A NUMERICAL STUDY OF SOME RECENTLY INTRODUCED TVD UPWINDING SCHEMES WITH APPLICATIONS IN FLUID DYNAMICS PROBLEMS

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Abstract. *An important issue in computational fluid dynamics is the appropriate approximation of the convection phenomena. For this, the TVD schemes are alternatives to the ENO/WENO techniques due to the robustness, low cost and simplicity of implementation. Within this scenario, the aim of this our work is to present a numerical study of some recently introduced polynomial TVD upwinding schemes - namely TOPUS and SDPUS-*C^1 *with applications in fluid dynamics problems. By using these new upwind schemes, numerical results for nonconvex nonlinear problem, 1D Euler equations, 2D advection of scalars and 2D MHD equations are presented. Comparison with the well recognized CFL-dependent ARORA-ROE and ADBQUICKEST schemes and the conventional SUPERBEE and MC schemes are assessed. The TOPUS and SDPUS-*C^1 *upwind schemes are developed in the context of normalized variables (NV) of Leonard and satisfy TVD constraints of Harten.*
Keywords: *high-resolution schemes, upwinding, conservation laws*

1. INTRODUCTION

To modelate convective terms in the field of computational fluid dynamics (CFD) it can be used, among others, different techniques namely: central schemes (CS), enhanced non-oscillatory - ENO (and his related Weighted ENO-WENO) and the total variation diminishing (TVD) upwind schemes. The CS can be a simple choice to obtain good numerical results but can develop spurious oscillations. With the ENO/WENO scheme (see Harten *et al.* (1987) and Liu *et al.* (1994)), it can be obtained excellent results in accuracy and approximation but the performance on 3D grid is relatively poor. The TVD upwind schemes are good alternatives to modelate problems with discontinuous solutions and shocks. The goal of this paper is to present a study of accuracy of two recently introduced TVD upwind schemes namely: Third-Order Polynomial Upwind Scheme (TOPUS) and Six-Degree Upwind Polynomial Scheme of C^1 class (SDPUS-C^1). In addition, a comparison of the results with other high-resolution TVD upwind schemes is assessed.

2. THE UPWIND APPROACH

For the sake of simplicity, we consider the 1D model for advection of a scalar

$$\phi_t + a\phi_x = 0, \quad a = \text{const.} > 0, \tag{1}$$

$$\phi(x,0) = \phi_0(x), \quad x \in \mathbb{R},$$

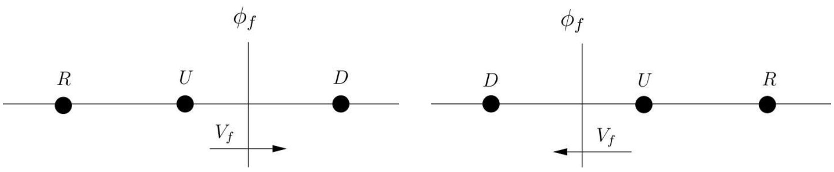
with the analytical solution given by $\phi(x) = \phi(x - at)$. The numerical approximation for (1) using the conservative finite difference methodology is

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

where ϕ_i^n is the numerical solution at mesh point $(i\delta x, n\delta t)$; δx and δt are the space and time increments, respectively. $\theta = a\delta t/\delta x$ is the Courant-Friedrichs-Lewy (CFL) number. The quantities $\phi_{i+1/2}^n$ and $\phi_{i-1/2}^n$ are the numerical flux functions, which depend on three selected neighboring mesh points, namely D (Downstream), U (Upstream) and R (Remote-upstream). These numerical fluxes are determined according to the convective velocity V_f at the faces $i + 1/2$ or $i - 1/2$, as shown in Fig.1.

In this way, the variable ϕ is transformed into the NV of Leonard (1988) by $\hat{\phi}_{()} = \frac{\phi_{()} - \phi_R}{\phi_D - \phi_R}$. The advantage of this formulation is that the interface value $\hat{\phi}_f$ depends on $\hat{\phi}_U$ only, since $\hat{\phi}_D = 1$ and $\hat{\phi}_R = 0$. In this context, it is possible to derive a nonlinear monotonic NV scheme by imposing the following conditions for $0 \le \hat{\phi}_U \le 1$: $\hat{\phi}_f(0) = 0$ (a necessary condition), $\hat{\phi}_f(1) = 1$ (a necessary condition), $\hat{\phi}_f(0.5) = 0.75$ (a necessary and sufficient condition to reach second order of accuracy) and $\hat{\phi}'_f(0.5) = 0.75$ (a necessary and sufficient condition to reach third order of accuracy).

