UPWIND SCHEMES FOR CONVECTION DOMINATED PROBLEMS

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Abstract. *The numerical solution of convection dominated fluid flows arises in many important areas in science and engineering. These problems occur in many applications such as in the transport of air and ground water pollutants, oil reservoir flow, in the modeling of semiconductors, and so forth. This work discusses modern high-order boundedness upwind schemes for solving the convection dominated fluid flow problems. These models are based on NVD approach by Leonard, Gaskell and Lau, and on TVD constraints by Harten, Yee and Roe. The purpose of this work is to provide a 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, finite difference*

1. Introduction

Achieving physical realism is a difficult task with all numerical solutions of the advection dominated models. Deficiences in this regard include numerical diffusion, spurious oscillations and peak clipping. The origin of these problems is the convective terms, which is not well resolved for traditional numerical techniques. Although much pioneering works in the development of advection schemes has been done during the 20 years, the perfect scheme that minimizes numerical diffusion, eliminates the spurious oscillation, captures the correct peak, is robust, is ease of implementing, and is efficient, is not appear yet. So, the research in this field is simmering in the CFD community. Classical schemes of first/second-order accurate such as FOU, CD, QUICK, SHARP, SMART, HLPA, VONOS, and so on, present some of the deficiences described above. Nowadays, two concepts have demonstrated to be of great utility in the construction of high-order schemes: the TVD (Harten, 1984)–(Sweby, 1984) constraints and the NVD (Gaskell and Law, 1988)–(Leonard, 1988) approach. The fundamental mechanism common to these two models is the use of the dissipative nature of first-order differencing schemes. TVD schemes, that is, schemes which satisfy the TVD constraints, 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 type model. The NVD approach, as mentioned before, was introduced by (Gaskell and Lau, 1988) and (Leonard, 1988) for steady state flows, and extended for unsteady flows by (Leonard, 1991). By using the TVD and NVD tools, (Song et al., 2000) proposed a third-order accurate and limited scheme named WACEB. 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., 2003). As a remedy for this, they devised a high resolution scheme named CUBISTA, which is based on TVD restrictions and associated with the Courant number. This paper describes an approach to discretize the convective terms in convection dominated problems, which given encouraging results for 1D wave equation and for 2D incompressible turbulent fluid flow problem.

2. Numerical Schemes

The features of convective-dominated systems can be illustrated by the linear unsteady advection equation

$$\phi_t(x,t) + f_x(\phi(x,t)) = 0 \tag{1}$$

with initial condition $\phi(x,0) = \phi_0(x)$, where ϕ is a scalar function and $f(\phi) = a\phi$ is the flux function with constant velocity a. This is possible because Eq. (1) has only a linear convection term. Its exact solution is given by $\phi(x,t) = \phi_0(ax - t)$. The numerical solution of Eq. (1), with its initial condition, is given 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 centre is x_i. We denote the value face $\phi_{i-1/2}$ by ϕ_ℓ and $\phi_{i+1/2}$ by ϕ_f. Therefore we can write the FOU, Lax-Wendroff and third-order accurate QUICKEST (QUICK with Estimated Streaming Terms (Leonard, 1979)) scheme, respectively, as

$$\phi_f = \frac{\phi_{i+1} + \phi_i}{2} - \frac{1}{2}sgn(a)(\phi_{i+1} - \phi_i), \tag{3}$$

$$\phi_f = \phi_i + \frac{1}{2}(1-\nu)\,(\phi_{i+1} - \phi_i), \tag{4}$$

$$\begin{aligned}\phi_f = {} & \frac{1}{2}[\phi_{i+1} + \phi_i - \nu(\phi_{i+1} - \phi_i)] \\ & -\frac{(1-\nu^2)}{6}\left[\frac{\phi_{i+2} - \phi_{i+1} - \phi_i + \phi_{i-1}}{2} - sgn(\nu)\frac{\phi_{i+2} - 3\phi_{i+1} + 3\phi_i - \phi_{i-1}}{2}\right]\end{aligned} \tag{5}$$

