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Pages 10: Equations (5.9a) "$U^L_{j-\frac{1}{2}}$" should be "$U^L_{j+\frac{1}{2}}$".

Pages 10: The vector "$\widehat{\phi}_{j+\frac{1}{2}}$" below equation (5.9b) and before equation (5.9c) should be "$\widehat{\Phi}_{j+\frac{1}{2}}$".

Page 10: Equation (5.9e) should be

$$\widehat{\alpha}_{j+\frac{1}{2}} = \widehat{R}^{-1}_{j+\frac{1}{2}}(U^R_{j+\frac{1}{2}} - U^L_{j+\frac{1}{2}})$$

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Abstract

The relative computational effort among the spatially five-point numerical flux functions of Harten, van Leer, and Osher and Chakravarthy is explored. These three methods typify the design principles most often used in constructing higher than first-order upwind total variation diminishing (TVD) schemes. For the scalar case the difference in operation count between any two algorithms may be very small and yet the operation count for their system counterparts might be vastly different. The situation occurs even though one starts with two different yet equivalent representations for the scalar case.

I. Introduction

Various high-resolution upwind difference schemes have been developed in recent years [1-9]. Of special interest are the extension of these methods to systems of nonlinear hyperbolic conservation laws in one and higher dimensions. Typical methods for systems are MUSCL [1,2], Osher [6], Harten [3], Roe [5], and van Leer [1]. Here van Leer method means using his methodology [1] to extend the first-order Roe's scheme [5] to higher than first-order and MUSCL means van Leer's pioneer work on extending the first-order Godunov scheme to higher-order. The MUSCL and Osher type of approach require considerably more computation and programming effort than with the latter three, especially for problems in multidimensions and in curvilinear coordinates. Harten and Roe's second-order schemes share many common features. Considering only the latter three, the way second-order accuracy is achieved and the form of limiters play an important role. For the scalar case, the difference in operation count between any two algorithms may be very small and yet the operation count for their system counterparts might be vastly different. This situation occurrs even though one starts with two different yet equivalent representations for the scalar case. An example will be given in section V.

Recently, Osher and Chakravarthy [10] extended their earlier work on five-point fully upwind second-order total variation diminishing (TVD) schemes to five-point second-order or third-order upwind biased TVD schemes. They also derived formulas for more than five points and higher than third-order cases. Only the second and third-order are discussed here. They claimed that their five-point second-order or third-order upwind biased scheme requires hardly anymore work

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than their five-point fully upwind second-order scheme. It was the investigation of their work which prompted the work of this note. As one can see later for system cases, their five-point upwind biased schemes require more operations than their fully upwind second-order scheme. Furthermore, their five-point fully upwind or upwind biased schemes require substantially more operations than the Harten or van Leer method. For the purpose of this paper, order of accuracy of a TVD scheme refers to the numerical solution that is away from extreme points.

Specifically, it is the objective of this note to discuss the relative computational effort among the spatially five-point TVD schemes of Harten, van Leer and Osher and Chakravarthy [3,7,10] for system cases via the Huang [11] and Roe's [12] generalization for systems. It is emphasized here that, the scalar schemes of Harten, van Leer and Osher and Chakravarthy are used. Then extensions to systems are employed by the same method (i.e. Huang or Roe), not by their original Riemann solver [1,13] for system cases. Huang and Roe's generalization to system cases is based on a local linearization which defines at each point a "local" system of characteristic fields, and then applies the scalar scheme to each of the scalar characteristic equations. Because of the freezing of coefficients, one can transform the local characteristic field back to the original field variables, and arrive at an algorithm for the nonlinear hyperbolic system case. Numerical experiments with these schemes on one and two-dimensional steady-state calculations [14-20] show that they produce similar shock resolution. In certain instances, the third-order scheme gives a slightly better result than the second-order method [20]. In general, the improvement from second-order to third-order is far less pronounced than from first-order to second-order TVD schemes [19]. This is due partly to the fact that all TVD schemes of higher than first-order reduce to first-order at points of extrema. Knowing their performance, it is relevant to compare their computational effort.

The comparison is only on the numerical flux function. No specific time discretization is involved. For simplicity in presentation, the forward Euler time differencing is assumed. One should notice that under the forward Euler time differencing only Harten's method is second-order in time and space; the other two are first-order in time and second-order in space. As a side remark, TVD schemes are not necessarily upwind [21-23], but upwind TVD schemes, in general, give sharper shocks than symmetric TVD schemes. The advantage of symmetric TVD schemes is that they are easier to implement and provide a more natural way of extending the scheme to two and three-dimensional problems. One can easily modify Harten's method to be non-upwind. In this note, only the aforementioned three upwind methods are considered.