Leonard also recommends that for values of $\hat{\phi}_U < 0$ or $\hat{\phi}_U > 1$, the scheme must be extended using the FOU (First Order Upwinding) scheme, which is defined by $\hat{\phi}_f = \hat{\phi}_U$. It is possible to rewrite the scheme in NV in the flux limiter form from the relationship $\hat{\phi}_f = \hat{\phi}_U + \frac{1}{2}\psi(r_f)(1 - \hat{\phi}_U)$, where $\psi_f = \psi(r_f)$ is the flux limiter function and r_f is the reason of two consecutive gradients (a sensor), given by $r_f = \frac{1}{1-\hat{\phi}_U}$. As explained in Hirsch (2007), the concept of flux limiter is based on a control of non-monotone schemes keeping the gradients within the proper bounds. Therefore it is controlled the formation of under and overshoots on discontinuities and shocks.



(a) $V_f > 0$ (b) $V_f < 0$

Figure 1. Position of computational nodes D, U and R according to the sign of V_f speed of a convective variable ϕ_f

The upwind schemes used in this works satisfy the TVD constraint of Harten (1983) and the convection boundedness criterion (CBC) of Gaskell and Lau (1988). The TVD concept ensures that spurious oscillations (unphysical noises) are removed from the numerical solution. Consider a sequence of discrete approximations $\phi(t) = \phi_i(t)_{i\in\mathbb{Z}}$ for a scalar quantity. The total variation (TV) at time t of this sequence is defined by $TV(\phi(t)) = \sum_{i\in\mathbb{Z}} |\phi_{i+1}(t) - \phi_i(t)|$. From this definition, the scheme is TVD if, for all data set ϕ^n, the values ϕ^{n+1} calculated by numerical method satisfy

$$TV(\phi^{n+1}) \leq TV(\phi^n), \quad \forall n. \tag{3}$$

The CBC establishes that a monotone scheme is limited if the scheme expressed in NV satisfies

$$\hat{\phi}_U \leq \hat{\phi}_f(\hat{\phi}_U) \leq 1, \qquad \text{if } \hat{\phi}_U \in [0,1], \tag{4}$$

$$\hat{\phi}_f = \hat{\phi}_f(\hat{\phi}_U) = \hat{\phi}_U, \qquad \text{if } \hat{\phi}_U \notin [0,1], \tag{5}$$

$$\hat{\phi}_f(0) = 0 \quad \text{and} \quad \hat{\phi}_f(1) = 1. \tag{6}$$

3. THE UPWIND SCHEMES

It is briefly described the high-resolution upwind schemes used in this work in terms of flux limiter.

ADBQUICKEST, by Ferreira *et al.* (2009):

$$\psi(r_f) = \max\left\{0,\ \min\left[2r_f, \frac{2+\theta^2-3|\theta|+(1-\theta^2)r_f}{3-3|\theta|}, 2\right]\right\}; \tag{7}$$

ARORA-ROE, by Arora and Roe (1997):

$$\psi(r_f) = \max\{0, \min[2r_f, \alpha(r_f-1)+1], 2\}, \quad \alpha = \frac{2-\theta}{3}; \tag{8}$$

MC, by van Leer (1977):

$$\psi(r_f) = \max\{0, \min(2r_f, 0.5(1+r_f), 2)\}; \tag{9}$$

SDPUS-C^1, by Lima *et al.* (2010):

$$\psi(r_f) = \max\left\{0,\ \frac{0.5(|r_f|+r_f)[(-8+2\alpha)r_f^3+(40-4\alpha)r_f^2+2\alpha r_f]}{(1+|r_f|)^5}\right\}, \quad \alpha = 12; \tag{10}$$

SUPERBEE, by Roe (1986):

$$\psi(r_f) = \max\{0, [\min(r_f, 2), \min(2r_f, 1)]\}; \tag{11}$$

TOPUS, by Queiroz and Ferreira (2010):

$$\psi(r_f) = \max\left\{0, \frac{0.5(|r_f|+r_f)[(-0.5\alpha+1)r_f^2+(\alpha+4)r_f+(-0.5\alpha+3)]}{(1+|r_f|^3)}\right\}, \quad \alpha = 2. \tag{12}$$

4. ERROR AND CONVERGENCE ORDER

With the aim of analyzing the errors in L_1 norm, the following definition is used

$$||E_{\delta x}||_1 = ||\Phi - \phi||_1 = \sum_{j=0}^{N} |\Phi_j^n - \phi_j^n|\delta x, \tag{13}$$

where ϕ and Φ are the numerical and reference and/or analytical solutions respectively. N is the total number of mesh points.

