DEVELOPMENT AND EVALUATION OF TWO NEW UPWIND SCHEMES FOR CONSERVATION LAWS

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Abstract. *This work deals with a computational evaluation of two new high resolution upwind schemes, namely ADBQUICKEST (Int. J. Numer. Meth. Fluids 2009; 60:1–26) and TOPUS (Comput. Fluids - Submitted), for solving general hyperbolic conservation laws. By using the finite difference methodology, the schemes are analyzed and implemented in the context of normalized variables of Leonard (1988). In order to access the performance of these schemes, a series of one-dimensional test problems are examined beginning with classical linear advection of scalars and ending with Riemann problems for Burgers, Buckley-Leverett, shallow water, and Euler equations. And, as application, the ADBQUICKEST and TOPUS schemes are used for the numerical simulation of 3D incompressible Navier-Stokes equations involving free surface.*

Keywords: *upwind differencing, high resolution schemes, convective transport, advective terms, incompressible flows*

1. INTRODUCTION

Successful simulation of the convective transport is one of the most challenging and interesting research branches in computational fluid dynamics (CFD), which has attract many workers for more than three decades (see, for instance, the review article of van Leer (2006)).

It is well known that stability, boundedness, and accuracy are the most important properties of modeling schemes for the convection terms (in general non-linear). Particularly, the approximation of the convective terms in hyperbolic conservation laws (or fluid flow problems at high Reynolds number) using bounded high resolutions schemes is today an area of intense activity. The main challenge is to derive a high resolution upwind scheme that reproduces good performance in a vast range of problems. Thus, this study is motivated by the desire to design an upwind scheme that combine simplicity and ability to capture discontinuities (shock waves) with robustness. These properties are needed to describe phenomena that occur in hyperbolic conservation laws and related fluid dynamics problems.

There is a specialized literature about high resolution upwind schemes for advection transport, but none of them does not show the process in details (see, for example, Waterson (2008)). We can also cite the following two new schemes: ADBQUICKEST ("ADaptative Bounded QUICKEST") of Ferreira et al (2009b) and TOPUS ("Third-Order Polynomial Upwind Scheme") Ferreira et al. (2009a). The ADBQUICKEST and TOPUS schemes were derived in the context of the NVD ("Normalized Variable Diagram") of Leonard (1988) and by enforcing the total variation diminishing (TVD) constraint of Harten (1983). Consequently, they satisfy the convection boundedness criterion (CBC) of Gaskell and Lau (1988).

The objective of this work is to evaluate the ADBQUICKEST and TOPUS schemes for solving advection of scalars and 1D Riemann problems for Burgers, Buckley-Leverett, shallow water, and Euler equations. Then, as an application, these schemes are used in the numerical simulation of 3D incompressible Navier-Stokes equations involving free surface.

The rest of the work is organized as follows. Section 2 deals with normalized variable, CBC and TVD constraints. The ADBQUICKEST and TOPUS schemes are summarily discussed in Sec. 3. In Sec. 4 we will exhibit our computational results and evaluation using as test a set of problems of increasing complexity. The conclusions are discussed in Sec. 5. The references are appended at the end.

2. NORMALIZED VARIABLE, CBC AND TVD CONSTRAINTS

The ADBQUICKEST and TOPUS schemes are used to interpolate the numerical flux u_f at the f face using the three neighboring grid points D (*Downstream*), U (*Upstream*) and R (*Remote-upstream*), and the convecting velocity, V_f, (upwinding) at this face. Figure 1 depicts, for one-dimensional problems, the two cases that occur in our implementation. For multidimensional problems, this upwind-biased strategy is handled in the same fashion, with each convective derivative approximated along the line of the relevant variable (direction-by-direction). By using this upwinding strategy, both ADBQUICKEST and TOPUS schemes are written in the following general form (in general non-linear)

$$u_f = u_f(D, U, R). \tag{1}$$

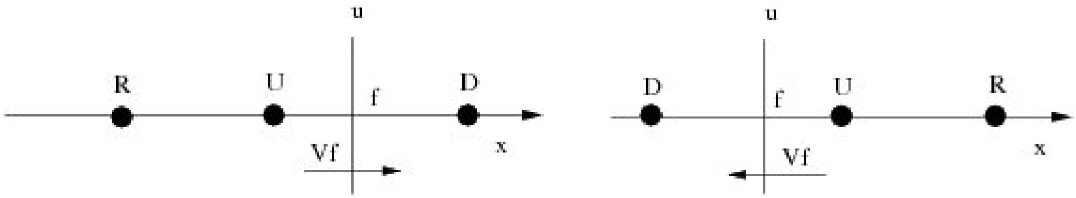


Figure 1. Interfaces and their related grid points for defining normalized variables.