II. Harten TVD Scheme

Consider a scalar hyperbolic conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \tag{2.1}$$

where f is the flux function and $a(u) = \partial f/\partial u$ is the characteristic speed. Let u_j^n be the numerical solution of (2.1) at $x = j\Delta x$ and $t = n\Delta t$, with Δx the spatial mesh size and Δt the time step. Consider a general five-point explicit difference scheme in conservation form

$$u_j^{n+1} = u_j^n - \lambda(\tilde{h}^n_{j+\frac{1}{2}} - \tilde{h}^n_{j-\frac{1}{2}}), \tag{2.2}$$

where $\tilde{h}^n_{j\pm\frac{1}{2}} = \tilde{h}(u^n_{j\mp1}, u^n_j, u^n_{j\pm1}, u^n_{j\pm2})$, and $\lambda = \Delta t/\Delta x$. Here $\tilde{h}$, commonly called a numerical flux function, is required to be consistent with the conservation law in the following sense

$$\tilde{h}(u,u,u,u) = f(u). \tag{2.3}$$

The numerical flux of the second-order explicit TVD scheme of Harten [3] can be expressed as

$$\tilde{h}^H_{j+\frac{1}{2}} = \frac{1}{2}\left[\tilde{f}_j + \tilde{f}_{j+1} - \psi(\tilde{a}_{j+\frac{1}{2}})\Delta_{j+\frac{1}{2}}u\right], \tag{2.4a}$$

where $\tilde{f}_j = f(u_j) + g_j$, $\tilde{a}_{j+\frac{1}{2}} = a_{j+\frac{1}{2}} + \gamma_{j+\frac{1}{2}}$, and $\Delta_{j+\frac{1}{2}}u = u_{j+1} - u_j$, with

$$\psi(z) = |z| \tag{2.4b}$$

$$a_{j+\frac{1}{2}} = \begin{cases} (f_{j+1} - f_j)/\Delta_{j+\frac{1}{2}}u & \Delta_{j+\frac{1}{2}}u \neq 0 \\ a(u_j) & \Delta_{j+\frac{1}{2}}u = 0 \end{cases} \tag{2.4c}$$

$$\begin{aligned} g_j &= S \cdot \max\left[0, \min(\sigma_{j+\frac{1}{2}}|\Delta_{j+\frac{1}{2}}u|, S\cdot\sigma_{j-\frac{1}{2}}\Delta_{j-\frac{1}{2}}u)\right] \\ S &= \operatorname{sgn}(\Delta_{j+\frac{1}{2}}u) \end{aligned} \tag{2.4d}$$

and

$$\gamma_{j+\frac{1}{2}} = \begin{cases} (g_{j+1} - g_j)/\Delta_{j+\frac{1}{2}}u & \Delta_{j+\frac{1}{2}}u \neq 0 \\ 0 & \Delta_{j+\frac{1}{2}}u = 0. \end{cases} \tag{2.4e}$$

Here $\sigma_{j+\frac{1}{2}} = \sigma(a_{j+\frac{1}{2}})$ and can be expressed as

$$\sigma(z) = \frac{1}{2}[\psi(z) - \lambda z^2] \geq 0 \tag{2.4f}$$

for time accurate calculations. With this choice of $\sigma(z)$, the scheme (2.2) together with (2.4) is second-order accurate in both time and space (except at points of extrema); see [3,4]. Also, with this choice of the g function, the scheme will automatically switch itself to first-order at points of extrema. This is one of the vehicles to prevent spurious oscillations near a shock.

Define a "minmod" function of a list of arguments to be the smallest number in absolute value if the list of arguments are of same sign, but to be zero if any argument is of the opposite sign. One can rewrite (2.4d) as $g_j = \operatorname{minmod}(\sigma_{j+\frac{1}{2}}\Delta_{j+\frac{1}{2}}u, \sigma_{j-\frac{1}{2}}\Delta_{j-\frac{1}{2}}u)$. It is a form of the so called "limiter" for the control of unwanted oscillations in numerical schemes. Other more general forms for g can be obtained following the line of argument of Roe [5]. As a side remark,

if one sets all the g_j's to zero in (2.4), the resulting scheme becomes Roe's first-order upwind method.

With the choice of the ψ function in(2.4b), the corresponding first-order upwind scheme is not consistent with an entropy inequality, and the scheme might converge to a nonphysical solution. A slight modification of the numerical viscosity term

$$\psi(z) = \begin{cases} |z| & |z| \geq \epsilon \\ (z^2 + \epsilon^2)/2\epsilon & |z| < \epsilon \end{cases} \tag{2.5}$$

can remedy the entropy violating problem [3,4], where $\epsilon > 0$ is a parameter. A formula for ϵ can be found in reference [24]. The $\psi(z)$ in (2.5) is a continuously differentiable positive approximation to $|z|$ in (2.4b).

For simplicity of presentation, assume $\psi(z)$ has the form (2.4b). The use of an entropy satisfying $\psi(z)$ is only a minor modification of what is about to be presented. Furthermore, since the main concern of this note is the spatial discretization, only the forward Euler time differencing is considered. Other explicit, implicit, or predictor and corrector types of time differencing do not alter the results.