In the 2D case, the L_1 norm error is defined by

$$||E_{\delta x}||_1 = \sum_{i,j}^{N} |\Phi_{ij}^n - \phi_{ij}^n|\delta x^2. \tag{14}$$

The observed order of convergence p is calculated by

$$p \approx \frac{\log(||E_{\delta x}||_1/||E_{\delta x/2}||_1)}{\log 2}. \tag{15}$$

5. NUMERICAL RESULTS

This section shows the numerical results for some 1D and 2D hyperbolic conservation laws of fluid dynamics. Firstly, it is computed the solutions for 1D nonlinear nonconvex scalar Buckley-Leverett and the Woodward-Colella blast waves problems. Then, it is solved a 2D scalar advection problem and the 2D Orszag-Tang MHD turbulence problem. For 1D problems and 2D advection of scalars, it is used $\theta = 0.5$. For the MHD problem it is considered $\theta = 0.75$. The numerical solutions for Buckley-Leverett and 2D linear advection problems are computed using an in-house computer program with a third order Runge-Kutta for marching time (Gottlieb and Chi-Wang-Shu, 1998). For 1D Euler and 2D MHD equations the numerical solutions are computed using the `CLAWPACK` code of Leveque (1999).

A 1D hyperbolic conservation law (HLC) is defined by

$$\phi_t + F(\phi)_x = 0, \tag{16}$$

where jacobian $F'(\phi)$ has real eigenvalues and a set of linearly independent eigenvectors. ϕ is the conservated variable and $F(\phi)$ is the flux of conservated variables.

In the 2D case, a HLC is

$$\phi_t + F(\phi)_x + G(\phi)_y = 0, \tag{17}$$

where the jacobians $F'(\phi)$ and $G'(\phi)$ have the same properties as in the 1D case. $F(\phi)_x$ and $G(\phi)_y$ are the fluxes of conservated variables on x and y respectively

5.1 The Buckley-Leverett equation

It is presented the numerical solution of the nonlinear nonconvex Buckley-Leverett equation where

$$\phi = u \qquad \text{and} \qquad F(\phi) = \frac{u^2}{4u^2 + (1-u)^2}. \tag{18}$$

This equation is used to model a two phase fluid flow in a porous media (see LeVeque (1992)). The initial condition is defined by

$$u = \begin{cases} 1, & 0.5 \le x \le 0, \\ 0, & \text{otherwise.} \end{cases} \tag{19}$$

The numerical solutions are computed with $N = 160$ and at final time $t = 0.4$. The reference solution is computed by using 1600 computational cells with the MC upwind scheme.

It can be concluded from Fig.2 that all schemes present, in general, good results, with TOPUS scheme presenting the best results near shocks. The CFL-dependent ADBQUICKEST and ARORA-ROE schemes show a small dissipative character near the shocks. The SUPERBEE scheme presents the best approximation on smooth regions.

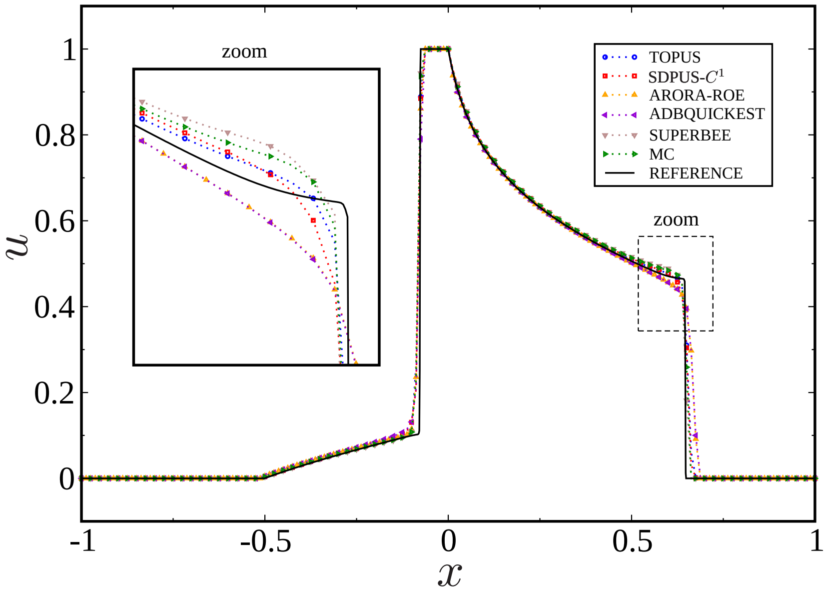


Figure 2. The Buckley-Leverett equation. $N = 160$, $\theta = 0.5$ at $t = 0.4$

5.2 The 1D Euler equations

The Woodward-Colella interacting blast waves problem for the Euler equations (see Woodward and Colella (1984); Kamm *et al.* (2008)) has been designed, among other things, for checking the capabilities of the upwind schemes. The Euler equations are given by using

$$\phi = (\rho, \rho u, \rho E)^T \qquad \text{and} \qquad F(\phi) = (\rho u, \rho u^2 + p, (\rho E + p)u)^T, \tag{20}$$

where ρ is the mass density, u is the velocity, p is the pressure, $E = e + u^2/2$ and e is the internal energy. The ideal gas law is $p = (\gamma - 1)\rho e$, where $\gamma = 7/5$ is the ratio of specific heats. Reflecting boundary conditions are implemented. The initial condition is defined by

$$(\rho, u, p)^T = \begin{cases} (1, 0, 1000)^T, & 0 < x < 0.1, \\ (1, 0, 0.01)^T, & 0.1 < x < 0.9, \\ (1, 0, 100)^T, & 0.9 < x < 1. \end{cases} \tag{21}$$

