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Modern Upwind Methodology for Scalar Transport

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Abstract: The goal of this article is to contribute to the development of the modern high-order boundedness adaptative QUICKEST scheme by Kaibara et al. as a new methodology for scalar transport. The scheme is based on NVD (Normalized Variable Diagram) approach by Leonard, Gaskell and Lau, and on TVD (Total Variation Diminishing) constraints by Harten, Yee and Roe. A flux limiter mechanism has been implemented in order to deal with steep gradients. After a short review of the various schemes and the associated limiters, we compare the adaptative QUICKEST scheme with several well known standard upwind schemes for solving the Euler equations of the gas dynamics and pure convection of scalar discontinuities.

***Keywords:* convection term discretization, convection boundedness criterion, bounded convection scheme, limiters, finite difference**

INTRODUCTION

During the last decades much progress has been achieved in designing bounded high order upwind approximation schemes for convection dominated problems, especially in fluid flows at high Reynolds and high Mach numbers. In these problems, numerical instabilities, shows up in the form of spurious oscillations, can be produced by step gradients which usually grow and break down the numerical algorithm. In recent years, efforts have been made to build such schemes which can give high order accuracy without introducing spurious oscillations and converge to physically correct solution. We refer interested reader to “Dorthea and Gour-Tsyh (1995)”, and reference listed therein, for an introduction to the field.

One of the major obstacles to be addressed in solving convection dominated problems is making the decision about which high order upwinding technique should be used to approximate the advection terms, in order to guarantee an accurate oscillation free solution without introducing excessive artificial dissipation. The first order upwind, for instance, is unconditionally bounded (within CFL conditions), but it can lead to large errors causing the solution grossly inaccurate. On the other hand, the scheme of “Lax and Wendroff (1960)” and the QUICK by “Leonard (1979)” can provoke spurious oscillations near discontinuities, causing numerical instabilities.

There are mainly two common ways to reduce spurious oscillations, namely: i) add an artificial viscosity; and ii) apply limiters. The disadvantage of adding artificial viscosity in model equations is that the performance is problem dependent, and the principal disadvantage of limiter approach is that the accuracy degenerates (to first order) near discontinuities. Control oscillations and, at the same time, minimize artificial dissipation by applying bounded high resolution schemes continue to be topics of importance and interest in the CFD (Computational Fluid Dynamics) community.

In this article, we will not discuss the technique of adding artificial viscosity in the equation models. We are interesting in a combination of NVD “Leonard (1988)” and TVD “Harten (1984)” approaches. The basic idea is to use a linear combination of a low order and a high order accurate scheme by using a limiter function. First, we give a short review of the NVD/TVD upwind methodologies for solving scalar transport equations. And then we present the development of the high order boundedness adaptative QUICKEST, proposed by “Kaibara et al. (2005)”, which is based on unsteady analysis of the 1D advection equation and retains the Courant (or CFL) number as a free parameter.

MATHEMATICAL FORMULATIONS

Harten’s TVD Concept

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 (1984)”. Here diminishing means non increasing. A desirable property for an approximate solution to share with the exact one is that its TV should decrease in time “Tadmor (1998)”. 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

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

where $H : \mathbb{R}^{2k+1} \to \mathbb{R}$ is a continuous function and ϕ_i^n denotes an approximation of the exact solution ϕ at the uniform grid point (x_i, t_n), being $x_i = i\Delta x$, $t_n = n\Delta t$, with Δx and Δt the spatial and the temporal grid spacing, respectively. By definition, the scheme (1) is TVD if

$$TV(\phi^{n+1}) \leq TV(\phi^n). \tag{2}$$

Before proceeding to the discussion of TVD schemes, it is essential to discuss the TVD constraints using the one dimensional scalar conservation law

$$\frac{\partial \phi}{\partial t} + a\frac{\partial \phi}{\partial t} = 0, \quad \mathrm{a} > 0. \tag{3}$$