The numerical solution of Eq. (1) using these schemes with $a = 1$ and initial condition given by

$$\phi_0(x) = \begin{cases} 1, & 0 \le x \le 0.13, \\ \sin^2(5\pi(x+0.11)), & 0.5 \le x \le 0.7 \\ \sqrt{1 - \dfrac{(x-1.2)^2}{1.12^2}}, & 1.1 \le x \le 1.31, \\ 0, & \text{otherwise,} \end{cases}$$

is plotted in Figs. 1, 2 and 3. In these figures the red line corresponds to the exact solution, while blue line the numerical solution. One can see from these figures that the solution obtained with FOU scheme is extremely dissipative in regions of corners and high gradients, e less dissipative in regions where the Courant number increases. For Lax-Wendroff scheme, one can note that it is dispersive and that it does not coincide with exact solution: it oscillates near descontinuities, and as the Courant number increases, the solution becomes less oscillatory. QUICKEST scheme is a good approximation everywhere, except in corners points where the solution is oscillatory.

The numerical solution computed by the discretization of convection term by 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 as, for example, Lax-Wendroff scheme, they always occur at the position where a steep gradient of dependent variable exists. Boundedness of a scheme may be defined as a property of the scheme in predicting no unphysical oscillations in regions of steep gradients. Boundedness is very important to keep numerical results physically reasonable. Lax-Wendroff scheme, for instance, is not TVD (see, Leveque, 1990), but as noted by Sweby (Sweby, 1984), its numerical flux in Eq. (4) can be viewed as the upwdind flux added to the antidiffusive term. From these observations, he modified the antidiffusive term in order to limit the scheme, i.e.,

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

where the limiter $\varphi_{i+1/2}$ is a function of the ratio of two consecutive gradients