The reference solution, using the Godunov method with a correction term associated with the MC flux limiter, is calculated with a mesh size of $N = 6400$ computational cells. Table 1 depicts the errors and the observed order for the upwind schemes, where it can be seen that in this nonlinear problem all schemes provided practically the same order of convergence.

Table 1. L_1 errors and convergence rates for the Woodward-Colella interacting blast waves problem

	TOPUS		SDPUS-C^1		ARORA-ROE		ADBQUICKEST		SUPERBEE		MC	
N	L_1	p	L_1	p	L_1	p	L_1	p	L_1	p	L_1	p
200	$3.36E-01$	$--$	$3.04E-01$	$--$	$2.79E-01$	$--$	$2.86E-01$	$--$	$1.91E-01$	$--$	$2.86E-01$	$--$
400	$1.78E-01$	0.92	$1.54E-01$	0.98	$1.37E-01$	1.03	$1.40E-01$	1.03	$6.41E-02$	1.58	$1.40E-01$	1.03
800	$8.26E-02$	1.11	$6.80E-02$	1.18	$6.00E-02$	1.19	$6.13E-02$	1.19	$1.66E-02$	1.95	$6.13E-02$	1.19
1600	$3.18E-02$	1.38	$2.41E-02$	1.50	$1.99E-02$	1.59	$2.04E-02$	1.59	$1.14E-02$	1.53	$2.04E-02$	1.59

Figure 3 details the numerical results for density as function of position. The peaks are developed at $x \approx 0.65$ (the first one) and $x \approx 0.745$ (the second one). From this figure, it is concluded that SUPERBEE scheme present the best approximation on the first peak. And the other schemes can be ranked on this peak as: ARORA-ROE, ADBQUICKEST, MC and SDPUS-C^1. The same conclusion is reached for the second peak. On the contact discontinuity at $x \approx 0.59$ the SUPERBEE scheme shown to be the best, while the other schemes are dissipative.

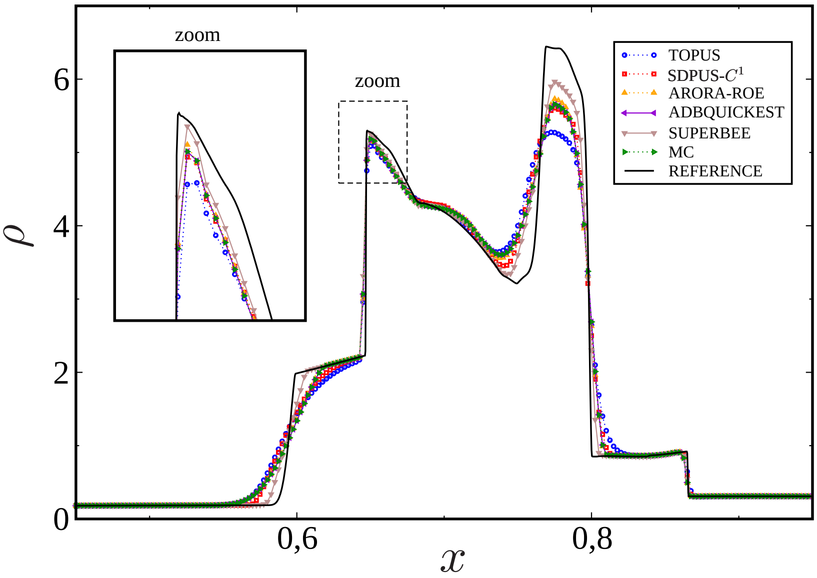


Figure 3. The Woodward-Colella interacting blast waves problem. The density at $t = 0.038$ for the $N = 400$, $\theta = 0.5$

5.3 The 2D linear advection equation

The 2D advection of scalars is defined using

$$\phi = u, \qquad F(\phi) = au \qquad \text{and} \qquad G(\phi) = bu, \tag{22}$$

where $a = b = 1$. The initial conditions is

$$u(x, y, 0) = \sin 2\pi x \sin 2\pi y, \qquad (x, y) \in (0, 1) \times (0, 1), \tag{23}$$

with periodic boundary conditions. The exact solution is given by

$$u(x, y, t) = \sin 2\pi(x - t) \sin 2\pi(y - t). \tag{24}$$

In this problem, a final time $t = 2.0$ and the meshes $N = 200, 400, 800, 1600$ are used.