An general explicit finite difference numerical scheme to the equation (3) is

$$\phi_i^{n+1} = \phi_i^n - C_{i-1/2}\delta_{i-1/2}\phi^n + D_{i+1/2}\delta_{i+1/2}\phi^n, \tag{4}$$

where δ is the central difference operator and $C_{i-1/2}$ and $D_{i+1/2}$ are functions of ϕ^n and, in general, the choice of these coefficients is not unique. By Harten’s lemma, the sufficient conditions to secure inequality (2) (the scheme to be TVD) are

$$C_{i+1/2} \geq 0 \quad D_{i+1/2} \geq 0 \quad \text{and} \quad \mathrm{C_{i+1/2} + D_{i+1/2}} \leq 1, \quad \text{for} \quad \text{all} \quad \text{i}. \tag{5}$$

For example, the first order upwind is a TVD scheme under de CFL condition $|a\Delta t/\Delta x| < 1$.

High Resolution Schemes and Flux Limiters

Any finite difference of the type (4) for the convective transport of a scalar property ϕ can generally be written as the sum of the first order upwind scheme and a anti diffusive flux as

$$\phi_i^{n+1} = \phi_i^n - \nu\delta_{i-1/2}\phi^n - \frac{1}{2}\nu(1-\nu)\Big[\frac{\psi(r_{i+1/2})}{r_{i+1/2}} - \psi(r_{i-1/2})\Big]\delta_{i-1/2}\phi^n, \tag{6}$$

where $\nu = a\Delta t/\Delta x$ is the Courant number (or CFL), $\psi(r)$ is the flux limiter function, taken to be nonnegative to maintain the anti diffusive flux, which dictates the order of the scheme and its boundedness properties, and the ratio of consecutive gradients

$$r_{i+1/2} = \frac{\delta_{i-1/2}\phi^n}{\delta_{i+1/2}\phi^n} \tag{7}$$

is a measure of the smoothness of the solution. High resolution schemes of the form (6) are a compromise between the classical first order upwind and high order difference schemes. The central idea of this formulation is to avoid numerical oscillations and, at the same time, to maintain the numerical diffusion as small as possible. For instance, second order accuracy can be attained by a hybridisation between Lax-Wendroff ($\psi = 1$) scheme and Beam-Warming ($\psi = r$) scheme (see “Warming and Beam” (1976)”)

$$\psi(r) = (1-\beta)\cdot 1 + \beta \cdot r, \quad 0 \leq \beta \leq 1. \tag{8}$$

It can be shown that the finite difference approximation (6), with the flux limiter given by (8), is not unconditionally bounded (TVD). Sweby showed that a TVD scheme of the form (6) can be obtained by setting the flux limiter respecting the constraints

$$\psi(r) = min(2r, 2) \quad \text{if} \quad r > 0 \quad \text{and} \quad \psi(r) = 0 \quad \text{if} \quad r \leq 0. \tag{9}$$

In order to satisfy the TVD principle (i.e., bounded) and, at the same time, to be second order, the scheme (6) must possess a flux limiter that lies within the shared area of Fig. 1. The reader is refereed to “Arora and Roe (1997)” for obtaining a discussion of how to obtain an ideal limiter.

A number of flux limiters have been developed over the years, being that the must well known are *Minmod*

$$\varphi(r) = min\{r, 1\}$$

and *Superbee*

$$\varphi(r) = max\{0, min\{1, 2r\}, min\{0, 2\}\}$$

by “Roe (1985)”, and

$$\varphi(r) = \frac{r + |r|}{1 + |r|}$$

by ”Van Leer (1974)”.

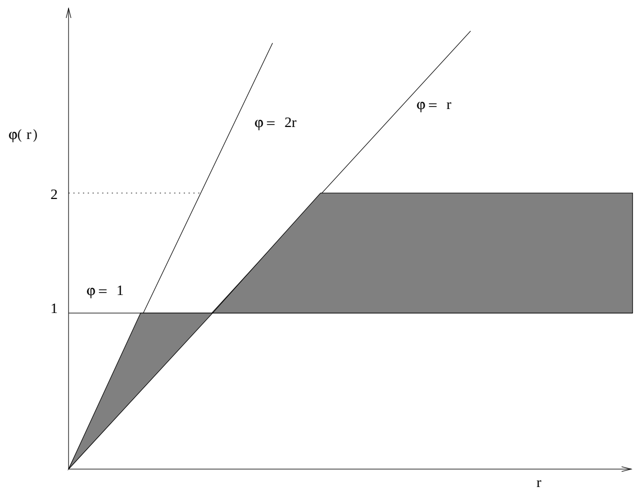

Figure 1 – Second order TVD region.