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

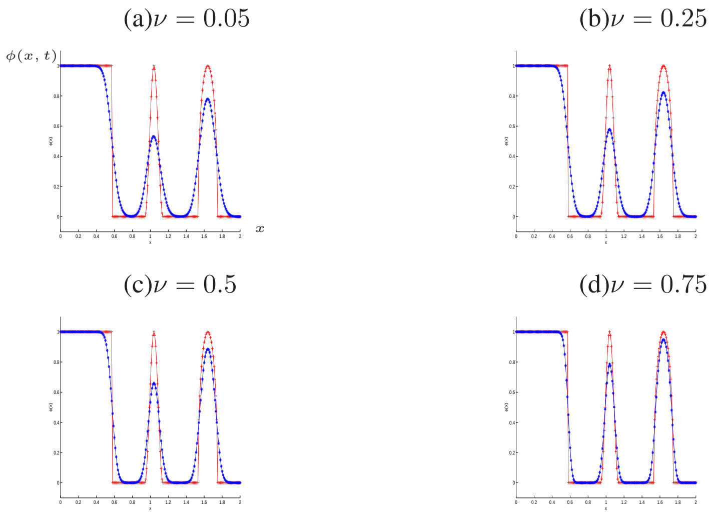

Figure 1. FOU scheme

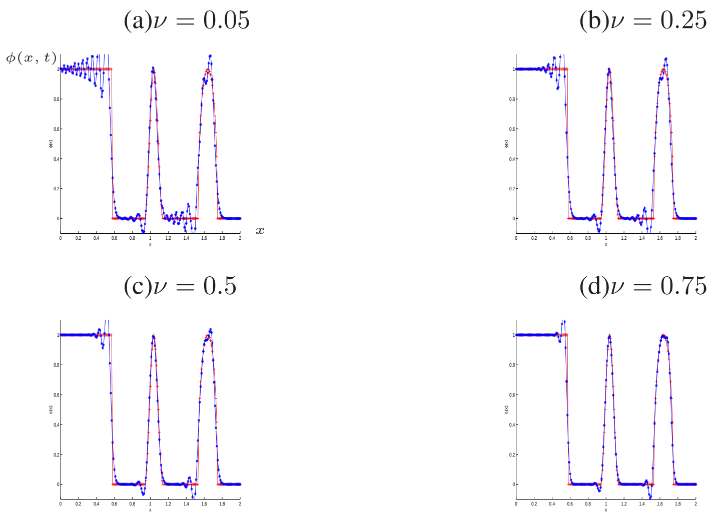

Figure 2. Lax-Wendroff scheme

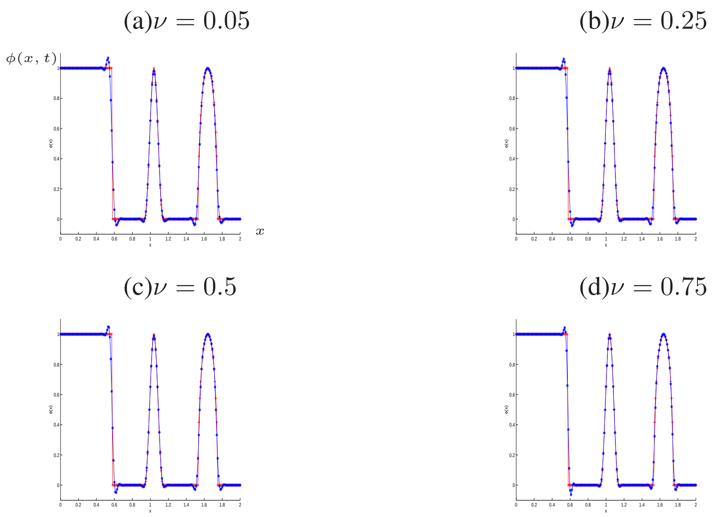

Figure 3. QUICKEST scheme

The Harten criteria (Harten, 1983) gives sufficient conditions on φ in order to the scheme (2), with numerical flux (6), to be TVD: If the function φ satisfies

$$\begin{cases} \varphi(r) = 0, & \text{if } r \leq 0 \\ 0 \leq \varphi(r) \leq \min\{2,\ 2r\}, & \text{if } r > 0, \end{cases} \tag{8}$$

then the scheme (2)–(6) is TVD, under the CFL (Courant-Friedrichs-Lewy) condition $0 \leq \nu \leq 1$, for $a > 0$. The condition (8) means that the graph of φ must lie in the shaded region of Fig. 4(a). Figure 4(b) shows the graphics of the FOU (the r-axis), the Lax-Wendroff (red line) and the Quickest (blue line) limiter (for $a > 0$). Note that the graphics are plotted out of TVD region, except the FOU scheme.

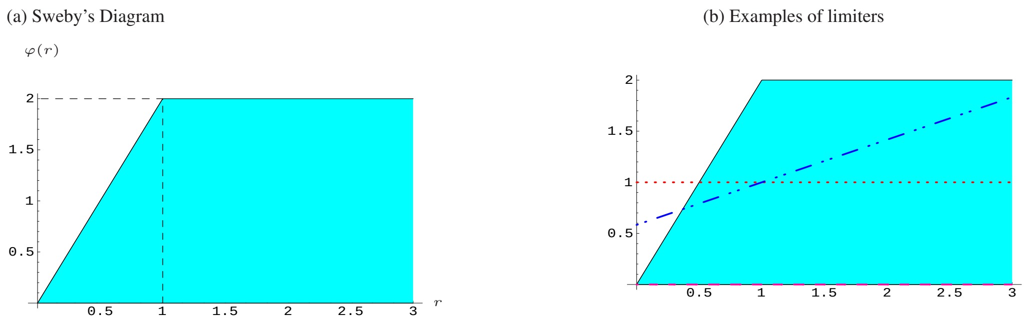

Figure 4. Limiters in TVD Region

Another usefull concept is that associated to the representation of flux function in normalized variable of (Gaskell and Lau, 1988) and (Leonard, 1988), (Leonard, 1991). A face value for ϕ_f can be determined by two nodes straddling the face and the next upstream node, which depends on the flow direction at the face f, that is, the signal of a. We represent this by the equation $\phi_f = \phi_f(\phi_D^n, \phi_U^n, \phi_R^n, \nu)$., where capital letters D, U and R indicates, respectively, the Downstream, Upstream and Remote-upstream locations. Note that the difference in the localization of these nodes depends on signal of a (see (Ferreira, 2001) for specific examples). So, in terms of original variables, variations in signal, flow direction and scale can be normalized defining the normalized variable variable as