Using the identity $|\tilde{a}_{j+\frac{1}{2}}| = \mathrm{sgn}(\tilde{a}_{j+\frac{1}{2}})\tilde{a}_{j+\frac{1}{2}}$ and $\tilde{a}_{j+\frac{1}{2}} = (\tilde{f}_{j+1} - \tilde{f}_{j+1})/(u_{j+1} - u_j)$, Harten's scheme can be rewritten as

$$u_j^{n+1} = u_j^n - \frac{\lambda}{2}\left[1 - \mathrm{sgn}(\tilde{a}^n_{j+\frac{1}{2}})\right](\tilde{f}^n_{j+1} - \tilde{f}^n_j) - \frac{\lambda}{2}\left[1 + \mathrm{sgn}(\tilde{a}^n_{j-\frac{1}{2}})\right](\tilde{f}^n_j - \tilde{f}^n_{j-1}). \tag{2.6}$$

Here, the numerical flux function becomes

$$\tilde{h}^H_{j+\frac{1}{2}} = \frac{1}{2}\left[1 - \mathrm{sgn}(\tilde{a}_{j+\frac{1}{2}})\right](\tilde{f}_{j+1} - \tilde{f}_j) + \tilde{f}_j. \tag{2.7}$$

Note that with the choice of g_j given in (2.4d), $\mathrm{sgn}(\tilde{a}^n_{j+\frac{1}{2}}) = \mathrm{sgn}(a^n_{j+\frac{1}{2}})$. Thus, one does not have to calculate $\gamma_{j+\frac{1}{2}}$. The $\tilde{h}^H_{j+\frac{1}{2}}$ can also be expressed as

$$\tilde{h}^H_{j+\frac{1}{2}} = \frac{1}{2}\left[1 - \mathrm{sgn}(a_{j+\frac{1}{2}})\right](\tilde{f}_{j+1} - \tilde{f}_j) + \tilde{f}_j. \tag{2.8}$$

With the use of the numerical flux (2.7) as an alternative, the g function of (2.4d) can be defined in a slightly different form.

$$g_j = \mathrm{minmod}\left(\overline{\sigma}_{j+\frac{1}{2}}\Delta_{j+\frac{1}{2}}f, \overline{\sigma}_{j-\frac{1}{2}}\Delta_{j-\frac{1}{2}}f\right) \tag{2.9a}$$

with $\overline{\sigma}_{j+\frac{1}{2}} = \overline{\sigma}(a_{j+\frac{1}{2}})$ and

$$\overline{\sigma}(z) = \frac{1}{2}\left[\mathrm{sgn}(z) - \lambda z\right]. \tag{2.9b}$$

Here the identities $\mathrm{sgn}(\Delta_{j+\frac{1}{2}}f)\mathrm{sgn}(a_{j+\frac{1}{2}}) = \mathrm{sgn}(u_{j+1} - u_j)$ and $|\Delta_{j+\frac{1}{2}}f| = |a_{j+\frac{1}{2}}||u_{j+1} - u_j|$ are used. The above limiter g_j of (2.9) can be considered as a flux limiter since the flux f is

limited. For scalar problems, equations (2.4a), (2.7) and (2.8) are equivalent. The difference in operation count are very minor. Equations (2.4d,f) are preferred over (2.9) for its straightforward extension to system cases because u appears rather than f. Furthermore, in the extension to nonlinear systems via Huang's and Roe's generalizations, (2.4a) results in a smaller operation count than (2.7) or (2.8).

III. van Leer Differencing

In references [7,19,25] van Leer and his collaborators adopted the original MUSCL [1] type of differencing to obtain a second and third-order flux vector splitting method. Very impressive results were obtained for steady-state airfoil calculations. Their result indicated that one does not have to resort to a Godunov type of Riemann solver in order to obtain good shock resolution. In this paper the application of the MUSCL type differencing to Roe's first-order scheme is proposed.

Consider a three point explicit difference scheme in conservation form

$$\begin{aligned} u_j^{n+1} &= u_j^n - \lambda\left(h_{j+\frac{1}{2}}^n - h_{j-\frac{1}{2}}^n\right) \\ &= u_j^n - \lambda\left[h(u_j^n, u_{j+1}^n) - h(u_{j-1}^n, u_j^n)\right] \end{aligned} \tag{3.1}$$

where $h_{j+\frac{1}{2}}^n = h(u_j^n, u_{j+1}^n)$, is a first-order numerical flux. Here $h_{j+\frac{1}{2}}$ without a " ~ " is used to distinguish a first-order numerical flux from the higher-order numerical flux $\tilde{h}_{j+\frac{1}{2}}$.

Roe's first-order scheme (without entropy fixed) can be written as

$$h_{j+\frac{1}{2}} = \frac{1}{2}\left[f_j + f_{j+1} - |a_{j+\frac{1}{2}}|\Delta_{j+\frac{1}{2}}u\right], \tag{3.2}$$

with $a_{j+\frac{1}{2}}$ defined in (2.4c).

The MUSCL approach to obtain a spatially higher order differencing is to replace the arguments u_{j+1} and u_j by $u_{j+\frac{1}{2}}^R$ and $u_{j+\frac{1}{2}}^L$ where

$$u_{j+\frac{1}{2}}^R = u_{j+1} - \frac{1}{4}\left[(1-\theta)\Delta_{j+\frac{3}{2}}u + (1+\theta)\Delta_{j+\frac{1}{2}}u\right] \tag{3.3}$$

$$u_{j+\frac{1}{2}}^L = u_j + \frac{1}{4}\left[(1-\theta)\Delta_{j-\frac{1}{2}}u + (1+\theta)\Delta_{j+\frac{1}{2}}u\right]. \tag{3.4}$$

Here the order of accuracy in space is determined by the value of θ. For example, if $\theta = -1$, the scheme is fully upwind and, if $\theta = 0$, it is the Fromm's scheme. When $\theta = 1/2$, the scheme is third-order and, when $\theta = 1$, it is the regular three-point central difference scheme.