NV Formulation and CB Criterion

The variation of a convected variable ϕ in a computational cell can be represented by a function linking the values ϕ_D, ϕ_U and ϕ_R, which represent, according to the convective velocity direction on a given f face of this computational cell, the Downstream, Upstream and Remote-upstream neighbouring nodes, respectively (see Fig. 2). If the functional relationship F involving these nodes is prescribed, then the facial value that is required at the f face of a computational cell can be determined. In order to construct a high order bounded convection scheme that preserves monotonicity, “Leonard (1988)”

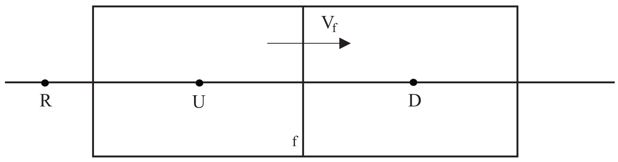

Figure 2 – Neighboring nodes D,U and R of the f face.

and “Leonard (1991)” introduced the Normalized Variable Formulation (NVF), while “Gaskell and Lau (1988)” proposed the Convection Boundedness Criterion (CBC). The NVF and CBC constitute the basis on which high-order oscillation-free convection schemes are constructed. From now on, we shall give a brief description of these two concepts.

Considering the f face of a computational cell (see Fig. 2), the normalized variable (NV) of Leonard (see “Leonard (1988)”) $\hat{\phi}$ is defined as

$$\hat{\phi}_f = \frac{\phi_f - \phi_R}{\phi_D - \phi_R}. \tag{10}$$

The advantage of this transformation is that a face value $\hat{\phi}_f$ depends on $\hat{\phi}_U$ only, because $\hat{\phi}_D = 1$ and $\hat{\phi}_R = 0$. If at most three neighbouring nodal values are used to approximate point values, such as those appearing in Eq. (10), then a necessary and sufficient condition for guaranting a bounded solution is the CBC. It can be formulated as

$$\hat{\phi}_f = \begin{cases} F(\hat{\phi}_U) \quad \text{Continuous} \\ F(\hat{\phi}_U) = 1 \quad \text{if} \quad \hat{\phi}_{\mathrm{U}} = 1 \\ \hat{\phi}_U < F(\hat{\phi}_U) < 1 \quad \text{if} \quad 0 < \hat{\phi}_{\mathrm{U}} < 1 \\ F(\hat{\phi}_U) = 0, \quad \text{if} \quad \hat{\phi}_{\mathrm{U}} = 0 \\ F(\hat{\phi}_U) = \hat{\phi}_U \quad \text{if} \quad \hat{\phi}_{\mathrm{U}} < 0 \quad \text{or} \quad \hat{\phi}_{\mathrm{U}} > 1 \end{cases} \tag{11}$$

The CBC is illustrated in Fig. 3, where the line $\widehat{\phi_F} = \widehat{\phi_U}$ and the shaded area form the region over which it is valid.

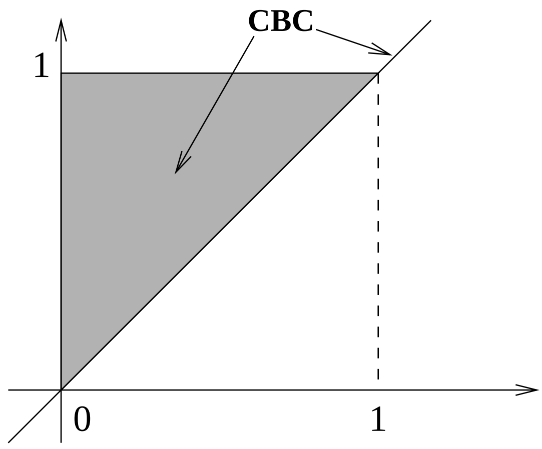

Figure 3 – CBC region in the $\widehat{\phi}_f - \widehat{\phi}_U$ plane.

