# UNIVERSIDADE DE SÃO PAULO

## Instituto de Ciências Matemáticas e de Computação

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**Part I: Theoretical Results**

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# Upwinding Finite-Difference Schemes for Convection Dominated Problems. Part I: Theoretical Results

Magda K. Kaibara[a], Valdemir G. Ferreira[b], Hélio A. Navarro[c]

[a]*Departamento de Matemática*
*Faculdade de Ciências/UNESP - Bauru*
*Av. Luiz Edmundo Carrijo Coube S/N, Vargem Limpa*
*CEP 17033-360, Bauru, SP*

[b]*Departamento de Ciências de Computação e Estatística*
*ICMC/USP - São Carlos*
*Caixa Postal 668*
*CEP 13560-970, São Carlos, SP*

[c]*Departamento de Estatística, Matemática Aplicada e Computação*
*IGCE/UNESP - Rio Claro*
*Caixa Postal 178*
*CEP 13506-700 Rio Claro, SP*

**Abstract**

This report discusses modern high-order boundedness upwind schemes. These models are based on NVD (Normalized Variable Diagram) approach by Leonard, Gaskell and Lau, and on TVD (Total Variation Diminishing) constraints by Harten, Yee and Roe. The purpose of this work is to provide a detailed discussion about upwinding type finite-difference numerical schemes for solving convection dominated fluid flow problems. Based on this review we derive a new approach for solving that type of problem.

**Keywords:** high-order upwind scheme, TVD constraints, NVD approach, convection-diffusion, convection term discretization, convective modelling, convection boundedness criterion, bounded convection scheme, limiters, finite diffrence,

# 1 Introduction

Standard finite-difference numerical schemes for approximating spatial derivatives may work well for problems with smooth solutions, but can give disastrous results when discontinuities are present, which are frequent in convection dominated processes. Currently, simulation of convection-diffusion equations is a most interesting/challenging subject in the computation of the fluid dynamics problems. For diffusive terms, the central second-order accurate finite difference scheme works well and it is adopted in many computational codes, while for convective terms, a variety of choices is possible.

In the development of a computational program for fluid flow and heat transfer problems, it is desirable adopting a scheme which models the convective terms with high accuracy, high stability, boundedness and with good performance. For our knowledge, in the literature there is no scheme that reaches these goals. Despite convective terms are represented by a simple first order derivative, its numerical representation has been one of the central subjects in computational fluid dynamic.

Classical schemes of first-order accurate, such as FOU (First Order Upwind), HYBRID and POWER-LAW, are unconditionally stable, however they introduce a large amount of numerical viscosity (artificial damping) that smooths the solution in the same way that physical viscosity. It presents a very serious problem to computational fluid dynamicists. The high order schemes, such as Central-Difference (CD), Second-Order Upwind (SOU) [16] and upwind of third order - QUICK (Quadratic Upstream Interpolation for Convective Kinematics) [9] improve the accuracy of the calculations. However, they have the problem of boundedness; that is, the solutions can display spurious oscillations when severe gradients (or discontinuities) are present. These spurious oscillations, very common in the shock wave problems [12], can be serious enough to cause numerical instabilities, which are introduced by round off errors, boundary conditions and non-linearities.

Since the nineties, efforts have been made to construct high order boundedness schemes. For steady problems, the SHARP (Simple High-Accuracy Resolution Program), proprosed by Leonard [10] in 1988, is an example of a scheme which has good performance. In his work, he developed the formulation of a scheme in the context of variable normalization and he devised a scheme that is limited and has high resolution. Another example is the scheme constructed by Gaskell and Lau [6]. They proposed the SMART (Sharp and Monotonic Algorithm for Realistic Transport) scheme, which uses the normalized variable formulation and is linear by parts. Both SHARP and SMART can reach third-order accurate, but for some problems, such as flow in shock tube [14], they are not limited. Besides, numerical tests (see [25]) disclose that SMART and SHARP schemes need an underrelaxation treatment in each face of the control volume in order to suppress the oscillatory convergent behavior. This difficulty increases the capacity of computational storage, especially for 3D fluid flow problem. In 1990, Zhu [24] proposed a hibrid scheme named HLPA (Hybrid Linear/Parabolic Approximation Scheme), which has only second-order accuracy. In 1998, Varonos and Bergeles [21] proposed the VONOS (Variable-Order Non-Oscillatory Scheme) model which emerged, according to Ferreira et al. [5], as an acceptable upwinding method for simulation of free surface flows.

Nowadays, two concepts have demonstrated to be of great utility in the construction of high-order schemes: the TVD [8]–[18] constraints and the NVD [6]–[10] approach. The fundamental mechanism common to these two models is the use of the dissipative nature of first-order differencing. TVD schemes, i.e. schemes which satisfy the TVD cosntraints, have attractive characteristics. The solutions obtained by them are well-resolved, oscillation-free and convergent. Usually, TVD schemes are applied for compressible flows in which the convective variables suffer high change in the gradient or in the case of discontinuities sprouting. Schemes that satisfy TVD conditions are always limited, and a good example is a MUSCL (Monotonic Upstream Scheme for Conservation Laws) type model. The NVD approach, as mentioned before, was introduced by Gaskell and Lau [6] and Leonard [10] for steady state flow problems, and extended for unsteady flows by Leonard [11]. This concept normalizes out the variation in sign, flow direction and scale.

By using the TVD and NVD tools, Song et al [17] proposed a third-order accurate and limited scheme named WACEB (Weighted-Average Coefficient Ensuring Boundedness). Numerical results for scalar convection problems, such as a sudden expansion of an oblique flow field and a laminar flow over a fence, show that this scheme has the ability of third-order QUICK scheme in the reduction of numerical diffusion without introducing overshoots or undershoots. However, this scheme still has convergence problems for some viscoelastic flows as noted by Alves et al. [1]. As a remedy for this, they devised a high resolution scheme named CUBISTA (Convergent and Universally Bounded Interpolation Scheme for Treatment of Advection), which is based on TVD restrictions and associated with the Courant number. The evaluation of the accuracy and the convergence properties of the scheme is measured for two dimensional numerical tests by using linear and non-linear problems and involving newtonian and non-newtonian fluid flows.

The main objective of this report is to present a study of upwinding type high-resolution finite-difference numerical schemes for convection dominated fluid flow problems. In view of this study we devised a new scheme which is based on adaptive flux computation. In the future, these techniques will be applied in order to compute effeciently and accurately time dependent numerical solution of linear and nonlinear problems.

## 2 TVD schemes

Given a sequence of discrete approximations $\phi(t) = \{\phi_i(t)\}_{i\in\mathbb{Z}}$ to a scalar, the Total Variation (TV) at time level $t$ of this sequence is defined by

$$TV(\phi(t)) = \sum_{i\in\mathbb{Z}} |\phi_{i+1}(t) - \phi_i(t)|.$$

Difference schemes which give rise to such TV diminishing are called TVD schemes, after Harten [8]. Here diminishing means nonincreasing. A desirable property for an approximate solution to share with the exact one is that its TV should decrease in time [19]. TVD is a purely scalar property, which ensures that spurious oscillations are completely removed from the numerical solution of a nonlinear conservation law.

Formally, consider the explicit difference scheme involving $(2k+1)$-points of the form

$$\phi_i^{n+1} = H(\phi_{i-k}^n, \cdots, \phi_{i+k}^n), \quad \forall n \geq 0, \quad i \in \mathbb{Z},$$

where $H : \mathbb{R}^{2k+1} \to \mathbb{R}$ is a continuous function and $\phi_i^n$ denotes an approximation of the exact solution $\phi$ at the uniform grid point $(x_i, t_n)$, being $x_i = i\Delta x,\ t_n = n\Delta t$, with $\Delta x$ and $\Delta t$ the spatial and the temporal steps, respectively. We say, by definition, that the above scheme is TVD if

$$TV(\phi^{n+1}) \leq TV(\phi^n).$$

We consider the unsteady linear advection equation of a scalar $\phi$ with constant velocity $a$, described by

$$\frac{\partial \phi}{\partial t} + a\frac{\partial \phi}{\partial x} = 0, \tag{1}$$

whose solution is approximated by the following numerical scheme in conservative form

$$\phi_i^{n+1} = \phi_i^n - \nu\ (\phi_{i+1/2} - \phi_{i-1/2}) \tag{2}$$

where $\nu = a\frac{\Delta t}{\Delta x}$ is the Courant number and $\phi_{i+1/2}$ is an approximation for the face value of the cell $[x_{i-1/2}, x_{i+1/2}]$ whose the center is $x_i$. We denote the value face $\phi_{i-1/2}$ by $\phi_\ell$ and $\phi_{i+1/2}$ by $\phi_f$. These points and values are ploted in Figure 1. Using these notations we can write