Various "slope" limiters are use to eliminate unwanted oscillations. A popular one is the "minmod" limiter; it modifies the upwind-biased interpolation (3.3)-(3.4) as follows:

$$u^R_{j+\frac{1}{2}} = u_{j+1} - \frac{1}{4}\left[(1-\theta)\widetilde{\Delta_{j+\frac{3}{2}}u} + (1+\theta)\widetilde{\widetilde{\Delta_{j+\frac{1}{2}}u}}\right] \tag{3.5}$$

$$u^L_{j+\frac{1}{2}} = u_{j+1} + \frac{1}{4}\left[(1-\theta)\widetilde{\widetilde{\Delta_{j-\frac{1}{2}}u}} + (1+\theta)\widetilde{\Delta_{j+\frac{1}{2}}u}\right] \tag{3.6}$$

where

$$\widetilde{\Delta_{j+\frac{1}{2}}u} = \text{minmod}\left(\Delta_{j+\frac{1}{2}}u, \beta\Delta_{j-\frac{1}{2}}u\right) \tag{3.7}$$

$$\widetilde{\widetilde{\Delta_{j+\frac{1}{2}}u}} = \text{minmod}\left(\Delta_{j+\frac{1}{2}}u, \beta\Delta_{j+\frac{3}{2}}u\right) \tag{3.8}$$

with

$$\text{minmod}(x, \beta y) = \text{sgn}(x) \cdot \max\left\{0, \min\left[|x|, \beta y \text{sgn}(x)\right]\right\} \tag{3.9}$$

and

$$\beta = \frac{3-\theta}{1-\theta}. \tag{3.10}$$

Therefore, a higher order scheme can be obtained by simply redefining the arguments of $h_{j\pm\frac{1}{2}}$ in equation (3.1); i.e.

$$u^{n+1}_j = u^n_j - \lambda\left[h(u^R_{j+\frac{1}{2}}, u^L_{j+\frac{1}{2}}) - h(u^R_{j-\frac{1}{2}}, u^L_{j-\frac{1}{2}})\right]^n. \tag{3.11}$$

Applied to Roe's scheme, the second-order numerical flux in (3.11) denoted by $\widetilde{h}^{VL}_{j+\frac{1}{2}}$ is

$$\begin{aligned}\widetilde{h}^{VL}_{j+\frac{1}{2}} &= h\left(u^R_{j+\frac{1}{2}}, u^L_{j+\frac{1}{2}}\right) \\ &= \frac{1}{2}\left[f(u^R_{j+\frac{1}{2}}) + f(u^L_{j+\frac{1}{2}}) - \left|\frac{f(u^R_{j+\frac{1}{2}}) - f(u^L_{j+\frac{1}{2}})}{(u^R_{j+\frac{1}{2}} - u^L_{j+\frac{1}{2}})}\right|(u^R_{j+\frac{1}{2}} - u^L_{j+\frac{1}{2}})\right].\end{aligned} \tag{3.12}$$

Anderson et al. [19] have demonstrated that the use of limiters is not necessary via the MUSCL differencing for some steady-state airfoil calculations. In reference [19], they use the fully one-sided unlimited second-order upwind scheme ($\theta = -1$ in (3.4)-(3.5)) via the flux vector splitting of both van Leer [7] and Steger and Warming [26]. Very accurate steady-state numerical solutions were obtained for some typical airfoil calculations with shocks.

For the fully upwind scheme with $\theta = -1$ and without limiter, $u^R_{j+\frac{1}{2}}$ and $u^L_{j+\frac{1}{2}}$ in (3.12) can be defined as

$$u^R_{j+\frac{1}{2}} = u_{j+1} - \frac{1}{2}\Delta_{j+\frac{3}{2}}u \tag{3.13}$$

$$u^L_{j+\frac{1}{2}} = u_j + \frac{1}{2}\Delta_{j-\frac{1}{2}}u \tag{3.14}$$

or the limited version

$$u^R_{j+\frac{1}{2}} = u_{j+1} - \frac{1}{2}\widetilde{\Delta_{j+\frac{3}{2}}u} \tag{3.15}$$

$$u^L_{j+\frac{1}{2}} = u_j + \frac{1}{2}\widetilde{\widetilde{\Delta_{j-\frac{1}{2}}u}}. \tag{3.16}$$

For the unlimited case (3.13)-(3.14), less computation is required for (3.11) than Harten's scheme (2.2). However, for the limited case (3.15)-(3.16) or (3.5)-(3.6) with $\theta \neq -1$, an extra limiter is required over the Harten scheme. This is due to the asymmetric nature of the scheme. In general (3.12) requires one more flux evaluation than Harten scheme requires.