TVD Principle in NVF

The relationships between TVD and CBC is what follows. First, note that the ratio of consecutive gradients

$$\frac{\phi_U - \phi_R}{\phi_D - \phi_R}$$

can be written in NV as

$$r_f = \frac{\hat{\phi}_U}{1 - \hat{\phi}_U}. \tag{12}$$

By using this relation and the TVD restrictions (9), the functional relationship between $\hat{\phi}_f$ and $\hat{\phi}_U$, that is $\hat{\phi}_f = F(\hat{\phi}_U)$, can be expressed as

$$\hat{\phi}_f = \begin{cases} \leq 1, \quad \leq 2\hat{\phi}_U \\ \geq \hat{\phi}_U \quad \text{if} \quad 0 < \hat{\phi}_{\text{U}} < 1 \\ = \hat{\phi}_U \quad \text{if} \quad \hat{\phi}_{\text{U}} \leq 0 \quad \text{or} \quad \hat{\phi}_{\text{U}} \geq 1 \end{cases} \tag{13}$$

In summary, in order to satisfy the TVD restrictions the value $\hat{\phi}_f$ must lie within the dashed line area in the monotonic region $0 < \hat{\phi}_U < 1$ and on the line $\hat{\phi}_f = \hat{\phi}_U$ outside the monotonic region (see Fig. 4).

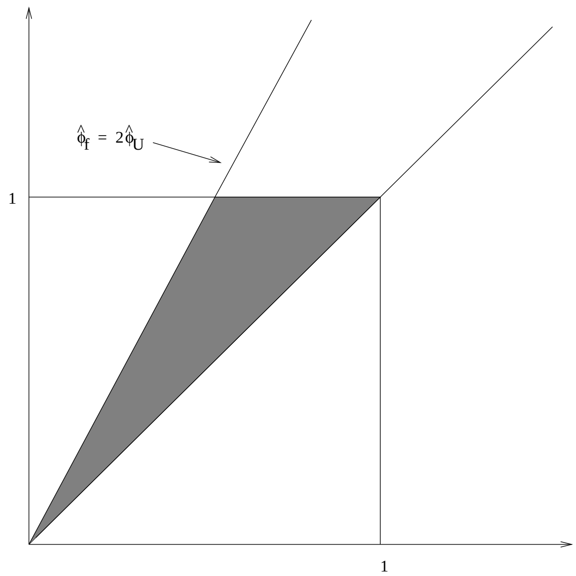

Figure 4 – TVD region in normalized variable

Adaptative QUICKEST Scheme

The discretization of the advective terms is performed by using the adaptative QUICKEST, a bounded high order upwind scheme proposed by "Kaibara et al. (2005)". This scheme was derived in the context of the NVF and by enforcing the TVD property. Consequently, it satisfies CBC. The main idea in the derivation of this scheme was to combine accuracy and monotonicity, while ensuring flexibility. It is based on unsteady analysis of the 1D advection equation and retains the Courant number as a free parameter. It can also ensure that total variation of the variables does not increase with time; thus no spurious numerical oscillations (maxima or minima) are generated. The numerical solution can be second or third order accurate in the smooth parts of the solution, but only first order near regions with large gradients. In summary, this advection scheme is implemented by the functional relationship

$$\hat{\phi}_f = \begin{cases} (2-\theta)\hat{\phi}_U, & 0 < \hat{\phi}_U < a \\ \hat{\phi}_U + \frac{1}{2}(1-|\theta|)(1-\hat{\phi}_U) - \frac{1}{6}(1-\theta^2)(1-2\hat{\phi}_U), & a \leq \hat{\phi}_U \leq b \\ 1-\theta+\theta\hat{\phi}_U, & b < \hat{\phi}_U < 1 \\ \hat{\phi}_U, & \text{elsewhere} \end{cases} \tag{14}$$

where θ=$V_f \cdot \Delta t/\Delta x$ is the local Courant number, V_f being a convective velocity, and the constants a and b are as follows

$$a = \frac{2-3|\theta|+\theta^2}{7-6\theta-3|\theta|+2\theta^2} \quad \text{and} \quad b = \frac{-4+6\theta-3|\theta|+\theta^2}{-5+6\theta-3|\theta|+2\theta^2}.$$