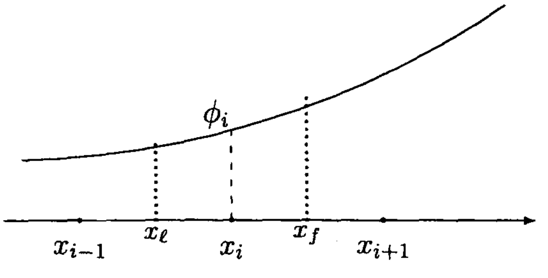


Figure 1: Interpolation stencil

- Upwind scheme

$$\phi_f = \frac{\phi_{i+1} + \phi_i}{2} - \frac{1}{2}sgn(a)(\phi_{i+1} - \phi_i).$$

- Lax-Wendroff scheme

$$\begin{aligned} \phi_i^{n+1} &= \phi_i^n - \frac{\nu}{2}\ (\phi_{i+1} - \phi_{i-1}) + \frac{\nu^2}{2}(\phi_{i+1} - 2\phi_i + \phi_{i-1}), &(3)\\ &= \phi_i^n - \nu\ (\phi_i - \phi_{i-1}) - \frac{1}{2}\nu(1-\nu)(\phi_{i+1} - 2\phi_i + \phi_{i-1}). &(4) \end{aligned}$$

Therefore

$$\phi_f = \phi_i + \frac{1}{2}(1-\nu)\ (\phi_{i+1} - \phi_i).$$

Note that the term $\frac{1}{2}\nu(1-\nu)(\phi_{i+1} - 2\phi_i + \phi_{i-1})$ in equation (4) may be viewed as an antidiffusive term added to the upwind scheme. It is known that the Lax-Wendroff scheme is not TVD. The antidiffusive term can be modified in order to limit the scheme

$$\phi_i^{n+1} = \phi_i^n - \nu\ (\phi_i - \phi_{i-1}) - \frac{1}{2}\nu(1-\nu)[\varphi_{i+1/2}(\phi_{i+1} - \phi_i) - \varphi_{i-1/2}(\phi_i - \phi_{i-1})], \tag{5}$$

then

$$\phi_f = \phi_i + \frac{1}{2}(1-\nu)\ \varphi_{i+1/2}(\phi_{i+1} - \phi_i). \tag{6}$$

We take the limiter $\varphi_{i+1/2}$ as being a function of the ratio of two consecutive gradients

$$\varphi_{i+1/2} = \varphi(r_{i+1/2}), \text{ with } r_{i+1/2} = \begin{cases} \dfrac{\phi_i - \phi_{i-1}}{\phi_{i+1} - \phi_i}, & \text{if a>0} \\ \\ \dfrac{\phi_{i+2} - \phi_{i+1}}{\phi_{i+1} - \phi_i}, & \text{if a<0 .} \end{cases} \tag{7}$$

**Remark 2.1** *Note that for $\varphi \equiv 1$, we obtain the Lax-Wendroff scheme.*

We give now a very useful criteria due to Harten [7], which ensures that a specific scheme is TVD. By using it, Sweby [18] deduces sufficient conditions for the scheme (5) to be TVD.

**Harten Criteria**: *Consider a scheme in the form*

$$\phi_i^{n+1} = \phi_i^n + C_{i+1/2}\ (\phi_{i+1}^n - \phi_i^n) - D_{i-1/2}\ (\phi_i^n - \phi_{i-1}^n) \tag{8}$$

*where the coefficients $C_{i+1/2}$ and $D_{i-1/2}$ depend on the $2k$ variables $\phi_{i-k+1}, \cdots, \phi_{i+k}$.*

*If the coefficients in (8) satisfy the following inequalities for all $i$,*

$$\begin{aligned} C_{i+1/2} &\geq 0, \\ D_{i+1/2} &\geq 0, \\ C_{i+1/2} + D_{i+1/2} &\leq 1, \end{aligned}$$

*then the scheme is TVD.*

**Proof:** We get

$$\begin{aligned} \phi_{i+1}^{n+1} - \phi_i^{n+1} &= \phi_{i+1}^n + C_{i+3/2}\ (\phi_{i+2}^n - \phi_{i+1}^n) - D_{i+1/2}\ (\phi_{i+1}^n - \phi_i^n) \\ &\quad -\phi_i^n - C_{i+1/2}\ (\phi_{i+1}^n - \phi_i^n) + D_{i-1/2}\ (\phi_i^n - \phi_{i-1}^n) \\ &= C_{i+3/2}(\phi_{i+2}^n - \phi_{i+1}^n) + (1 - C_{i+1/2} - D_{i+1/2})(\phi_{i+1}^n - \phi_i^n) + D_{i-1/2}(\phi_i^n - \phi_{i-1}^n) \end{aligned} \tag{9}$$

By hypothesis all coefficients in the right hand side of (9) are positive, thus

$$|\phi_{i+1}^{n+1} - \phi_i^{n+1}| \leq C_{i+3/2}|\phi_{i+2}^n - \phi_{i+1}^n| + (1 - C_{i+1/2} - D_{i+1/2})|\phi_{i+1}^n - \phi_i^n| + D_{i-1/2}|\phi_i^n - \phi_{i-1}^n|.$$

Adding-up these inequalities for all $i \in \mathbb{Z}$, and rearranging the sum in term of $|\phi_{i+1}^n - \phi_i^n|$, we get

$$TV(\phi^{n+1}) = \sum_i |\phi_{i+1}^{n+1} - \phi_i^{n+1}| \leq \sum_i |\phi_{i+1}^n - \phi_i^n| = TV(\phi^n).$$

□

Using the Harten Criteria, Sweby [18], in the next result, gives sufficient conditions on $\varphi$ in order to the scheme (5) to be TVD.

**Theorem 2.1** *Suppose that the function $\varphi$ satisfies*

$$\begin{cases} \varphi(r) = 0, & \text{if } r \leq 0 \\ 0 \leq \varphi(r) \leq \min\{2,\ 2r\}, & \text{if } r > 0, \end{cases} \tag{10}$$

*then the scheme (5) is TVD under the CFL (Courant-Friedrichs-Lewy) condition $0 \leq \nu \leq 1$, for $a > 0$.*

**Proof:** A possible choice for the coefficients $C_{i+1/2}$ and $D_{i-1/2}$ in Harten Criteria is

$$\begin{aligned} C_{i+1/2} &= 0, \\ D_{i-1/2} &= \nu + \frac{1}{2}\nu(1-\nu)\left(\frac{\varphi_{i+1/2}}{r_{i+1/2}} - \varphi_{i-1/2}\right). \end{aligned} \tag{11}$$

Under the conditions (10), let us check that we have $0 \leq D_{i-1/2} \leq 1$. Note that in this case, $\phi_i^{n+1}$ lies between $\phi_{i-1}^n$ and $\phi_i^n$, which illustrates the upwind propety of the scheme. Suppose first that

$$\left|\frac{\varphi(r)}{r} - \varphi(s)\right| \leq \Phi, \tag{12}$$

for all $r,\ s$ and for some $\Phi = \Phi(\nu)$. Since $0 < \nu < 1$, we have from (11) and (12)

$$\begin{aligned} 1 - (1-\nu)\frac{\Phi}{2} &\geq 0 \\ 1 + (1-\nu)\frac{\Phi}{2} &\leq \frac{1}{\nu}, \end{aligned}$$

and therefore $0 \leq D_{i-1/2}$ and $D_{i-1/2} \leq 1$, or equivalently

$$\Phi \leq \inf\left\{\frac{2}{\nu},\ \frac{2}{1-\nu}\right\} \quad \Rightarrow \quad 0 \leq D_{i-1/2} \leq 1.$$

Since $\nu \in (0,1)$, we must have $\Phi \leq 2$. It is clear from (11) that for $\nu = 0$ or $\nu = 1$ the Harten's criteria is satisfied.

Next, assuming $\varphi(r) = 0$ for $r \leq 0$, the equation (12) will hold with $\Phi = 2$ if $r > 0$

$$0 \leq \varphi(r) \leq 2r \quad \text{and} \quad \varphi(r) \leq 2$$

which leads to (10). □

The condition (10) means that the graph of $\varphi$ must lie in the shaded region of Figure 2.