IV. Osher and Chakravarthy TVD Schemes

Instead of using the MUSCL differencing, Osher and Chakravarthy [10] started with a one parameter family of semi-discrete schemes with numerical flux

$$\tilde{h}_{j+\frac{1}{2}} = h_{j+\frac{1}{2}} - \frac{(1-\theta)}{4}\left(\Delta_{j+\frac{3}{2}}f^-\right) - \frac{(1+\theta)}{4}\left(\Delta_{j+\frac{1}{2}}f^-\right) + \frac{(1+\theta)}{4}\left(\Delta_{j+\frac{1}{2}}f^+\right) + \frac{(1-\theta)}{4}\left(\Delta_{j-\frac{1}{2}}f^+\right) \tag{4.1}$$

where $h_{j+\frac{1}{2}} = h(u_j, u_{j+1})$ is the numerical flux of some first-order upwind TVD scheme. For comparison purposes, define $h_{j+\frac{1}{2}}$ as in (3.2). This five-point scheme again can be second or third-order depending on the value of the parameter θ. It is defined the same way as before. The superscript + or − denotes the flux difference across the wave with positive or negative wave speed. To obtain a TVD scheme, Osher and Chakravarthy used the flux limiter concept by simply modifying the last four terms on right hand side of (4.1); i.e., their numerical flux denoted by $\tilde{h}^{OC}_{j+\frac{1}{2}}$ is

$$\begin{aligned}\tilde{h}^{OC}_{j+\frac{1}{2}} = h_{j+\frac{1}{2}} &- \frac{(1-\theta)}{4}\left(\widetilde{\Delta_{j+\frac{3}{2}}f^-}\right) - \frac{(1+\theta)}{4}\left(\widetilde{\widetilde{\Delta_{j+\frac{1}{2}}f^-}}\right) \\ &+ \frac{(1+\theta)}{4}\left(\widetilde{\Delta_{j+\frac{1}{2}}f^+}\right) + \frac{(1-\theta)}{4}\left(\widetilde{\widetilde{\Delta_{j-\frac{1}{2}}f^+}}\right).\end{aligned} \tag{4.2}$$

The " ~ " shown over the flux difference values denotes the flux limited value and they are computed as follows

$$\widetilde{\Delta_{j+\frac{3}{2}}f^-} = \text{minmod}\left[\Delta_{j+\frac{3}{2}}f^-, \beta\Delta_{j+\frac{1}{2}}f^-\right] \tag{4.3a}$$

$$\Delta_{j+\frac{1}{2}}\widetilde{\widetilde{f}}^{-} = \text{minmod}\left[\Delta_{j+\frac{1}{2}}f^{-}, \beta\Delta_{j+\frac{3}{2}}f^{-}\right] \tag{4.3b}$$

$$\Delta_{j+\frac{1}{2}}\widetilde{f}^{+} = \text{minmod}\left[\Delta_{j+\frac{1}{2}}f^{+}, \beta\Delta_{j-\frac{1}{2}}f^{+}\right] \tag{4.3c}$$

$$\Delta_{j-\frac{1}{2}}\widetilde{\widetilde{f}}^{+} = \text{minmod}\left[\Delta_{j-\frac{1}{2}}f^{+}, \beta\Delta_{j+\frac{1}{2}}f^{+}\right] \tag{4.3d}$$

where the operator "minmod" is the same as (3.9) and is defined almost the same way as in (2.4d). The value β is the same as in (3.10). Due to the design principle of this scheme, the numerical flux (4.2) requires more computation than (2.4), (2.8) or (3.12). For $\theta = -1$, (4.2) together with (4.3) requires one more limiter than Harten's method. For $\theta \neq -1$, two more limiters than van Leer's method and three more limiters than Harten's method are required for (4.2)-(4.3). The extra computations will become even more apparent as we extend these schemes to system cases.

V. Generalization to Hyperbolic System of Conservation Laws

The procedure considered here for generalization to system cases is to extend the scalar scheme to system cases so that the resulting scheme is TVD for the "locally frozen" constant coefficient system. To do that, we define at each point a "local" system of characteristic fields, and then apply the scheme to each of the m scalar characteristic equations. Here m is the dimension of the hyperbolic system. The extension technique is a somewhat generalized version of the procedure suggested by Huang [11] and Roe [12]. For simplicity of presentation, only conservation laws in Cartesian coordinates with equal spatial step size will be discussed.

Consider a nonlinear hyperbolic system of conservation laws

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0, \qquad A(U) = \frac{\partial F(U)}{\partial U}. \tag{5.1}$$

Here U and $F(U)$ are column vectors of m components. Let the eigenvalues of A be $(a^1, a^2, ..., a^m)$. Denote R as the matrix whose columns are eigenvectors of A, and R^{-1} as the inverse of R. Define the characteristic variable of W with respect to the state U by

$$W = R^{-1}U. \tag{5.2}$$

In the constant coefficient case (5.1) decouples into m scalar equations for the characteristic variables

$$\frac{\partial w^l}{\partial t} + a^l\frac{\partial w^l}{\partial x} = 0, \tag{5.3}$$

with a^lconstant and w^l the elements of W. This offers a natural way of extending a scalar scheme to a constant coefficient system by applying it to each of the m scalar characteristic equations (5.3).