Figure 5 shows the adaptative QUICKEST scheme in the normalized variable diagram ($\hat{\phi}_U - \hat{\phi}_f$ plane).

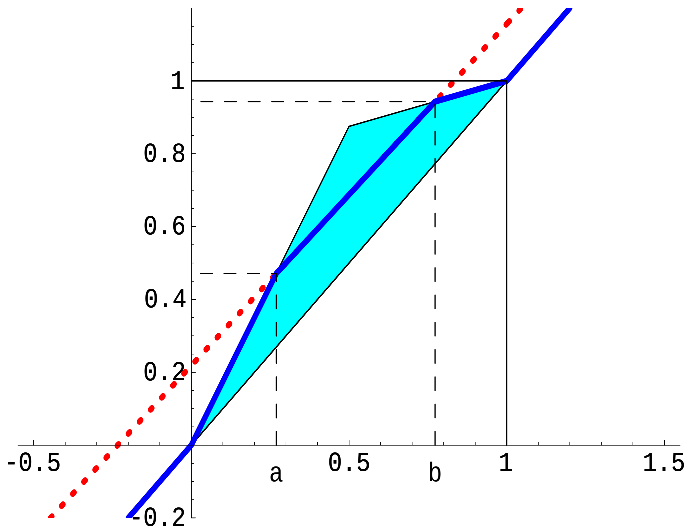

Figure 5 – Graphics in the normalized variable of $\hat{\phi}_f$ for QUICKEST (red) and adaptive QUICKEST with $\theta = 0.5$ (full) blue.

NUMERICAL TESTS

In this section, we compare numerical results of the adaptative QUICKEST scheme with those of the conventional Minmod, Superbee and Vanleer schemes. First, we assess the performance of the scheme for the 1D Euler equations, and then we simulate the convection of a step profile in a square domain.

Sod Tube problem

The 1D Euler equations of gas dynamics (see "Sod (1978)") are given by

$$\frac{\partial}{\partial t}\mathbf{U} + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{U}) = 0, \tag{15}$$

where $\mathbf{U} = (\rho, \rho v, E)^T$, $\mathbf{F}(\mathbf{U}) = (\rho v, \rho v^2 + p, v(E+p))^T$, and ρ, v, ρv, E, p are density, velocity, momentum, total energy and pressure, respectively. In order to solve the equation (15), the ideal gas equation of state $p = (\gamma - 1)(E - \frac{1}{2}\rho v^2)$, with

$\gamma = 1.4$, and initial conditions are required. In this case, the following initial conditions are used:

$$(\rho, v, p)^T = \begin{cases} (1,0,1)^T, & x < 0.5 \\ (0.125,0,0.1)^T, & x \geq 0.5. \end{cases}$$

Figures 6, 7, 8 and 9 depict, respectively, the graphical results obtained for Minmod, Superbee, Vanleer and adaptative QUICKEST schemes on mesh of 200 computational cells and at the output time $t = 0.245$s. In all figures the continuous line (blue) corresponds to the reference solution (obtained by applying the first order upwind scheme on a fine mesh of 1000 cells) and symbols (red) corresponds to the numerical solution. We see from Fig. 9 that the adaptative QUICKEST scheme suppresses the oscillations and give good resolution at corners, in the same way as Minmod, Superbee and Van Leer ones.