**Remark 2.2** *The Theorem 2.1 is valid in general case $|\nu| \leq 1$.*

## 2.1 Examples of Limiters

1. Sweby's limiter

$$\varphi_S(r) = \max\{0,\ \min(S\,r, 1),\ \min(r, S)\} \tag{13}$$

where $S$ is some parameter in the interval $[1,2]$. The function $\varphi_S$ is monotone increasing, having the "symmetry" property

$$\frac{\varphi_S(r)}{r} = \varphi_S\left(\frac{1}{r}\right). \tag{14}$$

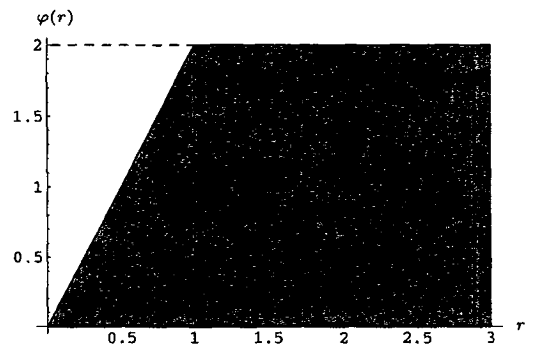

Figure 2: Sweby's Diagram

2. Roe's limiter
   For $S = 1$, in (13) we get Roe's MINMOD limiter and for $S = 2$ we get Roe's highly compressive limiter SUPERBEE.

3. Van Leer's limiter
   Van Leer's technique [20] leads to the limiter

$$\varphi(r) = \frac{r + |r|}{1 + |r|} = \begin{cases} 0, & r \leq 0 \\ \dfrac{2r}{1+r}, & r \geq 0 \end{cases}$$

Figure 3 plots the graphics of these examples of limiters. Note that all of them are in the TVD region.

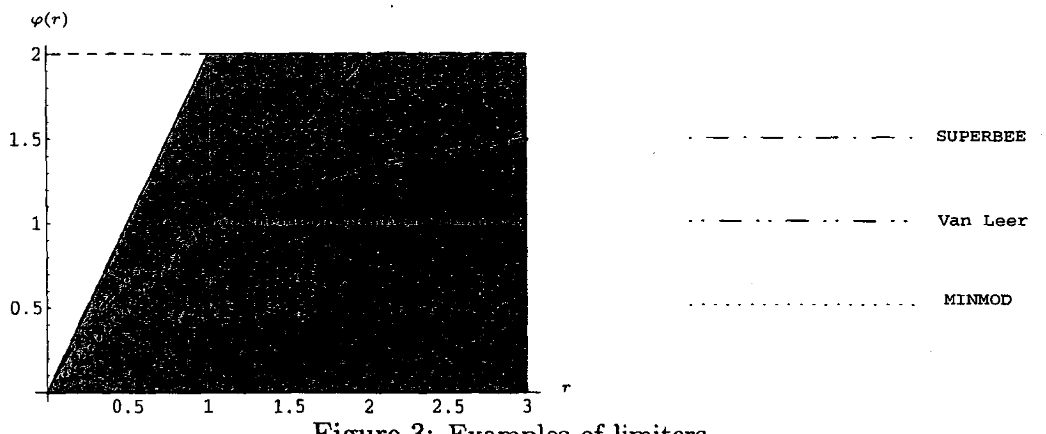

Figure 3: Examples of limiters

# 3 Normalized Variables

The concept of normalized variable that we describe now was introduced by Gaskell and Lau [6] and Leonard [10], [11].

The face value $\phi_f$ can be determined by the two nodes straddling the face and the next upstream node, which depends on the flow direction at the face $f$, i.e., the sign of $a$

$$\phi_f = \phi_f(\phi_D^n, \phi_U^n, \phi_R^n, \nu). \tag{15}$$

The capital letters $D$, $U$ and $R$ in equation (15) indicate, respectively, the downstream, upstream and remote-upstream positions. The value of $\phi$ at the point $x_i = U$ is denoted by $\phi_U$. The localization of the values $\phi_f$, $\phi_D$, $\phi_U$ and $\phi_R$ is illustrated in Figure 4. Note that the difference in the localization of these nodes depends on sign of $a$ (see Ferreira [4] for specific examples).

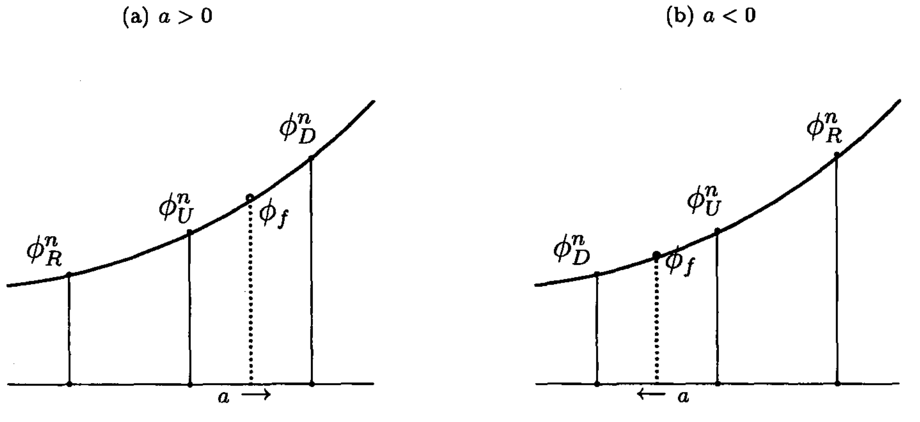


Figure 4: Localization of $\phi_R$, $\phi_U$, $\phi_D$ and $\phi_f$

Variations in sign, flow direction and scale in terms of original variables can be normalized by defining the normalized variable as

$$\hat{\phi}(x,t) = \frac{\phi(x,t) - \phi_R^n}{\phi_D^n - \phi_R^n}. \tag{16}$$

which implies that

$$\hat{\phi}_R^n = 0, \quad \hat{\phi}_D^n = 1.$$

and

$$\hat{\phi}_f = \phi_f(\hat{\phi}_U^n, \nu). \tag{17}$$

In case $a > 0$, we represent in Figure 5 the values of $\phi$ in terms of original variables and normalized variables.

Equation (17) includes first-order methods, second-order central and upwind schemes and third-order upwinding, in addition to second-order and third-order shock-capturing algorithms. Higher order methods involve more distant nodes but the normalized $\hat{\phi}_f$ will still depend most strongly on $\hat{\phi}_U^n$.

# 4 Convection Boundedness Criterion

The numerical solution computed by the discretization of convection term using a bounded scheme will never overpass the maximum or minimum values inherently determined by the physical process itself. If the numerical solution presents overshoot or undershoot, they always

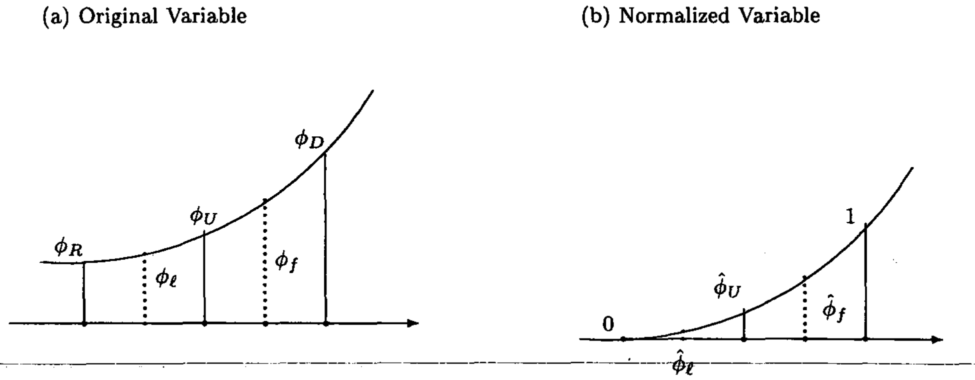


Figure 5: Interpolation of $\phi_f$

occur at the position where a steep gradient of dependent variable exists. *Boundedness* of a scheme may be defined as to predict no unphysical oscillations in regions of steep gradients. Boundedness is of immense importance to keep numerical results physically reasonable.

Gaskell and Lau [6] proposed a criterion named Convection Boundedness Criterion (CBC) for a convection scheme to possess the boundedness character. It is mainly applied to the incompressible flow. They proposed that a continuous function or a piecewise continuous function $\hat{\phi}_f = \hat{\phi}_f(\hat{\phi}_U^n)$ possess the boundedness if the following conditions are satisfied

$$\begin{aligned} \hat{\phi}_f &= \hat{\phi}_f(\hat{\phi}_U) = \hat{\phi}_U \text{ for } \hat{\phi}_U \leq 0 \\ \hat{\phi}_f &= \hat{\phi}_f(\hat{\phi}_U) = \hat{\phi}_U \text{ for } \hat{\phi}_U \geq 1 \\ \hat{\phi}_U &\leq \hat{\phi}_f(\hat{\phi}_U) \leq 1 \text{ for } 0 < \hat{\phi}_U < 1. \end{aligned} \tag{18}$$

The corresponding region in the normalized variable diagram is shown in Figure 6. In their

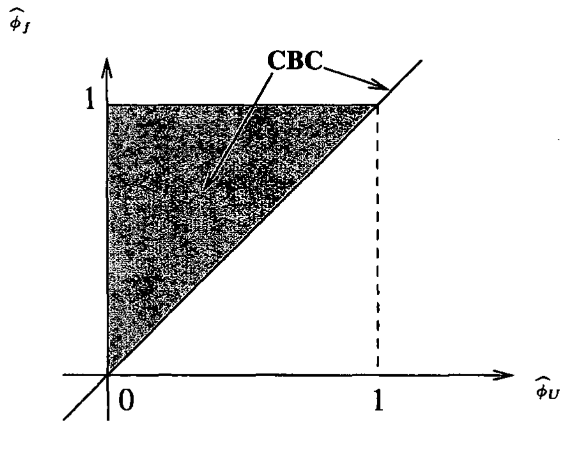


Figure 6: CBC region in $\widehat{\phi}_f - \widehat{\phi}_U$ plane

work they claimed that the definition line of a bounded scheme should be located within its region and vice-versa.

