# TVD Schemes, Positive Schemes, and the Universal Limiter

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3 July 1996 and 31 December 1996

ABSTRACT

Three approaches to building one-dimensional shape-preserving advection schemes, based on TVD (total variation diminishing) schemes, on positive schemes, and on the universal limiter, are shown to lead to the same constraints on the fluxes between grid boxes. Thus, although they have slightly different conceptual bases, the three approaches lead to mathematically equivalent schemes.

## 1. Introduction

Atmosphere and ocean dynamics on all scales is dominated by advection, so there is an ongoing effort to improve numerical advection schemes and to incorporate the best available schemes in numerical models of the atmosphere and ocean. However, the published literature on numerical methods in general, and on advection schemes in particular, is enormous and multidisciplinary. It is perhaps not surprising, then, that mathematically equivalent schemes may be invented independently more than once, often with different conceptual bases. For example, for a constant advecting velocity on a regular one-dimensional grid, it is well known that the second-order Crowley scheme (Crowley 1968; Tremback et al. 1987) is equivalent to the Lax–Wendroff scheme (Lax and Wendroff 1960), and that the third-order advective form Crowley scheme (Tremback et al. 1987) is equivalent to the QUICKEST scheme (Leonard 1979).

A desirable property of an advection scheme is that it should be ''monotonicity-preserving'' or ''shape-preserving''; that is, it should not create spurious extrema or cause spurious amplification of existing extrema in an advected quantity. This desirable property can be achieved by carefully constraining or ''limiting'' the advective fluxes calculated by the scheme. For one-dimensional advection, there are several superficially different approaches to limiting the fluxes. These include approaches based on total variation diminishing (TVD) schemes (e.g., Harten 1983; Sweby 1985), on positive schemes (Hundsdorfer et al. 1995), and on the universal limiter (Leonard 1991). For more complicated problems, the differences between these three approaches are important, not least because they can be extended in different ways. For example, the TVD approach can be applied to conservation laws other than the advection equation (e.g., Harten 1983; Sweby 1985); the positive schemes approach, by treating the space and time discretizations separately, allows different time stepping schemes to be used (Hundsdorfer et al. 1995); while the universal limiter approach has been extended to multidimensional advection on arbitrary meshes (Thuburn 1996). In this note, however, attention is restricted to the one-dimensional linear advection equation. In this case, as will be shown below, the three approaches then lead to equivalent schemes when appropriate choices are made.

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## 2. TVD schemes

Consider the advection of a mixing ratio–like quantity $q$ in one dimension by a velocity $u$, described by the equation

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} = 0, \quad (1)$$

and, to simplify the discussion, restrict attention to the case where $u$ is constant and positive. Let $q_k^m$ be a discrete approximation to $q$ in the $k$th grid box at time step $m$. The total variation TV at time step $m$ is defined by

$$\mathrm{TV}^m = \sum_k |q_{k+1}^m - q_k^m|. \quad (2)$$

A scheme is TVD if it ensures that

$$\mathrm{TV}^{m+1} \leq \mathrm{TV}^m. \quad (3)$$

The TVD property is a global property of an advection scheme. It goes some way toward preventing spurious amplification of extrema; for example, Harten (1983) proved that an initially monotonic profile $q$ remains monotonic after advection by a TVD scheme. However, the TVD property does not preclude the possibility that one extremum may grow while another nearby diminishes. This point will be addressed again at the end of section 3.

Suppose an advection scheme can be written in the form

$$q_k^{m+1} = q_k^m - C_{k-1/2}(q_k^m - q_{k-1}^m) + D_{k+1/2}(q_{k+1}^m - q_k^m), \tag{4}$$

where the $C$'s and $D$'s may depend on the $q$'s as well as on $u$. Harten (1983) showed that the conditions

$$0 \le C_{k+1/2}$$
$$0 \le D_{k+1/2}$$
$$C_{k+1/2} + D_{k+1/2} \le 1 \tag{5}$$

(for all $k$) are sufficient to ensure that the scheme is TVD. A strategy for building a TVD scheme, therefore, is to take a basic advection scheme, rewrite it in the form of (4), and then modify it so that it satisfies the conditions (5).