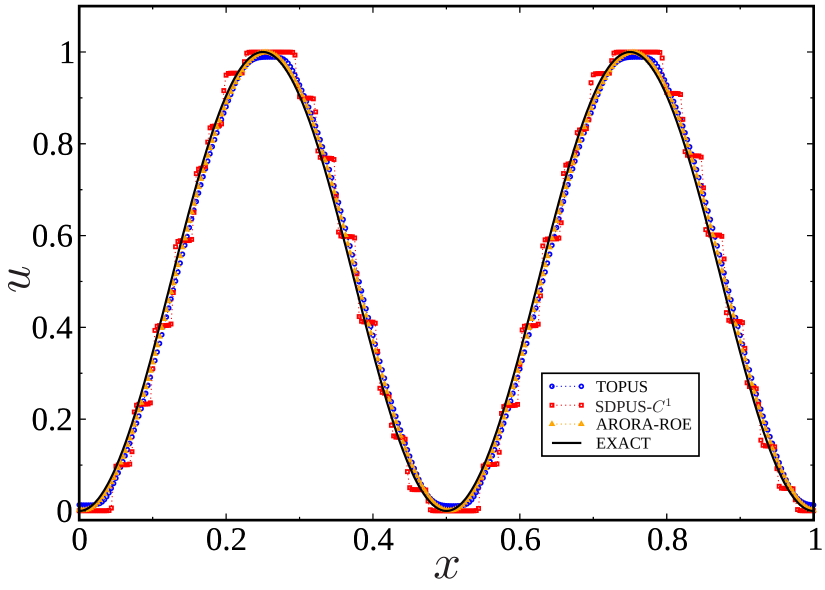
Table 2. L_1 errors and convergence rates for 2D linear advection equation

	TOPUS		SDPUS-C^1		ARORA-ROE		ADBQUICKEST		SUPERBEE		MC	
$N \times N$	L_1	p	L_1	p	L_1	p	L_1	p	L_1	p	L_1	p
20×20	$2.88E-02$	$--$	$1.73E-02$	$--$	$2.39E-02$	$--$	$2.45E-02$	$--$	$2.82E-02$	$--$	$2.19E-02$	$--$
40×40	$7.63E-03$	1.92	$5.49E-04$	4.98	$3.74E-03$	2.67	$6.74E-03$	1.86	$1.61E-04$	1.86	$2.85E-04$	6.27
80×80	$1.32E-03$	2.53	$5.71E-05$	3.26	$4.76E-04$	2.97	$1.68E-03$	2.00	$1.97E-05$	2.00	$3.28E-05$	3.12
160×160	$2.37E-04$	2.48	$7.94E-06$	2.85	$5.98E-05$	2.99	$4.13E-04$	2.03	$2.44E-06$	2.03	$3.99E-06$	3.04
320×320	$4.18E-05$	2.50	$1.43E-06$	2.47	$7.65E-06$	2.97	$1.01E-04$	2.03	$3.03E-07$	2.03	$4.93E-07$	3.01

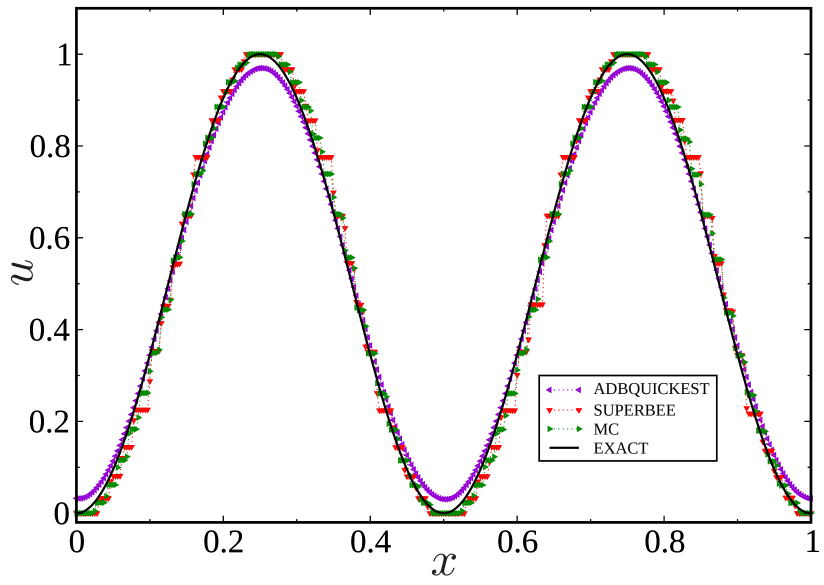
Table 2 shows, for this linear problem, the errors and the observed orders of convergence for upwind schemes. As it can be observed from this table, all schemes overcame the formal order, except the MC scheme which shown to be of third order of accuracy. Figure 4 shows a comparison of the results obtained with the upwind schemes. From Fig.4, one can clearly see that both TOPUS and ARORA-ROE schemes provide good solutions, while the ADBQUICKEST scheme presented a smeared solution (this behaviour has already been observed in test time for 1D advection of scalar (see Candezano *et al.* (2010)). The other schemes give similar results. Figure 5 depicts the space evolution of all upwind schemes for the 2D linear advection equation.