Let $U_{j+\frac{1}{2}}$ denote some symmetric average of U_j and U_{j+1} such as the arithmetic mean average of Huang or the Roe's average [11,12] for gas dynamics. Let $a^l_{j+\frac{1}{2}}$, $R_{j+\frac{1}{2}}$, $R^{-1}_{j+\frac{1}{2}}$ denote the quantities a^l, R, R^{-1} evaluated at $U_{j+\frac{1}{2}}$. Let w^l be the vector elements of W and let $\alpha^l_{j+\frac{1}{2}} = w^l_{j+1} - w^l_j$ be the component of $\Delta_{j+\frac{1}{2}}U = U_{j+1} - U_j$ for the lth characteristic; i.e.,

$$\alpha_{j+\frac{1}{2}} = R^{-1}_{j+\frac{1}{2}}\left(\Delta_{j+\frac{1}{2}}U\right) \tag{5.4a}$$

and

$$\Delta_{j+\frac{1}{2}}U = R_{j+\frac{1}{2}}\alpha_{j+\frac{1}{2}}. \tag{5.4b}$$

With the above notation, one can apply the scalar scheme to each of the locally defined characteristic variables of (5.3). Transforming back to the original variable locally, one gets

$$U^{n+1}_j = U^n_j - \lambda(\tilde{H}^n_{j+\frac{1}{2}} - \tilde{H}^n_{j-\frac{1}{2}}). \tag{5.5}$$

Numerical Flux for Harten Scheme

The corresponding numerical flux of (2.4) can be written as

$$\tilde{H}^H_{j+\frac{1}{2}} = \frac{1}{2}\left[F_j + F_{j+1} + R_{j+\frac{1}{2}}\Phi_{j+\frac{1}{2}}\right], \tag{5.6a}$$

where the elements of the $\Phi_{j+\frac{1}{2}}$ denoted by $\phi^l_{j+\frac{1}{2}}, l = 1, ..., m$ are

$$\phi^l_{j+\frac{1}{2}} = g^l_j + g^l_{j+1} - \psi(a^l_{j+\frac{1}{2}} + \gamma^l_{j+\frac{1}{2}})\alpha^l_{j+\frac{1}{2}} \tag{5.6b}$$

$$g^l_j = \text{minmod}(\sigma^l_{j+\frac{1}{2}}\alpha^l_{j+\frac{1}{2}}, \sigma^l_{j-\frac{1}{2}}\alpha^l_{j-\frac{1}{2}}) \tag{5.6c}$$

with $\psi(z)$ defined in (2.4b); $\sigma^l_{j+\frac{1}{2}}$ is (2.4f) with $z = a^l_{j+\frac{1}{2}}$, and

$$\gamma^l_{j+\frac{1}{2}} = \begin{cases} (g^l_{j+1} - g^l_j)/\alpha^l_{j+\frac{1}{2}} & \alpha^l_{j+\frac{1}{2}} \neq 0 \\ 0 & \alpha^l_{j+\frac{1}{2}} = 0, \end{cases} \tag{5.6d}$$

where $\alpha^l_{j+\frac{1}{2}}$ are the elements of (5.4a).

Extension of the scalar TVD scheme to nonlinear system cases is not unique. Take, for example, the case where the numerical flux $\tilde{h}_{j+\frac{1}{2}}$ in (2.4) is identical to $\tilde{h}_{j+\frac{1}{2}}$ in (2.8). The corresponding numerical fluxes for the system case have a different form depending on which of the scalars $\tilde{h}_{j+\frac{1}{2}}$ one started with. If one started with (2.8), the system can be expressed as

$$U^{n+1}_j = U^n_j - \frac{\lambda}{2}\left(I - \mathcal{A}^n_{j+\frac{1}{2}}\right)\left(\mathcal{F}^n_{j+1} - \mathcal{F}^n_j\right) - \frac{\lambda}{2}\left(I + \mathcal{A}^n_{j-\frac{1}{2}}\right)\left(\mathcal{F}^n_j - \mathcal{F}^n_{j-1}\right) \tag{5.7a}$$

where

$$A_{j+\frac{1}{2}} = R^{-1}_{j+\frac{1}{2}} \Lambda_{j+\frac{1}{2}} R_{j+\frac{1}{2}} \tag{5.7b}$$

$$\Lambda_{j+\frac{1}{2}} = \text{diag}\left[\text{sgn}(a^l_{j+\frac{1}{2}})\right], \tag{5.7c}$$

and one way to define $\mathcal{F}_j$ is

$$\mathcal{F}_j = F_j + R_j G_j \tag{5.7d}$$

with $G_j = (g^l_j, ..., g^m_j)^T$ and diag(z^l) denoting a diagonal matrix with diagonal elements z^l. The numerical flux $\tilde{H}_{j\pm\frac{1}{2}}$ can be of the form

$$\tilde{H}_{j+\frac{1}{2}} = \frac{1}{2}\left(1 - A_{j+\frac{1}{2}}\right)(\mathcal{F}_{j+1} - \mathcal{F}_j) + \mathcal{F}_j \tag{5.8a}$$

$$\tilde{H}_{j-\frac{1}{2}} = \mathcal{F}_j - \frac{1}{2}\left(1 + A_{j-\frac{1}{2}}\right)(\mathcal{F}_j - \mathcal{F}_{j-1}). \tag{5.8b}$$

Eventhough $R_{j+\frac{1}{2}}$ is needed in both (5.6) and (5.8), scheme (5.6) is preferred over (5.8) since R_j is not required in (5.6). In other words, for scalar cases (2.4) and (2.8) are identical, but in system cases (5.8a) requires more work than (5.6a).