To illustrate this approach, consider a regular grid of box size $\Delta x$. Because $u$ is constant, a conservative advection scheme can be written in the form

$$q_k^{m+1} = q_k^m - c(\hat{q}_{k+1/2} - \hat{q}_{k-1/2}), \tag{6}$$

where $c = u\Delta t/\Delta x$ and $\hat{q}$'s are mixing ratios at the grid box edges. One particular example is the Lax–Wendroff, or second-order Crowley scheme, in which the $\hat{q}$'s are defined by

$$\hat{q}_{k+1/2} = q_k^m + \frac{1}{2}(1 - c)(q_{k+1}^m - q_k^m). \tag{7}$$

To build a TVD scheme, this basic advection scheme is modified by introducing a factor, $\phi$, called the ''flux limiter'':

$$\hat{q}_{k+1/2} = q_k^m + \frac{1}{2}\phi_k(1 - c)(q_{k+1}^m - q_k^m). \tag{8}$$

When $\phi_k = 1$, the scheme reduces to the Lax–Wendroff scheme. When $\phi_k = 0$, the scheme reduces to the first-order upwind ''donor cell'' scheme. More generally, $\phi_k$ may depend on the $q$'s and so vary with position and time.

Equations (6) and (8) can be combined and rearranged into the form of (4) (with $D_{k+1/2} = 0$):

$$q_k^{m+1} = q_k^m - c(q_k^m - q_{k-1}^m)\left[1 - \frac{1}{2}(1 - c)\phi_{k-1} + \frac{1}{2}(1 - c)\frac{\phi_k}{r_{k+1/2}}\right], \tag{9}$$

where $r_{k+1/2} = (q_k^m - q_{k-1}^m)(q_{k+1}^m - q_k^m)^{-1}$. Then, provided that $c < 1$, the following conditions on $\phi_k$ imply the conditions (5) and therefore imply that the scheme is TVD:

$$0 \le \phi_k \le 2/(1 - c) \qquad \forall k,$$
$$0 \le \phi_k/r_{k+1/2} \le 2/c \qquad \forall k. \tag{10}$$

The dependence on $c$ can be avoided by accepting tighter conditions on $\phi_k$:

$$0 \le \phi_k \le 2 \qquad \forall k,$$
$$0 \le \phi_k/r_{k+1/2} \le 2 \qquad \forall k. \tag{11}$$

This is the form most commonly used and is often represented by means of what has become known as a Sweby diagram (e.g., Sweby 1985). However, the more general form (10) was known, for example, to Roe and Baines (1983), although they imposed some additional constraints. A particular example of a limiter satisfying (11) is van Leer's (1974):

$$\phi_k = \frac{r_{k+1/2} + |r_{k+1/2}|}{1 + |r_{k+1/2}|}. \tag{12}$$

TVD schemes are usually based on the Lax–Wendroff scheme (7), as described above. However, the same approach can, in fact, be followed for any high-order basic advection scheme. Let $\hat{q}_{k+1/2} = q_{k+1/2}^{(\mathrm{H})}$ be the box-edge mixing ratio implied by a high-order basic advection scheme. As before, this basic scheme is modified by introducing a flux limiter:

$$\hat{q}_{k+1/2} = q_k^m + \phi_k(q_{k+1/2}^{(\mathrm{H})} - q_k^m). \tag{13}$$

Again, $\phi_k = 1$ gives back the basic advection scheme while $\phi_k = 0$ gives the donor cell scheme. By substituting (13) in (6) and rearranging into the form of (4), it can be shown that the conditions on $\phi$,

$$0 \le \phi_k s_{k+1/2} \le 1 \qquad \forall k,$$
$$0 \le \phi_k s_{k+1/2}/r_{k+1/2} \le 1/c - 1 \qquad \forall k, \tag{14}$$

imply that the scheme is TVD, where $r_{k+1/2}$ is defined as above and $s_{k+1/2} = (q_{k+1/2}^{(\mathrm{H})} - q_k^m)(q_{k+1}^m - q_k^m)^{-1}$ (e.g., Zalesak 1987; Thuburn 1993).

## 3. Positive schemes

Hundsdorfer et al. (1995) call a spatial semidiscretization of (1) positive if, and only if, it satisfies

$$q_i = 0,\ q_j \ge 0\ \forall i \ne j \Rightarrow dq_i/dt \ge 0. \tag{15}$$

The requirement of positivity leads to a constraint on the fluxes implied by the semidiscretization. A full discretization of (1) is called positive if the spatial semidiscretization is positive and, in addition, no positive value of $q$ can become negative during one time step when all values are initially greater than or equal to zero. This leads to a second constraint involving the size of the time step. These two constraints will now be shown to be equivalent to (14).