5.4 The 2D Magnetohydrodynamics equations-MHD

The ideal MHD equations are a nonlinear system of hyperbolic conservation laws that characterize the flow of a conducting fluid in a presence of magnetic field. They are defined by



(a)



(b)

Figure 4. The 2D linear advection equation computed with $\theta = 0.5$, $N \times N = 320 \times 320$ at time $t = 2.0$: a) TOPUS, SDPUS-C^1 and ARORA-ROE; b) ADBQUICKEST, SUPERBEE and MC

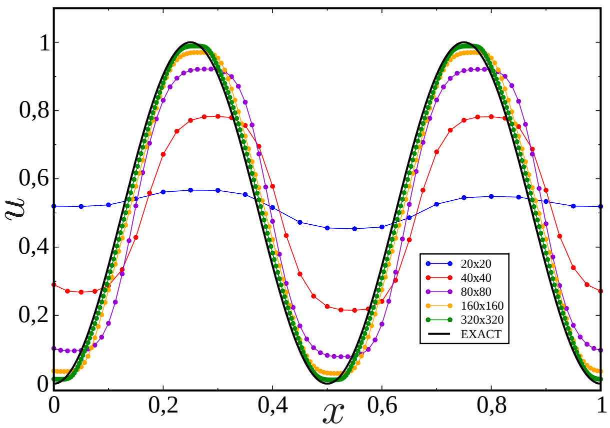
$$\phi = [\rho, \rho u, \rho v, \rho w, B_1, B_2, B_3, E]^T, \tag{25}$$

$$\begin{aligned} F(\phi) \quad = \quad & [\rho u, \rho u^2 + P^* - B_1^2, \rho uv - B_1 B_2, \rho uw - B_1 B_3, \\ & 0, uB_2 - vB_1, uB_3 - wB_1, u(E + P^*) - B_1(uB_1 + vB_2 + wB_3)]^T \end{aligned} \tag{26}$$

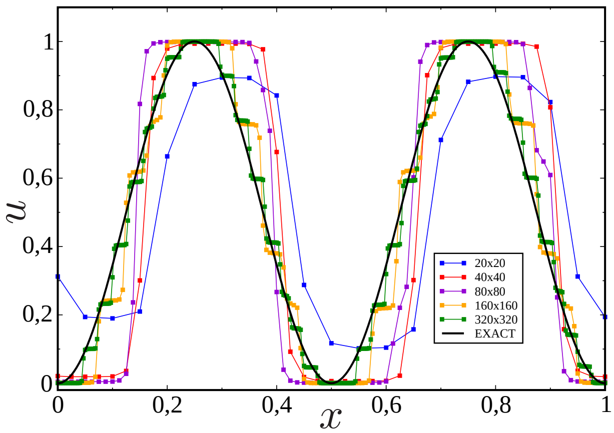
and

$$\begin{aligned} G(\phi) \quad = \quad & [\rho v, \rho vu - B_2 B_1, \rho v^2 + P^* - B_2^2, \rho vw - B_2 B_3, vB_1 - uB_2, \\ & 0, vB_3 - wB_2, v(E + P^*) - B_2(uB_1 + vB_2 + wB_3)]^T, \end{aligned} \tag{27}$$

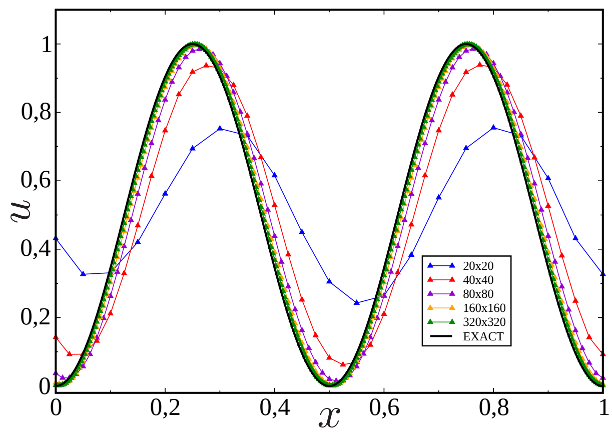
where ρ is the density, $\mathbf{u} = (u, v, w)$ is the fluid velocity, $\mathbf{B} = (\boldsymbol{B}_1, \boldsymbol{B}_2, \boldsymbol{B}_3)$ is the magnetic field, $E = \frac{1}{2}\rho||\mathbf{u}||^2 + \frac{1}{2}||\mathbf{B}||^2 + \frac{p}{(\gamma-1)}$ is the total energy. p is the thermal pressure, $P^* = p + \frac{1}{2}||\mathbf{B}||^2$ and $\frac{1}{2}||\mathbf{B}||^2$ is the magnetic pressure,