$$\hat{\phi}(x,t) = \frac{\phi(x,t) - \phi_R^n}{\phi_D^n - \phi_R^n}, \tag{9}$$

which implies that $\hat{\phi}_R^n = 0, \quad \hat{\phi}_D^n = 1$ and $\hat{\phi}_f = \phi_f(\hat{\phi}_U^n, \nu)$.

3. Relationship between Sweby's diagram and Normalized Variables

In the context of incompressible flow, (Gaskell and Lau ,1988) proposed the CBC (Convection Boundedness Criterion) for a convection scheme to possess the boundedness character. The CBC have been accepted as both a sufficient and necessary condition for a scheme possessing boundedness until recently, when Yu et al. (Yu, 2001) indicated that the CBC is only a sufficient condition; then, they proposed another CBC, named Extended CBC (ECBC). Based on the NVD, Ping-Li et al. in (Ping-Li, 2003) revealed the weakness of CBC by numerical example. They also proposed refinements to the CBC, based on careful consideration of the smoothness of the profile in normalized variable. The CBC can only guarantee the boundedness, without any accuracy consideration, and the new CBC guarantees not only the boundedness, but also high-order accuracy. Take into account that CBC and ECBC both do not work well for general problems (see Alves, 2003), we think it is more interesting to consider TVD schemes even in the incompressible case. Because even in this case, 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 the Normalized Variables.

The equations (6) and (7) in the normalized variables can be written (see (Leonard, 1991) and (Lin, 1991)) as

$$\hat{\phi}_f = \hat{\phi}_U + \frac{1}{2}(1-\nu)\,\varphi_{i+1/2}(1 - \hat{\phi}_U). \tag{10}$$

$$r_{i+1/2} = \frac{\hat{\phi}_U}{1 - \hat{\phi}_U}. \tag{11}$$

From relations (8) and (11), the relationship between $\hat{\phi}_f$ and $\hat{\phi}_U$, which satisfies the TVD principle, can be expressed as

$$\begin{cases} \hat{\phi}_U \leq \hat{\phi}_f \leq \min\{1-\nu+\nu\hat{\phi}_U, (2-\nu)\hat{\phi}_U\}, & \text{for } 0 < \hat{\phi}_U < 1, \\ \hat{\phi}_f = \hat{\phi}_U, & \text{for } \hat{\phi}_U \leq 0 \text{ or } \hat{\phi}_U \geq 1. \end{cases} \tag{12}$$

The region determined by relations (12) is depicted in Figure 5 (a) for $\nu = 0.25$. Note that for each value of $\nu \in [0, 1]$, the TVD region associated with ν must be contained in the global TVD region (which corresponds $\nu = 0$, for steady case) ploted in Figure 5(b).