The CBC and the corresponding region in the NVD have been accepted as both the sufficient and necessary condition for a scheme possessing boundedness. Recently, Yu et al. [22] indicated that the CBC is only a sufficient condition, and they proposed another CBC, named Extended CBC (ECBC).

Ping-Li et al. in [15] based on the NVD revealed the weakness of CBC by numerical example and made refinements to the CBC based on careful consideration of the smoothness of the profile variation pattern of the normalized variable. The analysis made by them demonstrated that the first and second constraints of CBC (Equation 19) are sufficient ones, and the third condition is a necessary and sufficient one for boundedness. The CBC can only guarantee the boundedness, without any accuracy consideration. The new CBC proposed guarantees not only the boundedness, but also high-order accuracy. They proposed that a continuous function or a piecewise continuous function $\hat{\phi}_f = F(\hat{\phi}_U^n)$ possess the boundedness with high accuracy if the following conditions are satisfied

$$\begin{aligned}
\hat{\phi}_U \in (-\infty, 0), &\quad \hat{\phi}_f(\hat{\phi}_U) \in [\hat{\phi}_U, 0.5\hat{\phi}_U) \\
\hat{\phi}_U \in [0, 0.5), &\quad \hat{\phi}_f(\hat{\phi}_U) \in [1.5\hat{\phi}_U, 0.5(1+\hat{\phi}_U), \\
\hat{\phi}_U \in [0.5, 2/3), &\quad \hat{\phi}_f(\hat{\phi}_U) \in [0.5(1+\hat{\phi}_U), 1.5\hat{\phi}_U), \\
\hat{\phi}_U \in [2/3, 1], &\quad \hat{\phi}_f(\hat{\phi}_U) \in (0.5(1+\hat{\phi}_U), 1], \\
\hat{\phi}_U \in (1, +\infty), &\quad \hat{\phi}_f(\hat{\phi}_U) \in (0.5(1+\hat{\phi}_U), \hat{\phi}_U].
\end{aligned}$$

The corresponding region in the NVD is shown in Figure 7.

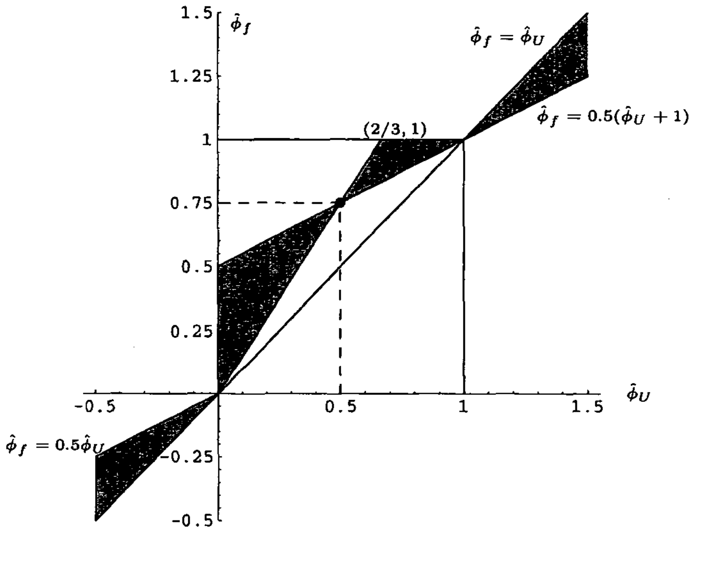


Figure 7: ECBC region in $\widehat{\phi}_f - \widehat{\phi}_U$ plane

In their work they claimed that the definition line of a bounded high-accuracy scheme should be located within its region and vice-versa.

# 5 Relationship between Sweby's diagram and Normalized Variables

GL-CBC and ECBC do not work well for general problems [1], so we think it is more interesting to lead with TVD schemes even for incompressible flows. Because it is assumed that the numerical solution evolves up to reach the equilibrium. So in this section we concentrate on explaining the relationship between Sweby's diagram and Normalized Variables.

The equations (6) and (7) in the normalized variables are written [11] and [14], respectively, as

$$\hat{\phi}_f = \hat{\phi}_U + \frac{1}{2}(1-\nu)\ \varphi_{i+1/2}(1-\hat{\phi}_U). \tag{19}$$

$$r_{i+1/2} = \frac{\hat{\phi}_U}{1-\hat{\phi}_U}. \tag{20}$$

From relations (10) and (20), the functional relationship between $\hat{\phi}_f$ and $\hat{\phi}_U$, which satisfies the TVD principle, can be expressed as

$$\begin{cases} \hat{\phi}_U \leq \hat{\phi}_f \leq \min\{1-\nu+\nu\hat{\phi}_U, (2-\nu)\hat{\phi}_U\}, & \text{for } 0 < \hat{\phi}_U < 1 \\ \hat{\phi}_f = \hat{\phi}_U, & \text{for } \hat{\phi}_U \leq 0 \text{ or } \hat{\phi}_U \geq 1 \end{cases} \tag{21}$$

This region is ploted in Figure 8 (a) for $\nu = 0.25$.

For each value of $\nu \in [0,1]$, the TVD region associated with $\nu$ must be contained in the global TVD region (which corresponds $\nu = 0$, for steady case) ploted in Figure 8(b), which is defined by the inequalities

$$\begin{cases} \hat{\phi}_U \leq \hat{\phi}_f \leq \min\{1, 2\hat{\phi}_U\}, & \text{for } 0 < \hat{\phi}_U < 1 \\ \hat{\phi}_f = \hat{\phi}_U, & \text{for } \hat{\phi}_U \leq 0 \text{ or } \hat{\phi}_U \geq 1 \end{cases}$$

**Remark 5.1** *The TVD constraint is more restritive than the CBC criterion. Schemes satisfying the TVD constraint are always bounded, but the reciprocal is not true.*

**Remark 5.2** *Usually, the TVD requirement is applied to the compressible flow in which the convected variable may experience sharp changes in gradients or discontinuity at a position where shock wave exists. The TVD constraint can guarantee that no unrealistic oscillatory results will occur in the computation of compressible flow. The CBC is mainly applied to the incompressible flow.*

# 6 Steady Case

In the steady case $\hat{\phi}_f$ depends only on $\hat{\phi}_U$, i.e.,

$$\hat{\phi}_f = \phi_f(\hat{\phi}_U^n). \tag{22}$$

Table 1 shows the expressions of $\phi_f$ and $\hat{\phi}_f$ for some well known schemes. Figures 9 and 10 depict these schemes in normalized variables.