In order to simplify the functional relationship Eq. (1) linking u_D, u_U and u_R, the original variables are transformed in normalized variables (NV) of Leonard (1988) as

$$\hat{u} = \frac{u - u_R}{u_D - u_R}. \tag{2}$$

The advantage of this new formulation is that the interface value $\hat{u}_f$ depends on $\hat{u}_U$ only, since $\hat{u}_D = 1$ and $\hat{u}_R = 0$.

Gaskell and Lau (1988) proposed the CBC, which states the conditions for boundedness as follows:

- $\forall \hat{u}_U \in [0,1], \quad \hat{u}_U \leq \hat{u}_f(\hat{u}_U) \leq 1;$
- $\forall \hat{u}_U \notin [0,1], \quad \hat{u}_f = \hat{u}_f(\hat{u}_U) = \hat{u}_U;$
- $\hat{u}_f(0) = 0$ and $\hat{u}_f(1) = 1$.

The CBC has long been accepted as both sufficient and necessary condition for a scheme possessing boundedness (see Gaskell and Lau (1988) and Zhu and Rodi (1991)). It can also be shown that the CBC can guarantee the stability of a scheme (see Yu et al. (2001)).

Another important convective stability is the TVD constraint of Harten (1983). TVD is a purely scalar property, which ensures that spurious oscillations are removed from the numerical solution of a non-linear conservation law. Formally, consider a sequence of discrete approximations $u(t) = u_i(t)_{i\in\mathbf{Z}}$ to a scalar. The total variation (TV) at time t of this sequence is defined by

$$TV(u(t)) = \sum_{i\in\mathbf{Z}} |u_{i+1}(t) - u_i(t)|. \tag{3}$$

We say, by definition, that the scheme is TVD if

$$TV(u^{n+1}) \leq TV(u^n), \quad \forall n. \tag{4}$$

Both ADBQUICKEST of Ferreira et al. (2009b) and TOPUS of Ferreira et al. (2009a) schemes satisfy CBC and preserve the TVD constraint. In summary, they are presented next.

3. DEVELOPMENT OF THE ADBQUICKEST AND TOPUS SCHEMES

The ADBQUICKEST and TOPUS schemes were derived in the context of the NVD of Leonard (1988) and by enforcing the TVD constraint of Harten (1983). Consequently they satisfy the CBC of Gaskell and Lau (1988). The numerical solutions obtained by these schemes can be second or third order accurate in the smooth parts of the solution, but only first order near regions with large gradients. The reader is referred to Ferreira et al. (2009b) and Ferreira et al. (2009a) for more details of the schemes. In summary, by using the CBC criterion and the recommendations of Leonard, namely the scheme passes at the points $O(0,0)$, $Q(0.5, 0.75)$, $P(1,1)$ and has inclination 0.75 at the point Q, the ADBQUICKEST (a linear piecewise function) and TOPUS (a four degree polynomial function) schemes are as follows.

• **ADBQUICKEST:** This scheme retains the Courant number θ in the formulation as a free parameter and is given by

$$\hat{u}_f = \begin{cases} (2-\theta)\hat{u}_U, & 0 < \hat{u}_U < a, \\ \hat{u}_U + \frac{1}{2}(1-|\theta|)(1-\hat{u}_U) - \frac{1}{6}(1-\theta^2)(1-2\hat{u}_U), & a \leq \hat{u}_U \leq b, \\ 1 - \theta + \theta\hat{u}_U, & b < \hat{u}_U < 1, \\ \hat{u}_U, & \text{elsewhere}, \end{cases} \tag{5}$$

where the constants a and b in Eq. (5) are given by

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

The corresponding flux limited is

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

$$r_f = \frac{\hat{u}_U}{1 - \hat{u}_U}. \tag{8}$$

• **TOPUS:** This scheme retains a free parameter α in the formulation and is given by

$$\hat{u}_f = \begin{cases} \alpha\hat{u}_U^4 + (-2\alpha+1)\,\hat{u}_U^3 + \left(\frac{5\alpha-10}{4}\right)\hat{u}_U^2 + \left(\frac{-\alpha+10}{4}\right)\hat{u}_U, & 0 \le \hat{u}_U \le 1, \\ \hat{u}_U, & \text{elsewhere}, \end{cases} \tag{9}$$

where the parameter $-2 \le \alpha \le 2$ ensures that it satisfy the CBC criterion. If α equal to 2, then TOPUS is entirely contained in the TVD region of Harten (1983). The o corresponding flux limited is

$$\psi(r_f) = \frac{0.5\,(|r_f| + r_f)\left[(-0.5\alpha+1)r_f^2 + (\alpha+4)r_f + (-0.5\alpha+3)\right]}{(1+|r_f|)^3}. \tag{10}$$

