latter scheme. This improvement involves an increase in computing time of only about a factor 4/3. The improvement over Godunov's scheme is even more obvious, but involves an increase in computing time of about a factor 4. On the other hand, Godunov's scheme can reach the accuracy of the monotonic version of Fromm's scheme only through a reduction of the mesh width of about a factor 3 in the case of Fig. 2, and about a factor 2 in the case of Fig. 3. This leads to an increase in computing time of a factor 9 and a factor 4, respectively. Thus, for a given accuracy, Godunov's scheme requires at least as much computing time as the monotonic version of

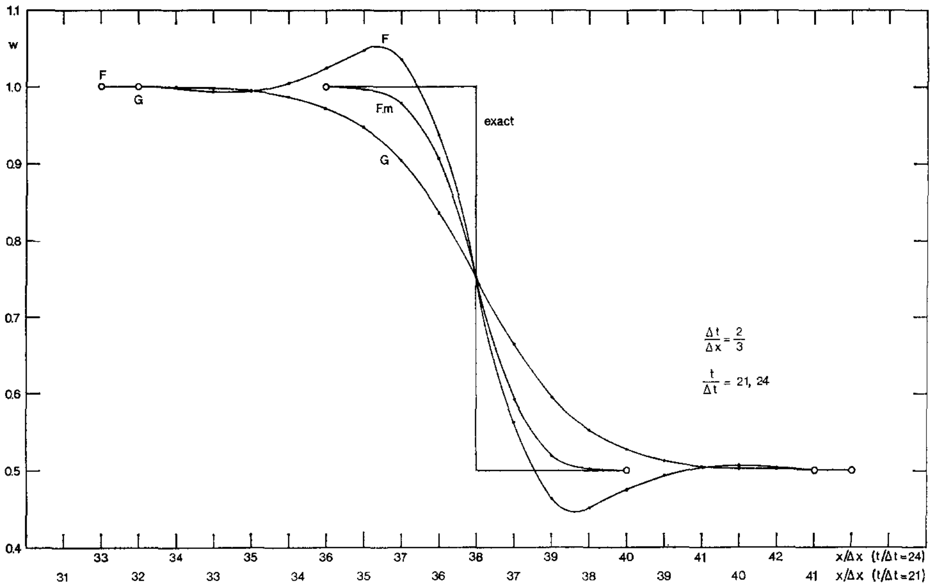

FIG. 3. Same as Fig. 2, but for a compression wave.

Fromm's scheme. This makes the latter scheme the most economic one of the schemes tested.

In the next paper of the present series, I shall discuss the application of Fromm's scheme and its monotonic version to the Lagrangean flow equations.

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