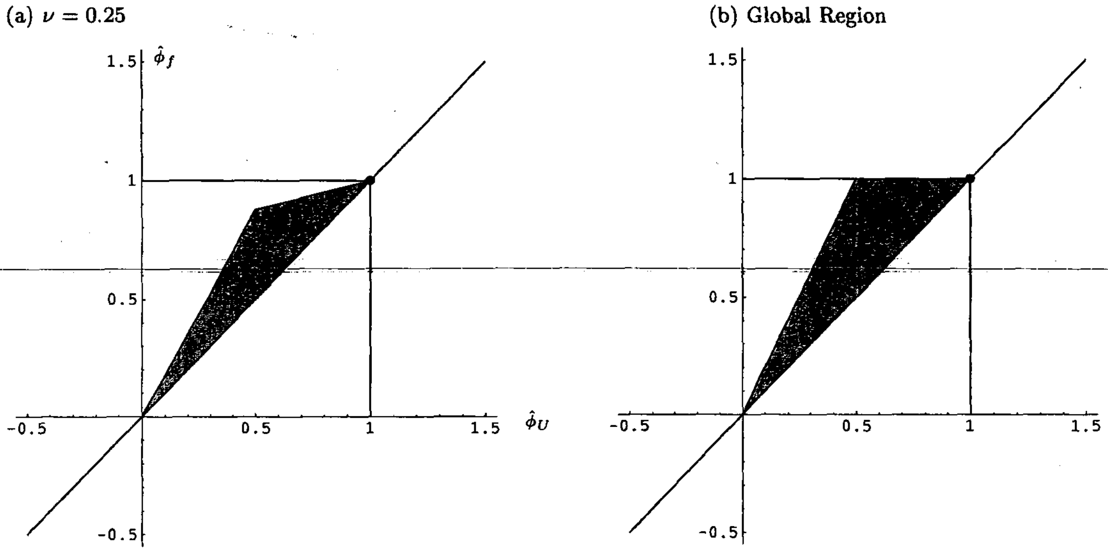


Figure 8: TVD region in Normalized Variables

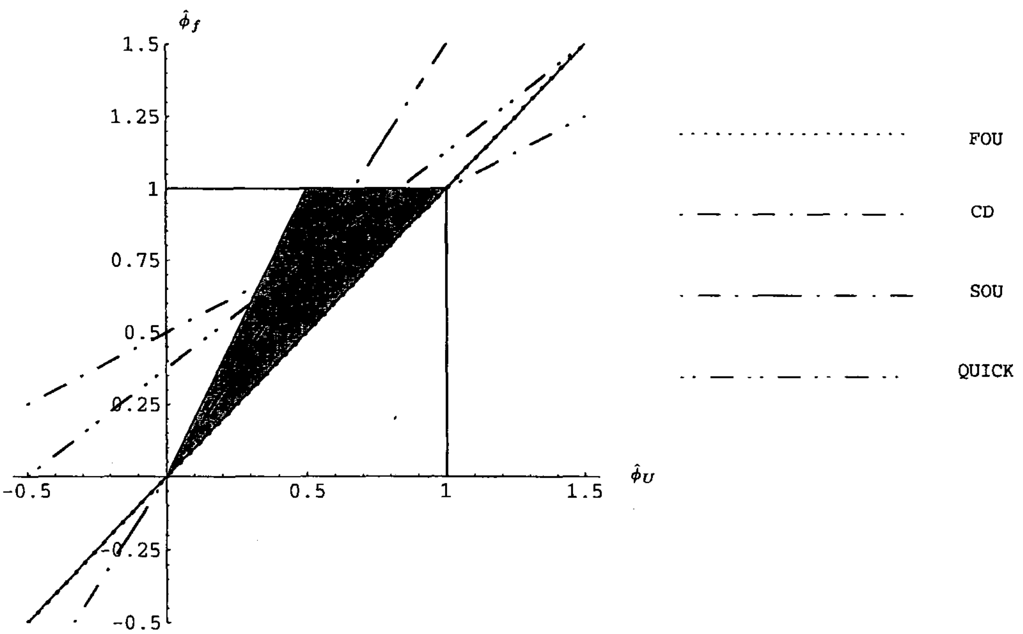


Figure 9: Examples of schemes in normalized variables

| Scheme | $\phi_f$ | $\hat{\phi}_f$ |
|---|---|---|
| FOU | $\phi_U$ | $\hat{\phi}_U$ |
| CD | $\frac{1}{2}(\phi_D + \phi_U)$ | $\frac{3}{4} + \frac{1}{2}(\hat{\phi}_U - \frac{1}{2})$ |
| SOU | $\frac{3}{2}\phi_U - \frac{1}{2}\phi_R$ | $\frac{3}{2}\hat{\phi}_U$ |
| QUICK | $\frac{1}{8}(3\phi_D + 6\phi_U - \phi_R)$ | $\frac{3}{4}\hat{\phi}_U + \frac{3}{8}$ |
| SMART | $\begin{cases} \phi_U, \\ 3\phi_U - 2\phi_R, \\ \frac{1}{8}(3\phi_D + 6\phi_U - \phi_R), \\ \phi_D. \end{cases}$ | $\begin{cases} \hat{\phi}_U & \text{if } \hat{\phi}_U \notin [0,1], \\ 3\hat{\phi}_U & \text{if } \hat{\phi}_U \in [0,1/6), \\ \frac{3}{4}\hat{\phi}_U + \frac{3}{8} & \text{if } \leq \hat{\phi}_U \in [1/6,5/6), \\ 1 & \text{if } \hat{\phi}_U \in [5/6,1). \end{cases}$ |
| VONOS | $\begin{cases} \phi_U, \\ 10\phi_U - 9\phi_R, \\ \frac{1}{8}(3\phi_D + 6\phi_U - \phi_R), \\ 1,5\phi_U - 0.5\phi_R, \\ \phi_D. \end{cases}$ | $\begin{cases} \hat{\phi}_U & \text{if } \hat{\phi}_U \notin [0,1], \\ 10\hat{\phi}_U & \text{if } \hat{\phi}_U \in [0,3/74), \\ \frac{3}{8}(1 + 2\hat{\phi}_U) & \text{if } \hat{\phi}_U \in [3/74,1/2), \\ 1,5\hat{\phi}_U & \text{if } \hat{\phi}_U \in [1/2,2/3), \\ 1 & \text{if } \hat{\phi}_U \in [2/3,1]. \end{cases}$ |
| HLPA | $\begin{cases} \phi_U \\ \phi_U + (\phi_D - \phi_U)\hat{\phi}_U. \end{cases}$ | $\begin{cases} \hat{\phi}_U & \text{if } \hat{\phi}_U \notin [0,1], \\ (2 - \hat{\phi}_U)\hat{\phi}_U & \text{if } \hat{\phi}_U \in [0,1]. \end{cases}$ |
| SHARP | $A \pm \sqrt{(\phi_D - A)(\phi_R - A)}$ where $A = \frac{\phi_D\phi_R - \phi_U^2}{\phi_D - 2\phi_U + \phi_R}$ | $\begin{cases} \frac{[\hat{\phi}_U(1-\hat{\phi}_U)^3]^{1/2} - \hat{\phi}_U^2}{1-2\hat{\phi}_U} & \text{if } \hat{\phi}_U \in [0,0.35] \cup [0.65,1], \\ \frac{3}{4}\hat{\phi}_U + \frac{3}{8} & \text{if } \hat{\phi}_U \in [0.35,0.65] \cup (-\infty,-1] \cup [1.5,+\infty), \\ \frac{3}{8}\hat{\phi}_U & \text{if } \hat{\phi}_U \in [-1,0], \\ \hat{\phi}_U & \text{if } \hat{\phi}_U \in [1,1.5]. \end{cases}$ |

Table 1: Expression for $\phi_f$ and $\hat{\phi}_f$

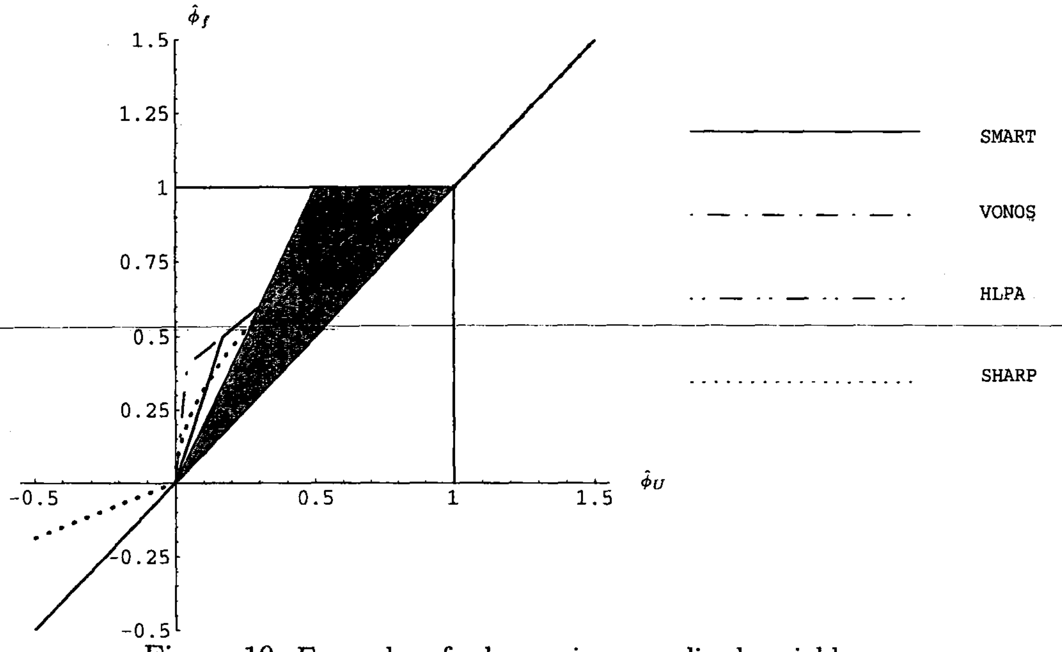

Figure 10: Examples of schemes in normalized variables

It is important to note that, except for the FOU scheme, all the schemes in Figures 9 and 10 pass through the point $Q(0.5, 0.75)$. As point out by Leonard [10], it is not difficult to show that for any scheme passing through $Q$ is necessary and sufficient for second-order accuracy, and passing through $Q$ with slope of 3/4 is necessary and sufficient for third-order accuracy. Schemes passing through $Q$ can be written as

$$\hat{\phi}_f = \frac{3}{4} + S(\hat{\phi}_U - \frac{1}{2}), \tag{23}$$

where $S$ represents the line slope. Using the original variables the equation (23), by one hand, is giving by

$$\phi_f = \frac{1}{2}(\phi_D + \phi_U) - \left(\frac{S}{2} - \frac{1}{4}\right)(\phi_D - 2\phi_U + \phi_R). \tag{24}$$