Consider a scheme written in the form (6) with $\hat{q}_{k+1/2}$ given by

$$\hat{q}_{k+1/2} = q_k^m + \frac{1}{2}\psi_{k+1/2}(q_k^m - q_{k-1}^m), \tag{16}$$

where $\psi_{k+1/2}$ may depend on the $q$'s. Any scheme may be written in this form by a suitable definition of $\psi_{k+1/2}$ (except possibly when $q_k^m - q_{k-1}^m = 0$). Substituting (16) in (6) gives

$$q_k^{m+1} = q_k^m - c(q_k^m - q_{k-1}^m)\left(1 + \frac{1}{2}\psi_{k+1/2} - \frac{1}{2}\psi_{k-1/2}r_{k-1/2}\right), \tag{17}$$

where $r_{k+1/2}$ is defined as above. First, consider the case $q_k^m = 0$, $q_{k-1}^m \geq 0$. Here, $q_k^{m+1}$ will be greater than or equal to zero for all $k$, that is, the spatial semidiscretization will be positive, under the condition

$$0 \leq 1 + \frac{1}{2}\psi_{k+1/2} - \frac{1}{2}\psi_{k-1/2}r_{k-1/2} \leq K \qquad \forall k \tag{18}$$

for any $K \geq 1$. The following pair of conditions imply (18):

$$0 \leq \psi_{k+1/2} \leq \delta \qquad \forall k,$$
$$0 \leq \psi_{k+1/2}r_{k+1/2} \leq 2 \qquad \forall k, \tag{19}$$

where $\delta = 2(K - 1)$. Now consider the case $q_k^m > 0$, $q_{k-1}^m = 0$. Here, $q_k^{m+1}$ will be greater than or equal to zero, that is, the fully discretized scheme will be positive, if, in addition to (18), the following condition holds:

$$cK \leq 1. \tag{20}$$

Rewriting (20) in terms of $\delta$ rather than $K$ and substituting in (19) leads to the following pair of conditions for the scheme to be positive:

$$0 \leq \psi_{k+1/2} \leq 2(1/c - 1) \qquad \forall k,$$
$$0 \leq \psi_{k+1/2}r_{k+1/2} \leq 2 \qquad \forall k. \tag{21}$$

Hundsdorfer et al. note that if a positive scheme satisfies the linear invariance property

$$p_k = \alpha q_k + \beta \quad \forall k \Rightarrow \hat{p}_{k+1/2} = \alpha\hat{q}_{k+1/2} + \beta \quad \forall k, \tag{22}$$

where $p$ is a second mixing ratio–like quantity and $\alpha$ and $\beta$ are constants, then there will be no spurious generation or amplification of extrema. In fact, it is clear from the derivation above that the conditions (21) imply that $q_k^{m+1}$ must lie between $q_{k-1}^m$ and $q_k^m$, so there will be no spurious generation or amplification of extrema even if the linear invariance property does not hold.

Now note that the substitution $\psi_{k+1/2} = 2\phi_k s_{k+1/2}$ makes (16) equivalent to (13) and makes the positivity constraints (21) equivalent to the TVD constraints (14). Furthermore, it is now clear that the constraints (14) imply not just the global TVD property (3), but also the stronger, local property that $q_k^{m+1}$ must lie between $q_{k-1}^m$ and $q_k^m$ for all $k$.

## 4. The universal limiter

As noted in section 3, the constraints (21) [or, equivalently, (14)] imply that $q_k^{m+1}$ must lie between $q_{k-1}^m$ and $q_k^m$. A scheme for which $q_k^{m+1}$ must lie between $q_{k-1}^m$ and $q_k^m$ is said to have the *local bounding* property (e.g., Roe and Baines 1983). This local bounding concept extends in an obvious way to nonconstant flow, larger stencils, and multidimensions. It is a natural and direct discrete analog of the absence of amplification of extrema in the continous equation. This suggests that advection schemes might be constructed directly so as to be locally bounding (rather than TVD or positive). This approach was used, for example, by van Leer (1974) and is the approach underlying the universal limiter (Leonard 1991).

The design of the universal limiter begins from (6). (Here the notation used is different from that of Leonard.) The universal limiter aims to ensure the local bounding property

$$\min(q_{k-1}^m, q_k^m) \leq q_k^{m+1} \leq \max(q_{k-1}^m, q_k^m) \ \forall k \tag{23}$$

by placing constraints on the value at the outflow edge $\hat{q}_{k+1/2}$. To do this, it is necessary to first place reasonable a priori constraints on the value at the inflow edge $\hat{q}_{k-1/2}$:

$$\min(q_{k-1}^m, q_k^m) \leq \hat{q}_{k-1/2} \leq \max(q_{k-1}^m, q_k^m) \ \forall k. \tag{24}$$

Combining (23) and (24) with (6) and rearranging shows that the required constraints at the outflow edge are

$$q_{\min,k}^{\text{out}} \leq \hat{q}_{k+1/2} \leq q_{\max,k}^{\text{out}} \ \forall k, \tag{25}$$

where

$$q_{\min,k}^{\text{out}} = \frac{1}{c}[q_k^m + (c - 1)\max(q_{k-1}^m, q_k^m)],$$

$$q_{\max,k}^{\text{out}} = \frac{1}{c}[q_k^m + (c - 1)\min(q_{k-1}^m, q_k^m)]. \tag{26}$$

In practice, the universal limiter may be applied by first calculating preliminary values for $\hat{q}_{k+1/2}$ using the chosen basic advection scheme and then adjusting those preliminary values if necessary to satisfy (24)–(26).