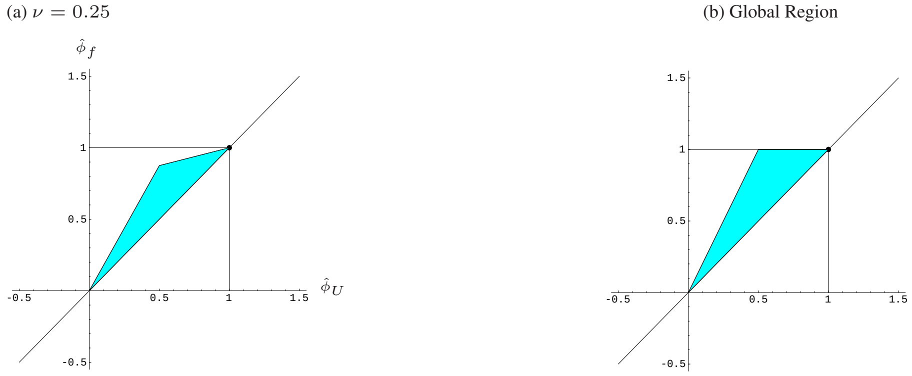

Figure 5. TVD region in Normalized Variables

4. Recent schemes

Recent schemes have a piecewise linear representation in the normalized diagram and are composed by three segments in the TVD region. The basic difference scheme is third-order, formally, accurate QUICK (Quadratic Upstream Interpolation for Convective Kinematics) scheme (Leonard, 1979), which is used in regions where the solution is smooth. For the steady case, $\hat{\phi}_f$ depends only on $\hat{\phi}_U$. The mostly recent scheme devised for steady case is the WACEB (Weighted-Average Coefficient Ensuring Boundedness) (Song et al., 2000) (see also (Lin et al., 1997)) scheme, that is a third-order accurate/limited scheme. In this method the normalized cell face is computed by

$$\hat{\phi}_f = \begin{cases} 2\hat{\phi}_U, & 0 < \hat{\phi}_U < 0.3 \\ \frac{3}{4}\hat{\phi}_U + \frac{3}{8}, & 0.3 \leq \hat{\phi}_U \leq \frac{5}{6} \\ 1, & \frac{5}{6} < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere.} \end{cases} \tag{13}$$

Figure 6(a) shows, in blue line, its characteristic curve, while red line represents the characteristic curve of QUICK scheme. For unsteady case, a recent scheme is the CUBISTA scheme presented in (Alves et al., 2003). It is obtained by considering the TVD restrictions (12). Also, it is proved that if $\nu = 0$, CUBISTA scheme reduces to the WACEB scheme. However, for some flows, this scheme still has convergence problems. So, in (Alves et al., 2003) the authors devised a scheme with a fixed $\nu = 0.25$. The results in all cases tested by (Alves et al., 2003) were convergents. This value of ν satisfies a following compromises; increasing ν in order to promove convergence and decreasing ν to improve resolution of sharp gradients. The scheme is given by Eq.(14) and its characteristic curve is depicted in Fig. 6(b) (blue line).

$$\hat{\phi}_f = \begin{cases} \frac{7}{4}\hat{\phi}_U, & 0 < \hat{\phi}_U < \frac{3}{8} \\ \frac{3}{4}\hat{\phi}_U + \frac{3}{8}, & \frac{3}{8} \leq \hat{\phi}_U \leq \frac{3}{4} \\ \frac{1}{4}\hat{\phi}_U + \frac{3}{4}, & \frac{3}{4} < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere.} \end{cases} \tag{14}$$

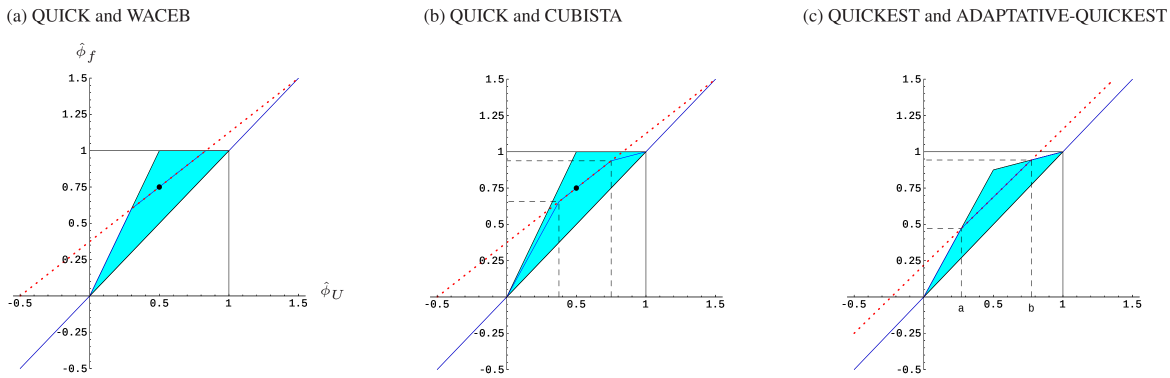

Figure 6. Characteristic line for WACEB, CUBISTA and ADAPTATIVE QUICKEST scheme on the TVD region