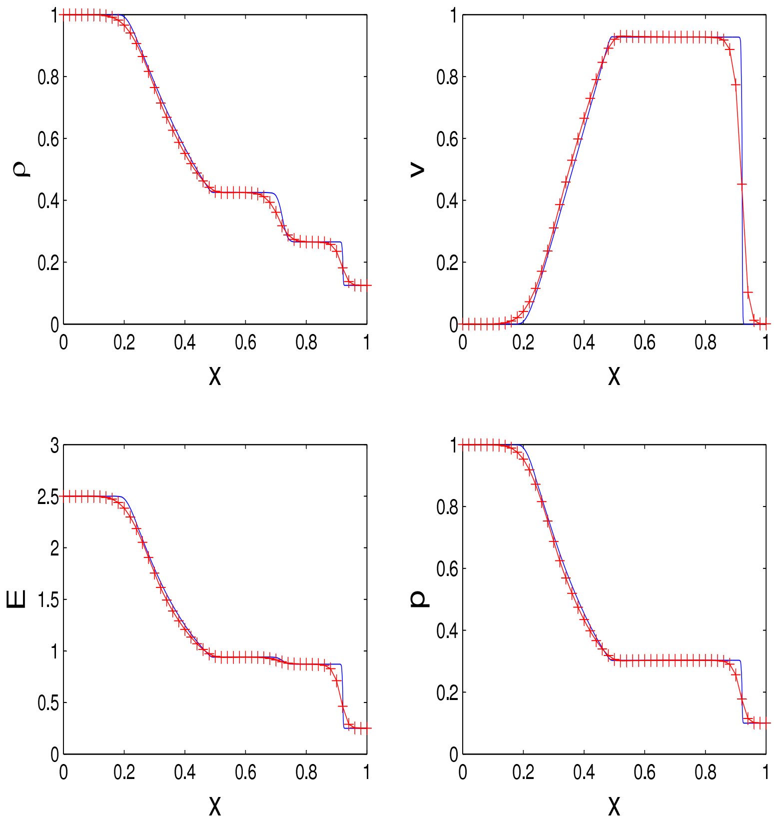

Figure 6 – Computed (red symbol) and reference (blue line) solutions for the Euler equation using the Minmod scheme.

Convection of Species

From now on, we consider the oblique convection of species across a square domain with initial distribution equal to zero along the bottom and one along the left side. A constant velocity on diagonal direction is prescribed everywhere. The MFIX (Multiphase Flow with Interphase eXchanges) code (see "Syamlal et al. (1993)"), adaptated with the adaptative QUICKEST scheme (the Minmod, Superbee, and Van Leer are default methods in MFIX), was run on this problem until the simulation time of 7.0s, by which the steady state is reached. The calculations with the adaptative QUICKEST were performed by using Courant number equal to 0.75 and zero. A uniform mesh of 8100 computational cells is used, and, initially, species mass fraction is set to zero everywhere into the domain. The exact solution for this problem is zero on the lower triangular region and one on the upper one. Figure 10 shows that the adaptative QUICKEST scheme with Courant number 0.75 is more diffusive when compare with other schemes. However, in case of Courant number equal to zero it compare favorably to the other schemes, eventhough the Superbee to be the best.