4. NUMERICAL RESULTS

We now discuss the performance of the ADBQUICKEST and TOPUS schemes based on the computational results for one-dimensional hyperbolic conservation laws and for three-dimensional incompressible Navier-Stokes equations.

4.1 One-dimensional hyperbolic conservation laws

In this subsection, we are concerned with solving the conservation laws in one-dimension defined by

$$u_t + f(u)_x = 0, \tag{11}$$

where u is the conserved variable and $f(u)$ is the flux function. Equation (11) is supplemented with initial and boundary conditions on a closed domain. The following cases are considered:
– Advection equation, where the flux function is $f(u) = u$;
– Burgers equation, where the convex flux function is $f(u) = \frac{1}{2}u^2$;
– Buckley-Leverret equation, where the flux function (non-convex) is $f(u) = u^2/[u^2 + \frac{1}{4}(1-u)^2]$;
– Shallow water equations, where $u = (h, hv)^T$ is the vector of the conserved quantities, $f(u) = (hv, hv^2 + \frac{1}{2}gh^2)^T$ is the vector flux function, being h and g the height and the gravitational constant, respectively;
– Euler equations, where $u = (\rho, \rho v, E)^T$ is the vector of the conserved quantities, $f(u) = (\rho v, \rho v^2 + P, v(E+P))^T$ is the vector flux function, and ρ, v, ρv, E, P are density, velocity, momentum, total energy and pressure, respectively. In order to solve this system, the ideal gas equation of state $P = (\gamma - 1)(E - \frac{1}{2}\rho v^2)$ was considered, where $\gamma = 1.4$ is the ratio of ratio specific heats.

4.1.1 Advection equation

One of the simplest hyperbolic systems arising from the conservation laws is the linear advection equation, which describes the advection (or transport) of a scalar u along the x-axis direction and wave speed 1. With appropriate initial conditions $u(x, 0)$, this equation has exact solution given by $u(x, t) = u_0(x - t)$. In the following, two tests problems are set with specific initial and periodic boundary conditions.

Test Problem 1: The first test problem considered is linear advection equation with initial condition given by

$$u_0(x) = \begin{cases} 1, & 0 \le x \le 0.2, \\ 4x - \frac{3}{5}, & 0.2 < x \le 0.4, \\ -4x + \frac{13}{5}, & 0.4 < x \le 0.6, \\ 1, & 0.6 < x \le 0.8, \\ 0, & \text{otherwise}. \end{cases} \tag{12}$$

This problem is a good test for the shock-capturing ability of the high order upwind schemes study here. The exact solution and numerical results obtained with ADBQUICKEST and TOPUS schemes on a mesh size of 400 computational cells over $x \in [-1, 1]$, at $t = 1$ and $\theta = 0.3$ are presented Fig. 2. We can see from this figure that, qualitatively, the results are similar between these two schemes. In particular, the ADBQUICKEST accurately captured the peaks.