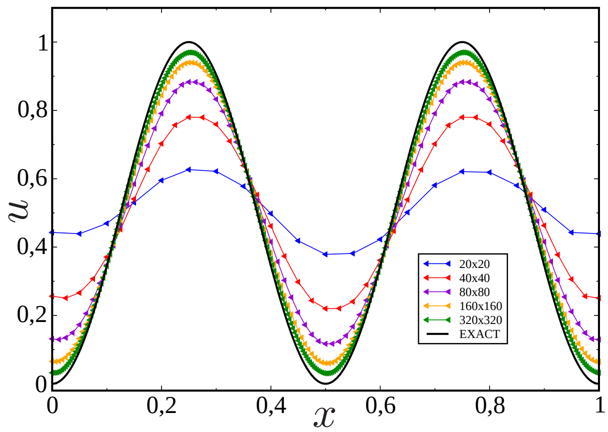
(a) TOPUS



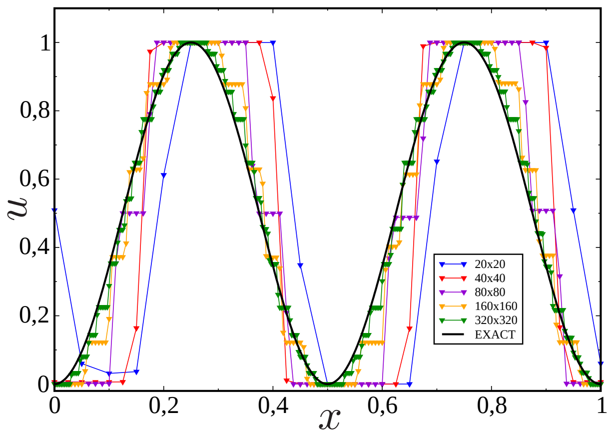
(b) SDPUS-C^1



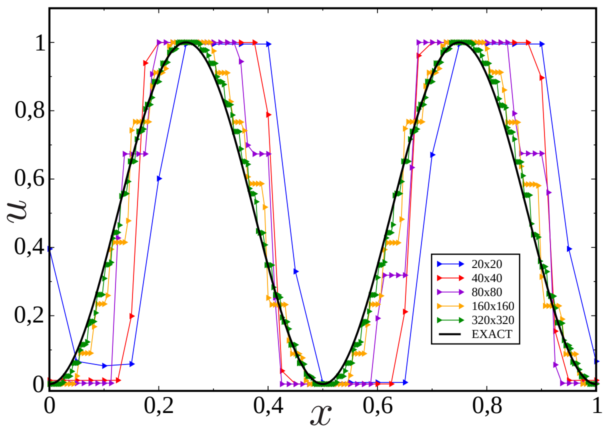
(c) ARORA-ROE



(d) ADBQUICKEST



(e) SUPERBEE



(f) MC

Figure 5. Space evolution for 2D linear advection equation

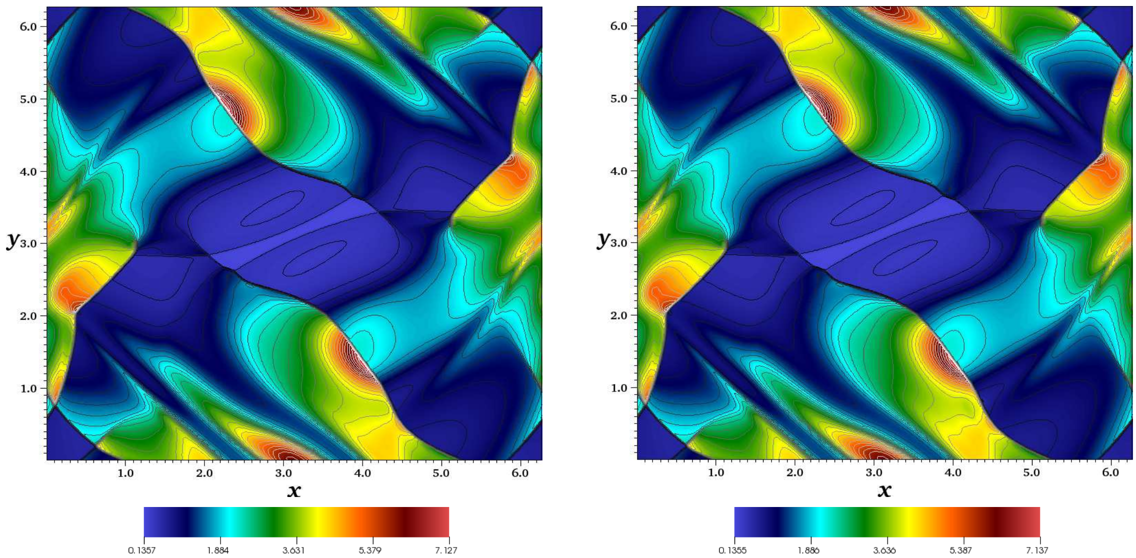
$\gamma = 5/3$ is the ratio of the specific heats. The system has eight unknowns $\phi = (\rho, \rho\mathbf{u}, E, \mathbf{B})$ and eight equations. In addition, for physical reasons the magnetic field must satisfy the free divergence condition, $\nabla \cdot \mathbf{B} = 0$. From now on, the results for the Orszag-Tang turbulence problem (Orszag and Tang, 1979) are presented. This problem describes the evolution of a vortex system involving the interaction between several shock's waves traveling at various speed regimes. From numerical point of view, this test is very interesting. The computational domain is $[0, 2\pi] \times [0, 2\pi]$. The grid sizes are: $16 \times 16, 32 \times 32, 64 \times 64, 128 \times 128$ and 256×256. The initial conditions are given by: $\rho = \gamma^2, u = -\sin y, v = \sin x, w = 0, B_1 = -\sin y, B_2 = sin2x, B_3 = 0, p = \gamma$. Periodic boundary conditions are implemented.

Table 3. L_1 errors and convergence rates for density of the Orszag-Tang turbulence problem

	TOPUS		SDPUS-C^1		ARORA-ROE		ADBQUICKEST		SUPERBEE		MC	
$N \times N$	L_1	p	L_1	p	L_1	p	L_1	p	L_1	p	L_1	p
16×16	$1.06E+00$	$--$	$1.07E+00$	$--$	$1.07E+00$	$--$	$1.08E+00$	$--$	$1.09E+00$	$--$	$1.07E+00$	$--$
32×32	$2.72E-01$	1.97	$2.74E-01$	1.97	$4.46E-01$	1.27	$2.77E-01$	1.96	$2.83E-01$	1.94	$2.76E-01$	1.96
64×64	$6.60E-02$	2.04	$6.63E-02$	2.04	$6.70E-02$	2.74	$6.69E-02$	2.05	$6.79E-02$	2.06	$6.68E-02$	2.04
128×128	$1.43E-02$	2.20	$1.43E-02$	2.21	$1.43E-02$	2.22	$1.44E-02$	2.22	$1.45E-02$	2.23	$1.44E-02$	2.22