Approximating the value of $\phi_f$ by quadratic polynomial interpolation based on the values $\phi_D$, $\phi_U$ and $\phi_R$ we get

$$\begin{aligned} \phi_f &= \phi_U + \frac{\phi_D - \phi_R}{4} + \frac{1}{8}(\phi_D - 2\phi_U + \phi_R) \quad (25)\\ &= \frac{1}{2}(\phi_D + \phi_U) - \frac{1}{8}(\phi_D - 2\phi_U + \phi_R). \quad (26) \end{aligned}$$

So, by other hand, defining the value of $\phi_f$ in terms of the Curvature Factor (CF) as made in [10] we have

$$\phi_f = \frac{1}{2}(\phi_D + \phi_U) - CF(\phi_D - 2\phi_U + \phi_R). \tag{27}$$

Therefore from (24) and (27) we obtain

$$S = 2\,CF + \frac{1}{2}. \tag{28}$$

According to (28) we have

- SOU: $CF = 1/2$, $S = 3/2$
- CD: $CF = 0$, $S = 1/2$
- QUICK: $CF = 1/8$, $S = 3/4$.

**Remark 6.1** *The term $(\phi_D+\phi_U)/2$ corresponds to the value of $\phi_f$ obtained by linear polynomial interpolation. Also, if $CF = 1/8$, Equation (27) is the value of $\phi_f$ obtained by quadratic polynomial interpolation.*

**Remark 6.2** *The Lax-Wendroff scheme can also be viewed as a quadratic interpolation as the one above.*

In normalized variables, Equation (27) is given by

$$\hat{\phi}_f = \frac{1}{2}(1+\hat{\phi}_U) - CF(1-2\hat{\phi}_U). \tag{29}$$

As mentioned by Leonard [10] any (non-linear) functional relation between $\hat{\phi}_f$ and $\hat{\phi}_U$ passing through $Q$ can be written in the same form as (29), since $CF$ is a function of $\hat{\phi}_U$, i.e., $CF = CF(\hat{\phi}_U)$. In his work, he concluded that any scheme written in the form (29), with $CF = CF(\hat{\phi}_U)$, has at least second order accuracy. If $CF(1/2) = 1/8$ then the scheme is third-order accuracy.

## 6.1 WACEB Scheme

This subsection describes the proposed third-order accurate and limited scheme named WACEB (Weighted-Average Coefficient Ensuring Boundedness) derived by Song et al. [17], see also [13]. In original variables, the higher-order interpolation schemes can be written as the following form

$$\phi_f = \phi_U + \frac{\phi_D - \phi_R}{4} + \frac{\kappa}{4}(\phi_R - 2\phi_C + \phi_D), \tag{30}$$

where $\kappa$ is a weighted-average coefficient. In the normalized variables Equation 30 is

$$\hat{\phi}_f = \hat{\phi}_U + \frac{1}{4}[(1+\kappa)(1-\hat{\phi}_U) + (1-\kappa)\hat{\phi}_U]. \tag{31}$$

To obtain a high-order scheme in order to ensure boundedness, the TVD constraints can be used. The Taylor series expansion shows that the two leading truncation error terms of the interpolation scheme (30) are

$$\frac{1}{4}\left(\kappa - \frac{1}{2}\right)\Delta x^2 \phi'' \text{ and } \frac{1}{8}(1-\kappa)\Delta x^3 \phi''',$$

therefore the scheme is at least second order accurate, as mentioned by Leonard [10]. Maximum accuracy (thrid-order) is achieve if $\kappa$ is equal to $1/2$. Then the scheme is constructed in such a way that $\kappa$ lies as close as possible to $1/2$, while satisfying TVD constraints. So, the proposed method by [17] et al. to compute the normalized cell face is given by

$$\hat{\phi}_f = \begin{cases} 2\hat{\phi}_U, & 0 < \hat{\phi}_U < 0.3 \\ \frac{3}{4}\hat{\phi}_U + \frac{3}{8}, & 0.3 \leq \hat{\phi}_U \leq \frac{5}{6} \\ 1, & \frac{5}{6} < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere.} \end{cases} \tag{32}$$

Figure 11 shows the characteristic curve of the WACEB scheme.

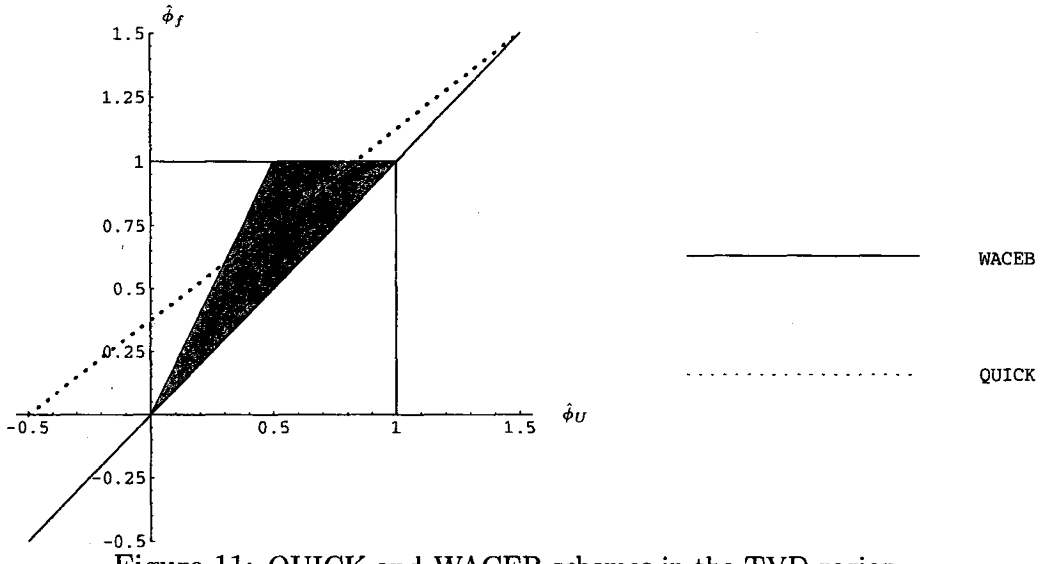

Figure 11: QUICK and WACEB schemes in the TVD region

# 7 Unsteady Case

In this section we will make some notes about the FOU, Lax-Wendroff and third-order accurate QUICKEST (QUICK with Estimated Streaming Terms [9]) schemes.

For the schemes FOU, Lax-Wendroff and QUICKEST, $\phi_f$ reads

- FOU

$$\hat{\phi}_f = \hat{\phi}_U.$$

- Lax-Wendroff

$$\hat{\phi}_f = \hat{\phi}_U + \frac{1}{2}(1-\nu)(1-\hat{\phi}_U) = \frac{(1-\nu)}{2}(1+\hat{\phi}_U) + \nu\hat{\phi}_U.$$

- QUICKEST

$$
\begin{aligned}
\hat{\phi}_f &= \frac{1}{2}[\phi_{i+1} + \phi_i - \nu(\phi_{i+1} - \phi_i)] \\
&\quad - \frac{(1-\nu^2)}{6}\left[\frac{\phi_{i+2} - \phi_{i+1} - \phi_i + \phi_{i-1}}{2} - sgn(\nu)\frac{\phi_{i+2} - 3\phi_{i+1} + 3\phi_i - \phi_{i-1}}{2}\right] \\
&= \hat{\phi}_U + \frac{1}{2}(1 - |\nu|)(1 - \hat{\phi}_U) - \frac{1-\nu^2}{6}(1 - 2\hat{\phi}_U) \\
&= \frac{(1-|\nu|)}{2}(1 + \hat{\phi}_U) + |\nu|\hat{\phi}_U - \frac{1-\nu^2}{6}(1 - 2\hat{\phi}_U)
\end{aligned}
$$

Figures 13 and 14 show the curves defined by $\hat{\phi}_f = \hat{\phi}_f(\hat{\phi}_U)$ in the corresponding TVD region associated with Courant number. From these figures and Figure 12 we remark:

- Increasing the value of $\nu$, the associated TVD region is going restricted.
- When $\nu$ approximates to 0 we have, respectively, for FOU, Lax-Wendroff and QUICKEST schemes
  - $\hat{\phi}_f = \hat{\phi}_U$
  - $\hat{\phi}_f \rightarrow \dfrac{1 + \hat{\phi}_U}{2}$
  - $\hat{\phi}_f \rightarrow \dfrac{1 + \hat{\phi}_U}{2} - \dfrac{1}{6}(1 - 2\hat{\phi}_U) = \dfrac{1}{3} + \dfrac{5}{6}\hat{\phi}_U$
- For $\hat{\phi}_U = 1/2$ and $\nu \rightarrow 0$, the correspondent value of $\hat{\phi}_f \rightarrow 3/4$ for Lax-Wendroff and QUICKEST scheme (see Figures 13(f) and 14(f)).