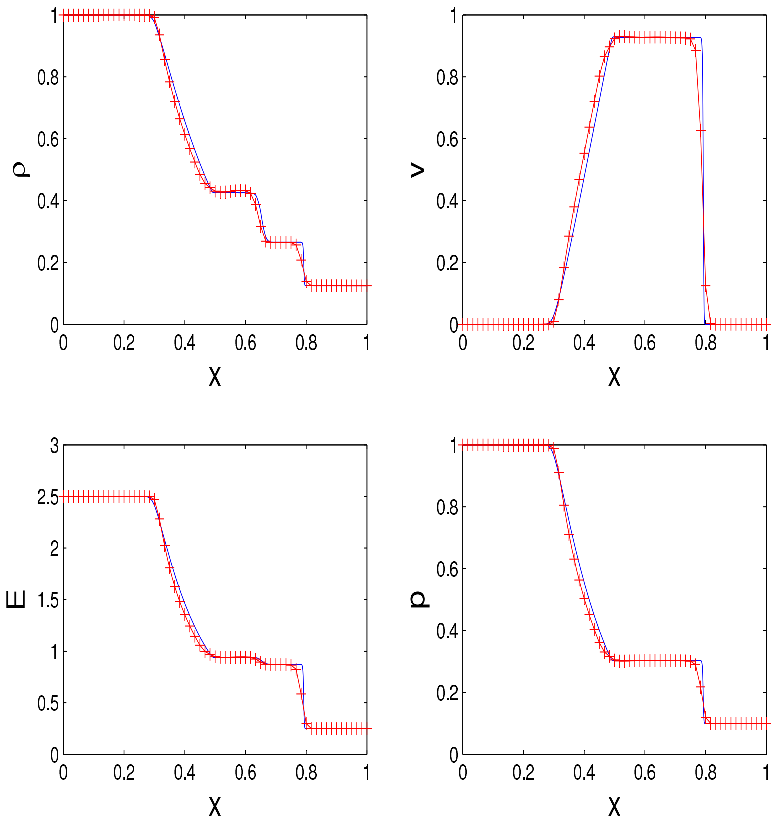

Figure 7 – Computed (red symbol) and reference (blue line) solutions for the Euler equation using the Superbee scheme.

CONCLUSIONS

The main objective of the present study was to contribute for development of the modern high-order boundedness adaptative QUICKEST scheme as a new methodology for scalar transport. The numerical results of the adaptative QUICKEST scheme, for Euler equations and convection of species, show to be in accordance with those obtained with well known schemes (Minmod, Superbee and Vanleer). A important advantage of the adaptative QUICKEST scheme is the choice of the Courant number, and this is a way of improving the numerical results.

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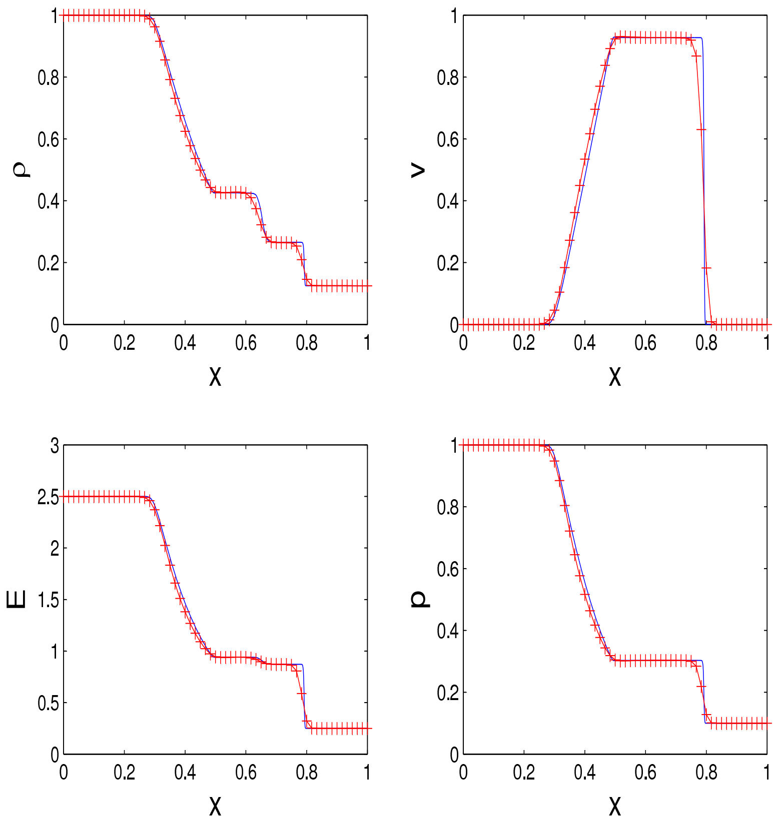

Figure 8 – Computed (red symbol) and reference (blue line) solutions for the Euler equation using the Van Leer scheme.