Numerical Flux for van Leer Differencing

The numerical flux in this case is

$$\tilde{H}^{VL}_{j+\frac{1}{2}} = \frac{1}{2}\left[F(U^R_{j+\frac{1}{2}}) + F(U^L_{j+\frac{1}{2}}) - \hat{R}_{j+\frac{1}{2}}\hat{\Phi}_{j+\frac{1}{2}}\right], \tag{5.9a}$$

where $\hat{R}_{j+\frac{1}{2}}$ is the eigenvector of A evaluated at some symmetric average of $U^R_{j+\frac{1}{2}}$ and $U^L_{j+\frac{1}{2}}$; i.e.,

$$\hat{R}_{j+\frac{1}{2}} = R(U^R_{j+\frac{1}{2}}, U^L_{j+\frac{1}{2}}) \tag{5.9b}$$

and the elements of $\hat{\Phi}_{j+\frac{1}{2}}$ are

$$\hat{\phi}^l_{j+\frac{1}{2}} = |\hat{a}^l_{j+\frac{1}{2}}|\hat{\alpha}^l_{j+\frac{1}{2}} \tag{5.9c}$$

where again $\hat{a}^l_{j+\frac{1}{2}}$ and $\hat{\alpha}^l_{j+\frac{1}{2}}$ are evaluated at some symmetric average of $U^R_{j+\frac{1}{2}}$ and $U^L_{j+\frac{1}{2}}$ and

$$\hat{a}^l_{j+\frac{1}{2}} = a^l(U^R_{j+\frac{1}{2}}, U^L_{j+\frac{1}{2}}) \tag{5.9d}$$

$$\hat{\alpha}_{j+\frac{1}{2}} = \hat{R}^{-1}_{j+\frac{1}{2}}(U^R_{j+\frac{1}{2}} - U^L_{j+\frac{1}{2}}) \tag{5.9e}$$

with

$$U^R_{j+\frac{1}{2}} = U_{j+1} - \frac{1}{4}\left[(1-\theta)\Delta\widetilde{_{j+\frac{3}{2}}U} + (1+\theta)\Delta\widetilde{\widetilde{_{j+\frac{1}{2}}U}}\right] \tag{5.9f}$$

$$U^L_{j+\frac{1}{2}} = U_j + \frac{1}{4}\left[(1-\theta)\Delta\widetilde{\widetilde{_{j-\frac{1}{2}}U}} + (1+\theta)\Delta\widetilde{_{j+\frac{1}{2}}U}\right] \tag{5.9g}$$

where each element of the quantities are defined in the same way as in (3.7) and (3.8).

Numerical Flux for Osher and Chakravarthy Schemes

Their numerical flux for a system can be written as

$$\begin{aligned}\tilde{H}^{OC}_{j+\frac{1}{2}} = H_{j+\frac{1}{2}} &- \frac{(1-\theta)}{4}R_{j+\frac{3}{2}}\widetilde{\mathcal{A}^-_{j+\frac{3}{2}}} - \frac{(1+\theta)}{4}R_{j+\frac{1}{2}}\widetilde{\widetilde{\mathcal{A}^-_{j+\frac{1}{2}}}} \\ &+ \frac{(1+\theta)}{4}R_{j+\frac{1}{2}}\widetilde{\mathcal{A}^+_{j+\frac{1}{2}}} + \frac{(1-\theta)}{4}R_{j-\frac{1}{2}}\widetilde{\widetilde{\mathcal{A}^+_{j-\frac{1}{2}}}}.\end{aligned} \tag{5.10a}$$

Here the $H_{j+\frac{1}{2}}$ is the first-order numerical flux

$$H_{j+\frac{1}{2}} = \frac{1}{2}\left[F_j + F_{j+1} - R_{j+\frac{1}{2}}\hat{\hat{\Phi}}_{j+\frac{1}{2}}\right], \tag{5.10b}$$

where the elements of $\hat{\hat{\Phi}}_{j+\frac{1}{2}}$ are $\phi^l_{j+\frac{1}{2}} = |a^l_{j+\frac{1}{2}}|\alpha^l_{j+\frac{1}{2}}$

The elements of the $\mathcal{A}^{\pm}$'s are

$$\mathcal{A}^{l-}_{j+\frac{1}{2}} = a^{l-}_{j+\frac{1}{2}}\alpha^l_{j+\frac{1}{2}} \tag{5.10c}$$

$$\mathcal{A}^{l+}_{j+\frac{1}{2}} = a^{l+}_{j+\frac{1}{2}}\alpha^l_{j+\frac{1}{2}} \tag{5.10d}$$

with $a^{l\pm}_{j+\frac{1}{2}} = 0.5(a^l_{j+\frac{1}{2}} \pm |a^l_{j+\frac{1}{2}}|)$, and $a^l_{j+\frac{1}{2}}$ is (5.4), and

$$\widetilde{\mathcal{A}^{l-}_{j+\frac{3}{2}}} = \text{minmod}\left[\mathcal{A}^{l-}_{j+\frac{3}{2}}, \beta\mathcal{A}^{l-}_{j+\frac{1}{2}}\right] \tag{5.10e}$$