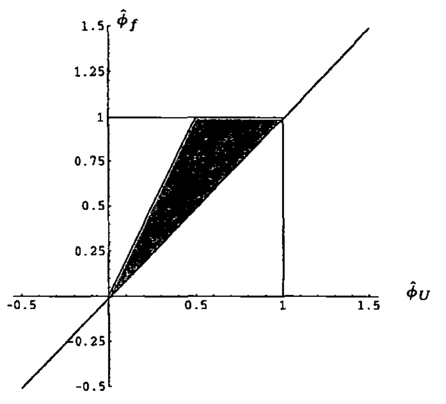


Figure 12: FOU scheme in TVD region

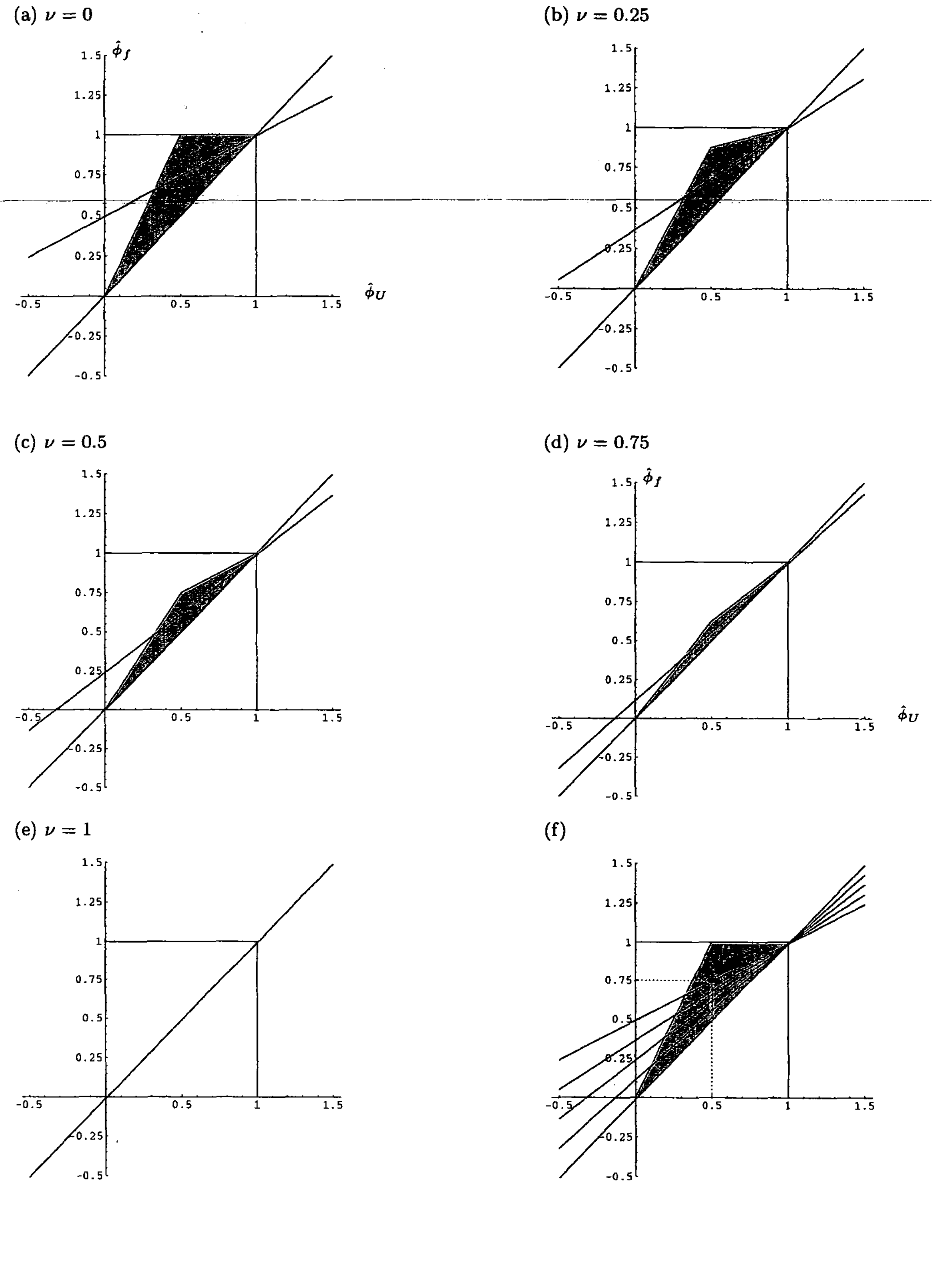


Figure 13: Lax-Wendroff scheme in the TVD region

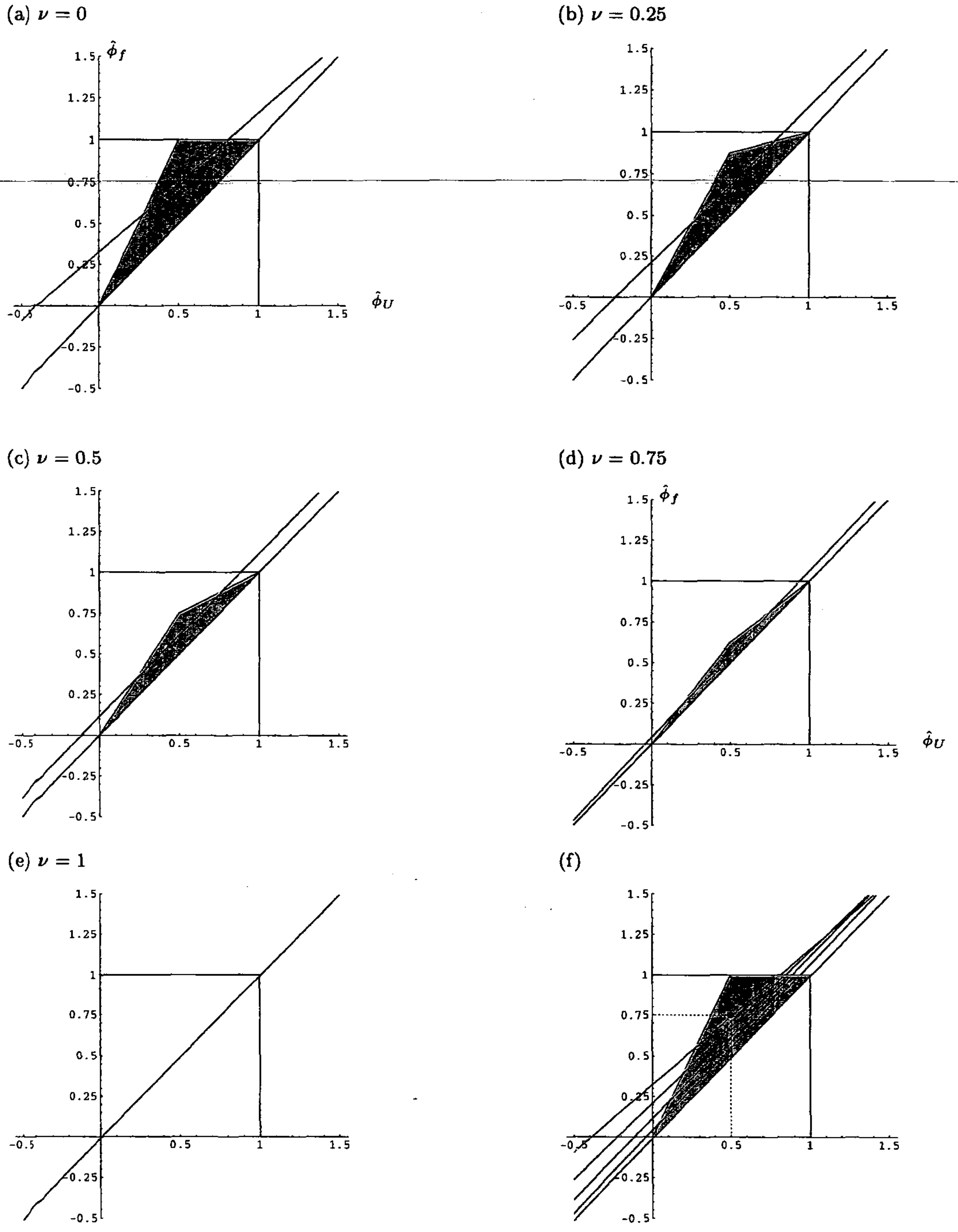


Figure 14: QUICKEST scheme in TVD region

### 7.1 CUBISTA Scheme

In this subsection we describe the CUBISTA scheme presented in [1], which has a piecewise linear representation in the normalized diagram and is composed by three segments in the TVD region, namely: on the left $\hat{\phi}_U \approx 0$; on the middle QUICK line corresponding to the smooth flow regime; and on the right the TVD limiter $\hat{\phi}_U \approx 1$.