5. ADAPTATIVE-QUICKEST Scheme

As mentioned before CBC and ECBC do not work well for general problems (see Alves et al., 2003). So, from now on, we devised a more interesting TVD scheme, even for incompressible flows. In summary, inspired on the design of WACEB and CUBISTA schemes we suggest the following new scheme, named ADAPTATIVE-QUICKEST, by

$$\hat{\phi}_f = \begin{cases} (2-\nu)\hat{\phi}_U, & 0 < \hat{\phi}_U < a \\ \hat{\phi}_U + \frac{1}{2}(1-\nu)(1-\hat{\phi}_U) - \frac{1}{6}(1-\nu^2)(1-2\hat{\phi}_U), & a \le \hat{\phi}_U \le b \\ 1-\nu+\nu\hat{\phi}_U, & b < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere} \end{cases} \tag{15}$$

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 6(c) (blue line) shows the characteristic line for this new scheme. Here we are assuming, in general, that the numerical solution evolves up to reach the equilibrium. Note that in the ADAPTATIVE-QUICKEST, the Courant number is not fixed as in the WACEB and CUBISTA scheme.

6. Numerical Results

For the wave equation, the numerical results using the schemes given by Eq. (2) with numerical flux Eqs. (13), (14) and (15), for $\nu = 0.05,\ 0.25,\ 0.5,\ 0.75$, are displayed in Figs. 7, 8 and 9. In these figures, the red line corresponds to the exact solution, while blue line the numerical solution. Figure 7 shows the results for WACEB scheme. The numerical solution is better approximated near shock region, it is less dissipative than FOU scheme and does not present spurious oscillations except when $\nu = 0.75$. This behaviour makes sense since this scheme is constructed considering steady state problems. The numerical solution with CUBISTA is plotted in Fig. 8. One can see that the same notes of WACEB can be made for CUBISTA. By comparing the numerical solutions in region of shock for WACEB scheme with small value to ν and for CUBISTA scheme with $\nu = 0.25$, we conclude that the solution obtained with CUBISTA scheme is better, as mentioned by Alves et al. in (Alves, 2003). Figure 9 exhibits the solution derived by ADAPTATIVE-QUICKEST scheme. Note that it presents better solutions in all cases of ν. This is explained by adaptative character of the numerical scheme defined by Eq. (15).

Table 1 presents the numerical values of the reattachment point for flow over a backward-facing step. This length was estimated by using the standard $\kappa - \varepsilon$ turbulence model, updated with the VONOS, WACEB and CUBISTA schemes, in three different meshes. The experimental value for this length is ≈ 7.1 (see, for example, (Thangam, 1992)). One can see from this table that the VONOS scheme provided the worst result in all meshes; this occours because it is not a TVD scheme. On the other hand, the CUBISTA scheme provided the better results in both medium and fine meshes. And this occours because it was constructed by transient flows, while the WACEB scheme not. We are surprise with the value provided by the WACEB scheme; we believe that the coarse mesh influenced the result. For ADAPTATIVE-QUICKEST scheme we expect better value for the reattachment point.