$$\widetilde{\widetilde{\mathcal{A}^{l-}_{j+\frac{1}{2}}}} = \text{minmod}\left[\mathcal{A}^{l-}_{j+\frac{1}{2}}, \beta\mathcal{A}^{l-}_{j+\frac{3}{2}}\right] \tag{5.10f}$$

$$\widetilde{\mathcal{A}^{l+}_{j+\frac{1}{2}}} = \text{minmod}\left[\mathcal{A}^{l+}_{j+\frac{1}{2}}, \beta\mathcal{A}^{l+}_{j-\frac{1}{2}}\right] \tag{5.10g}$$

$$\widetilde{\widetilde{\mathcal{A}^{l+}_{j-\frac{1}{2}}}} = \text{minmod}\left[\mathcal{A}^{l+}_{j-\frac{1}{2}}, \beta\mathcal{A}^{l+}_{j+\frac{1}{2}}\right]. \tag{5.10h}$$

Collecting terms of $R_{j+\frac{1}{2}}$, (5.10a) can be rewritten as

$$\tilde{H}^{OC}_{j+\frac{1}{2}} = \frac{1}{2}\left\{ F_j + F_{j+1} - R_{j+\frac{1}{2}} \left[\hat{\hat{\Phi}}_{j+\frac{1}{2}} + \frac{(1+\theta)}{4} \widetilde{\widetilde{\mathcal{A}^-_{j+\frac{1}{2}}}} - \frac{(1+\theta)}{4} \widetilde{\mathcal{A}^+_{j+\frac{1}{2}}} \right] \right.$$
$$\left. - \frac{(1-\theta)}{4} R_{j+\frac{3}{2}} \widetilde{\mathcal{A}^-_{j+\frac{3}{2}}} + \frac{(1-\theta)}{4} R_{j-\frac{1}{2}} \widetilde{\widetilde{\mathcal{A}^-_{j-\frac{1}{2}}}} \right\}. \tag{5.11}$$

The terms that are common to the numerical fluxes of Harten's $\tilde{H}^H_{j+\frac{1}{2}}$ (5.6), van Leer's $\tilde{H}^{VL}_{j+\frac{1}{2}}$ (5.9) and Osher and Chakravarthy's $\tilde{H}^{OC}_{j+\frac{1}{2}}$ (5.11) are F_{j+1}, F_j, $R_{j+\frac{1}{2}}$ and $\alpha_{j+\frac{1}{2}}$. Both $\tilde{H}^H$ and $\tilde{H}^{VL}$ require one matrix-vector multiplication $R_{j+\frac{1}{2}}\Phi_{j+\frac{1}{2}}$ or $\hat{R}_{j+\frac{1}{2}}\hat{\Phi}_{j+\frac{1}{2}}$. Comparing (5.6b)-(5.6d) and (5.9c)-(5.9g), the computational effort between $\tilde{H}^H$ and $\tilde{H}^{VL}$ is very competitive. The first three terms on the right hand side of $\tilde{H}^{OC}_{j+\frac{1}{2}}$ in (5.11) require similar operation count as $\tilde{H}^H$ and $\tilde{H}^{VL}$. The last two terms of (5.11) consist of approximately 2/5 of the computation of the numerical flux $\tilde{H}^{OC}_{j+\frac{1}{2}}$. They are the extra computation that are not present in $\tilde{H}^H$ and $\tilde{H}^{VL}$. Therefore, for $\theta \neq -1$, $\tilde{H}^{OC}$ is approximately 40-45% more expensive to use than $\tilde{H}^H$ or $\tilde{H}^{VL}$. For $\theta = -1$, $\tilde{H}^{OC}$ is approximately 20-25% more expensive than the other two schemes.

Concluding Remarks

The current note addresses an aspect of implementating three existing spatially five-point upwind schemes for systems of hyperbolic conservation laws. The reason for choosing the above methods is that they represent typical design principles often used in constructing second-order (or higher-order) upwind TVD schemes. The current conclusion on the relative computational effort among the three methods mainly addresses unsteady calculations.

It is observed that the five-point upwind TVD scheme of Osher and Chakravarthy requires more operations than Harten or van Leer. The reason lies mainly in the different way of arriving the spatially second and third-order TVD schemes. The indication is that one can achieve the same spatial order of accuracy as Osher and Chakravarthy by using the lower operation count method of van Leer or Harten. Moreover, for the forward Euler time differencing, only Harten's method is second-order in time and space; the other two are first-order in time but second-order in space. To achieve second-order in time as well as space, additional work is required for the van Leer and for the Osher and Chakravarthy methods.

For steady-state applications, aside from accuracy requirements, convergence rate of a scheme is equally or more important than the CPU time per time step. The performance of an individual scheme in terms of convergence rate is highly problem dependent. Therefore the discussion here requires extensive numerical testing before a clearer picture can be drawn for steady-state applications.

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16. Abstract

The relative computational effort among the spatially five-point numerical flux functions of Harten, van Leer, and Osher and Chakravarthy is explored. These three methods typify the design principles most often used in constructing higher than first-order upwind total variation diminishing (TVD) schemes. For the scalar case the difference in operation count between any two algorithms may be very small and yet the operation count for their system counterparts might be vastly different. The situation occurs even though one starts with two different yet equivalent representations for the scalar case.

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