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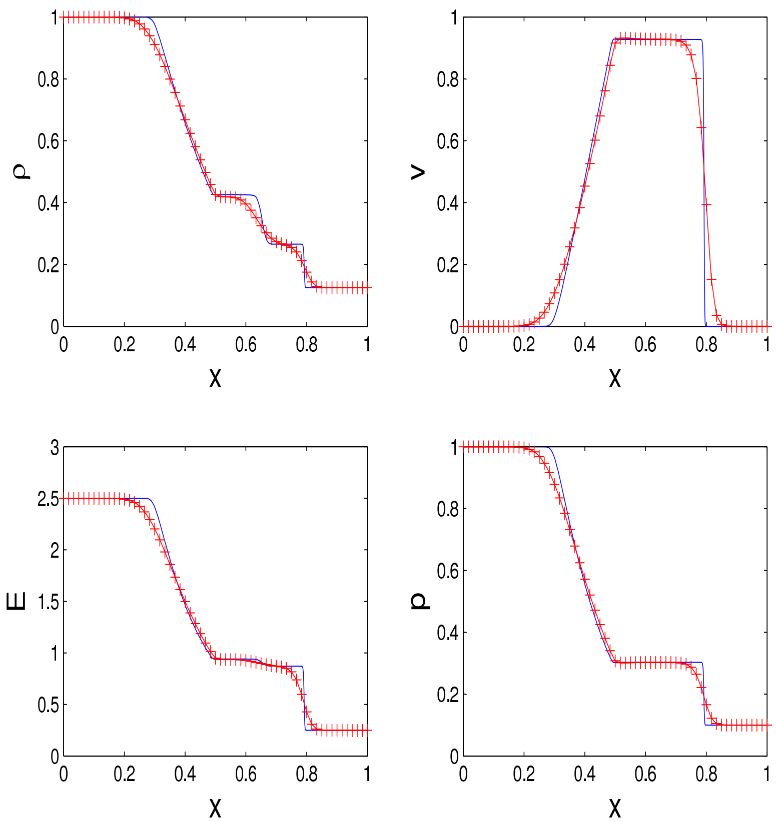

Figure 9 – Computed (red symbol) and reference (blue line) solutions for the Euler equation using the adaptative QUICKEST with CFL 0.34.

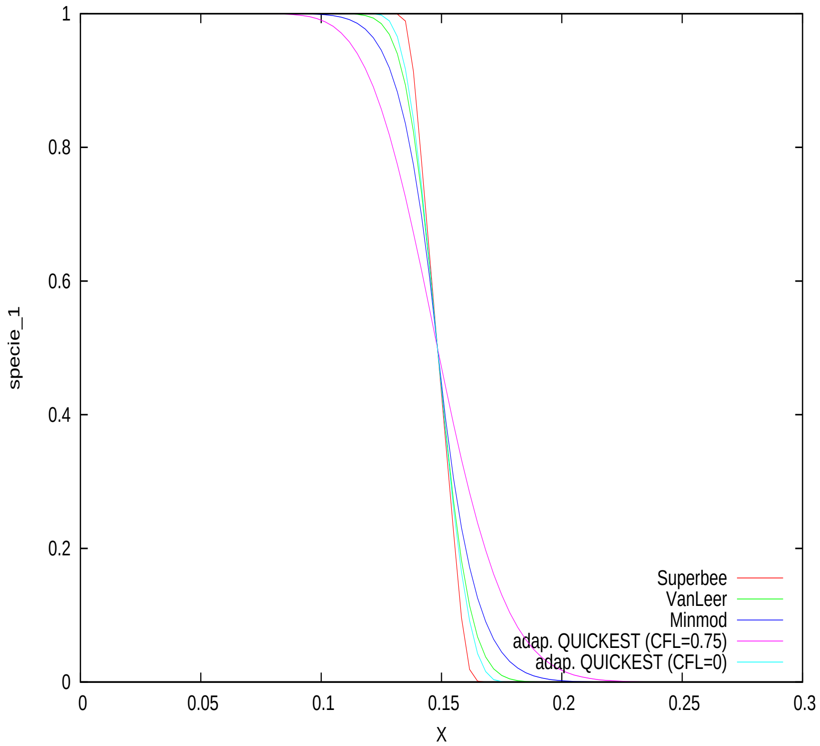

Figure 10 – Step profile calculed by various schemes.