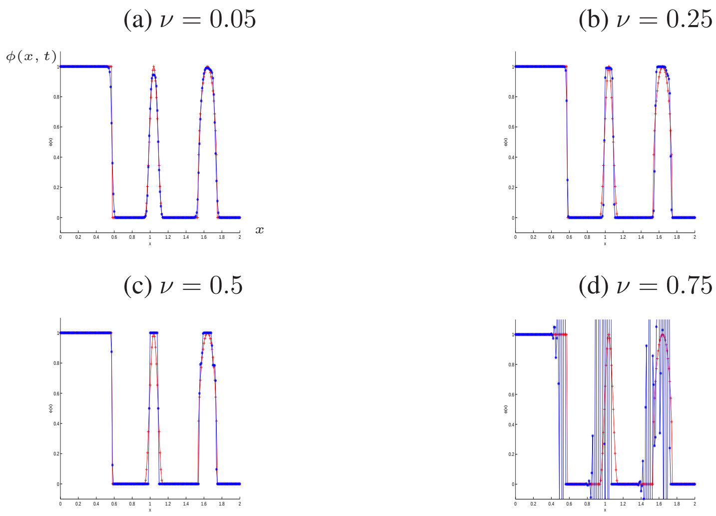

Figure 7. WACEB scheme

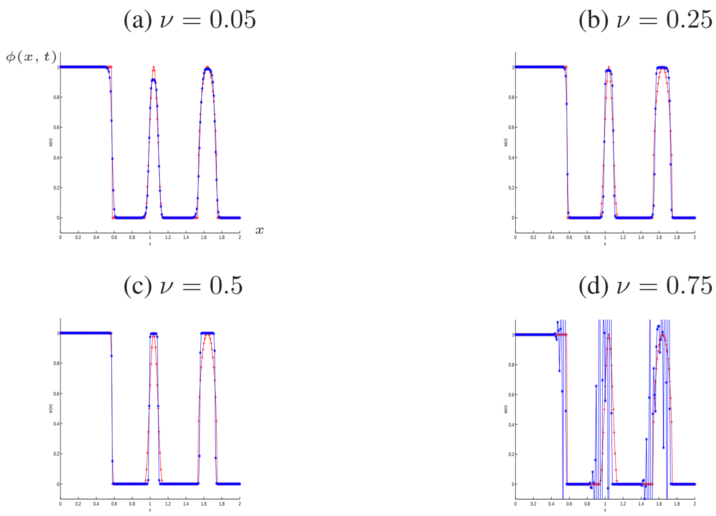

Figure 8. CUBISTA scheme

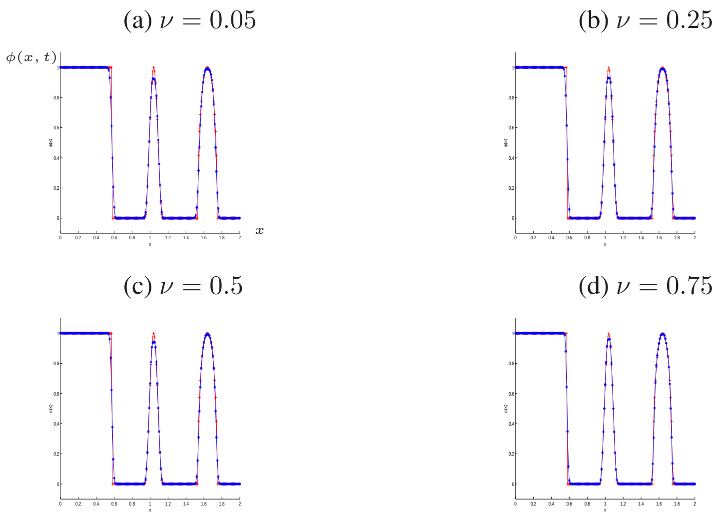

Figure 9. ADAPTATIVE-QUICKEST scheme

Table 1. Comparison among numerical results using the CUBISTA, WACEB and VONOS schemes.

mesh	CUBISTA	WACEB	VONOS
coarse	7.13	7.10	6.12
medium	6.10	6.06	5.76
fine	5.51	5.50	5.42

7. 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. The first results obtained for linear advection equation are encouraged. In the future, these techniques will be applied, by the authors, to compute efficiently and accurately time dependent numerical solution of 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.

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