It is straightforward to verify that (24)–(26) are equivalent to (14) or (21). The equivalence of (14) to the universal limiter was noted without proof in the appendix of Thuburn (1993).

## 5. Minimal constraints

It is sometimes considered desirable to make the minimum modifications to a basic advection scheme to make it locally bounding (or TVD, or positive). According to the constraints discussed above, this means (i) choosing $\phi_k = 1$ whenever this satisfies (14), and otherwise choosing $\phi_k$ to be as close as possible to 1 subject to (14); or, equivalently, (ii) choosing $\psi_{k+1/2} = 2s_{k+1/2}$ whenever this satisfies (21), and otherwise choosing $\psi_{k+1/2}$ to be as close as possible to $2s_{k+1/2}$ subject to (21); or, equivalently, (iii) choosing $\hat{q}_{k+1/2}$ to be the preliminary value given by the basic advection scheme whenever this satisfies (24)–(26), and otherwise choosing $\hat{q}_{k+1/2}$ to be as close as possible to the preliminary value subject to (24)–(26).

In fact, the local bounding property can be achieved under weaker constraints than these. Let $\hat{q}'_{k-1/2}$ be the value obtained by adjusting the preliminary value of $\hat{q}_{k-1/2}$ to lie within the inflow constraints for box $k$ (24). First, note that the upwind value $q^m_k$ always satisfies the outflow constraints for box $k$:

$$q^{\text{out}}_{\min,k} \le q^m_k \le q^{\text{out}}_{\max,k}. \tag{27}$$

Similary, the upwind value $q^m_{k-1}$ always satisfies the outflow constraints for box $k - 1$. Consequently, the outflow constraints for box $k - 1$ will cause $\hat{q}_{k-1/2}$ to lie between the value $\hat{q}'_{k-1/2}$ and the upwind value $q^m_{k-1}$. Therefore, after the inflow constraints have been imposed, the value at the inflow edge of box $k$ is known to lie in a narrower range than (24); namely

$$\min(q^m_{k-1}, \hat{q}'_{k-1/2}) \le \hat{q}_{k-1/2} \le \max(q^m_{k-1}, \hat{q}'_{k-1/2}) \qquad \forall k. \tag{28}$$

This means that the local bounding property (23) can be guaranteed under weaker outflow constraints than (26); namely,

$$\tilde{q}^{\text{out}}_{\min,k} \le \hat{q}_{k+1/2} \le \tilde{q}^{\text{out}}_{\max,k} \ \forall k, \tag{29}$$

where

$$\tilde{q}^{\text{out}}_{\min,k} = \max(q_{k-1}, \hat{q}'_{k+1/2}) + \frac{1}{c}[q^m_k - \max(q^m_{k-1}, q^m_k)],$$

$$\tilde{q}^{\text{out}}_{\max,k} = \min(q_{k-1}, \hat{q}'_{k+1/2}) + \frac{1}{c}[q^m_k - \min(q^m_{k-1}, q^m_k)]. \tag{30}$$

Note that these weaker outflow constraints do depend on the preliminary value at the inflow edge, and so they are not independent of the basic advection scheme used. A refinement of this sort, allowing weaker outflow constraints, is useful in building multidimensional locally bounded schemes that cause minimal distortion of the advected profile (Thuburn 1996).

## 6. Summary

The TVD schemes approach, the positive schemes approach, and the universal limiter approach to building shape-preserving schemes for one-dimensional advection have been shown to lead to mathematically equivalent constraints on the advective fluxes. Note, by the way, that some approaches not discussed in this note, such as the flux corrected transport approach (e.g., Boris and Book 1973; Zalesak 1979), do lead to mathematically distinct schemes, even for the one-dimensional advection problem.

A refinement of the universal limiter approach leads to weaker constraints on the advective fluxes than those given by the standard versions of the three approaches discussed.

*Acknowledgments.* This work was carried out under the U.K. Universities Global Atmospheric Modelling Programme funded by the U.K. Natural Environment Research Council.

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