The basic difference scheme is the formally third-order accurate QUICK scheme which is used in the region where the solution is smooth, i.e., almost everywhere in the domain. The scheme should respect the TVD restrictions (21), with $\nu$ taken as an empirical parameter, and it is not a real Courant number, to be found by numerical experiments and theoretical calculations. It is proved that if $\nu = 0$, we would end up with the WACEB scheme [17]. However, for some flows, this scheme still has convergence problems. For $\nu = 0.25$, the results in all cases tested by Alves et al. [1] were convergents. $\nu$ satisfies a compromise between increasing $\nu$ in order to promove convergence, and decreasing $\nu$ to improve resolution of sharp gradients. Symmetric limiter was required, i. e., the limiter $\varphi$ must satisfy the equation (14).

Translating the proposed scheme from the NVD to Sweby's diagram, using the relation

$$\varphi = \frac{\hat{\phi}_f - \hat{\phi}_U}{0.5(1 - \hat{\phi}_U)} \quad \text{and} \quad r = \frac{\phi_U - \phi_R}{\phi_D - \phi_U} = \frac{\hat{\phi}_U}{1 - \hat{\phi}_U}$$

one obtains

$$\varphi(r) = \max\{0, \min[2r(1 - C_1), \frac{3}{4} + \frac{r}{4}, 2(1 - C_2)]\},$$

where $C_1 = 2 - \nu$ and $C_2 = \nu$. So it is obtained that $\nu$ must be 0.25. Therefore, the scheme is given by

$$\hat{\phi}_f = \begin{cases} \frac{7}{4}\hat{\phi}_U, & 0 < \hat{\phi}_U < \frac{3}{8} \\ \frac{3}{4}\hat{\phi}_U + \frac{3}{8}, & \frac{3}{8} \le \hat{\phi}_U \le \frac{3}{4} \\ \frac{1}{4}\hat{\phi}_U + \frac{3}{4}, & \frac{3}{4} < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere.} \end{cases} \tag{33}$$

Figure 15 shows the characteristic curve of the CUBISTA scheme.

# 8 Adaptive QUICKEST Scheme

From observing Figures 13, 14 and inspired by the design of WACEB and CUBISTA scheme we proposed the following new scheme

$$\hat{\phi}_f = \begin{cases} (2 - \nu)\hat{\phi}_U, & 0 < \hat{\phi}_U < a \\ \hat{\phi}_U + \frac{1}{2}(1 - \nu)(1 - \hat{\phi}_U) - \frac{1}{6}(1 - \nu^2)(1 - 2\hat{\phi}_U), & a \le \hat{\phi}_U \le b \\ 1 - \nu + \nu\hat{\phi}_U, & b < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere} \end{cases} \tag{34}$$

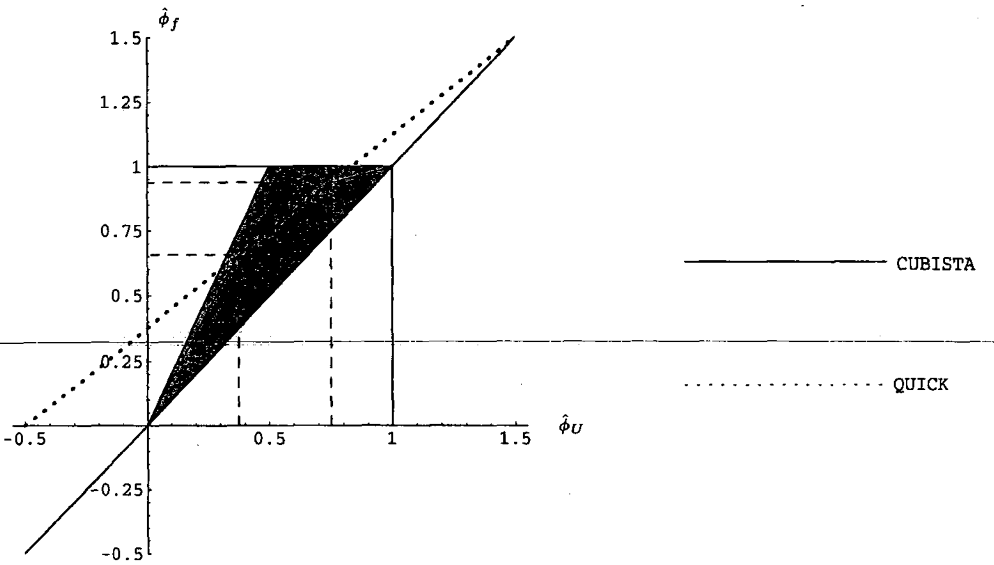


Figure 15: QUICK and CUBISTA schemes

where $a$ and $b$ are, respectively, the intersection points between the curves defined by QUICKEST scheme and $\hat{\phi}_f = (2-\nu)\hat{\phi}_U$, and by QUICKEST scheme and $\hat{\phi}_f = 1-\nu+\nu\hat{\phi}_U$. Figure 16 shows this new scheme in $\hat{\phi}_U - \hat{\phi}_U$ plane.

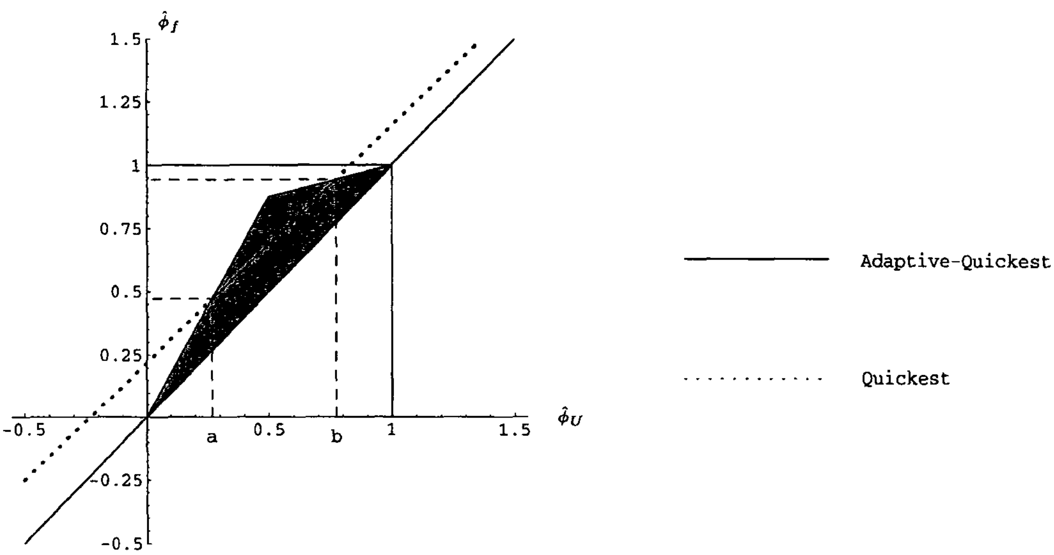


Figure 16: Caracteristic Curves of QUICKEST and Adaptive-QUICKEST schemes

# 9 Concluding Remarks

This work has been concerned with modern high-order upwind techniques for numerical solution of fluid flow problems. The NVD and TVD approaches were considered. We end the report by devising a new adaptative scheme.

In the future, these techniques will be applied, by the authors, to compute efficiently and accurately time dependent numerical solution of linear and nonlinear problems. We plan to exploit the potential of the TVD upwind shock capturing techniques by modelling complex unsteady 3D flows such as those involving a moving free surface.


**Resumo**

Nestas notas esquemas "upwind" modernos de alta ordem e limitados são discutidos. Esses modelos são baseados em variáveis normalizadas de Leonard, Gaskell e Lau, e na restrição TVD ("Total Variation Diminishing") introduzida por Harten, Yee e Roe. O objetivo desse trabalho é fornecer uma discussão detalhada sobre esquemas de diferenças tipo "upwind" para a solução numérica de prolemas de escoamentos de fluidos dominados por convecção. Tendo como base este estudo, nós derivamos uma nova estratégia para resolver este tipo de problema.


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