256×256	$2.39E-03$	2.57	$2.39E-03$	2.58	$2.39E-03$	2.59	$2.39E-03$	2.59	$2.39E-03$	2.60	$2.39E-03$	2.59

Table 3 displays the errors and the observed orders of convergence at final time $t = 0.5$. In this nonlinear complex problem, all schemes overestimated the formal order of the numerical method.

Figure 6 shows the pressure contours obtained with TOPUS and SDPUS-C^1 schemes for the Orszag-Tang turbulence problem, at final time $t = 2$, with a mesh 256×256. These results are in good agreement with those given by Balbás *et al.* (2004). In particular, it can be observed that TOPUS and SDPUS-C^1 schemes capture well the complex evolution of the system and the formation of all shocks involved in this problem.



(a) TOPUS (b) SDPUS-C^1

Figure 6. The Orszag-Tang MHD turbulence problem. The pressure on 256×256 grids points, $\theta = 0.75$ at time $t = 2$, with 30 contour lines

6. CONCLUSION

In this work, it was presented a study of the accuracy for two recently introduced TVD upwind schemes, namely TOPUS and SDPUS-C^1. Some fluid dynamics problems, such as 1D nonconvex nonlinear Buckley-Leverett, 1D Euler equations, 2D linear advection equation and 2D MHD equations, were solved. By using these problems, comparisons were assessed with respect to the errors and observed orders of convergence. In general, it was observed that both TOPUS and SDPUS-C^1 upwind schemes overestimated the formal order of accuracy, with exception of the Woodward-Colella problem where it was observed that orders were underestimated. In the case of advection of scalars in 2D, the TOPUS scheme presented a solution very near to the exact one. In the Orszag-Tang problem the TOPUS and SDPUS-C^1 scheme captured well the shock interactions. For the future, the authors are planning to use the TOPUS and SDPUS-C^1 scheme for solving 3D incompressible free surface flows in a turbulent regime.

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