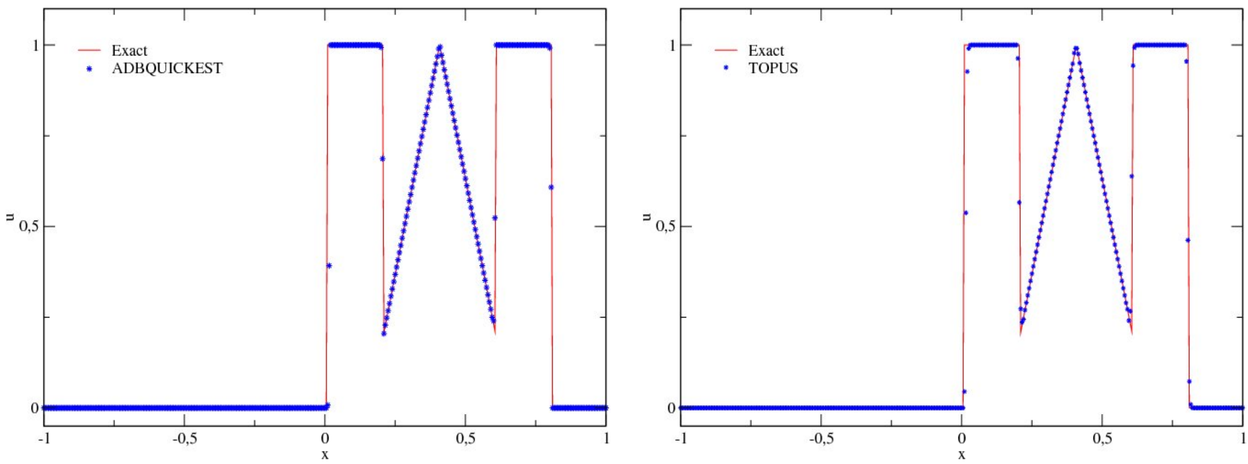


Figure 2. Numerical and analytic (Exact) solutions for the linear advection equation using the initial data of the Eq. (12).

Test Problem 2 (Long time simulation:) The ability of the ADBQUICKEST and TOPUS schemes to perform long time integration is evaluated in this test. Long time integration is important in many practical applications, such as aeroacoustic and LES (Large Eddy Simulation) (see, for example, Ekaterinaris (2004)). In the simulation, it is considered the linear advection equation with the initial condition

$$u_0(x) = \cos(0,75|\mathrm{x}|)\mathrm{e}^{-0,1|\mathrm{x}|}. \tag{13}$$

The exact solution and numerical results obtained with theses schemes on a mesh size of 9000 computational cells over $x \in [-55, 245]$, at $t = 200$ and $\theta = 0.5$ are presented Fig. 3. It can be seen from this figure that the numerical results are in good agreement with the analytical (Exact) solution. We can also see that both ADBQUICKEST and TOPUS schemes are capable of obtaining a sufficiently accurate solution for long time integration. In addition, the ADBQUICKEST scheme solves this equation with a better satisfactory resolution than the TOPUS scheme.

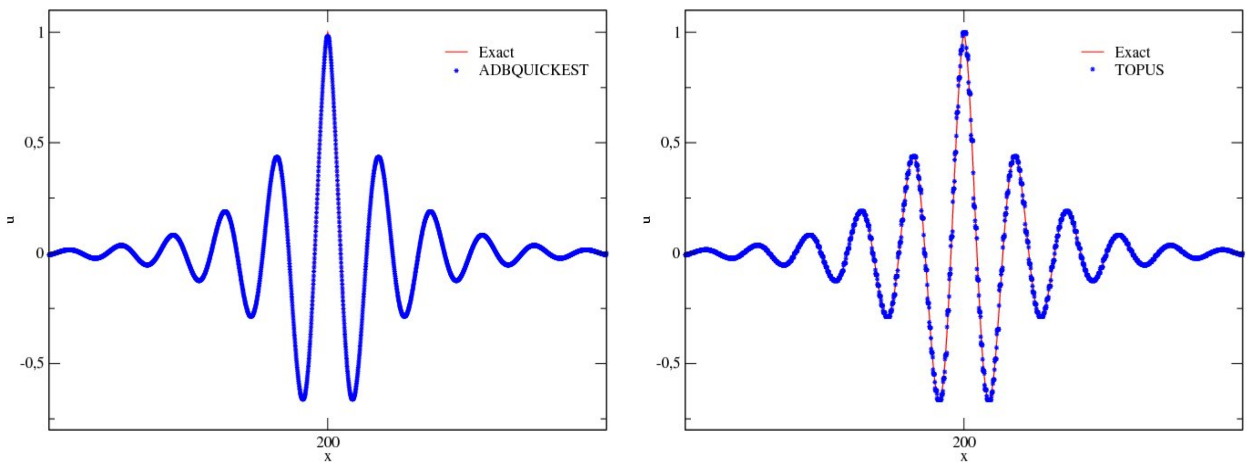


Figure 3. Numerical and analytic (Exact) solutions for the linear advection equation using the initial data of the Eq. (13).

4.1.2 Burgers equation

The performance of the ADBQUICKEST and TOPUS schemes is now analyzed by applying them to the non-linear inviscid Burgers equation. Burgers equation serves as a good model for understanding discontinuities (shock) formation and turbulence, and has similar features with the Navier-Stokes equations due to its non-linearity.

Test Problem 3 (Error analysis): In this test problem, Burgers equation is solved on $[0, \pi]$ with periodic boundary conditions and with initial condition given by

$$u_0(x) = \sin(\mathrm{x}). \tag{14}$$

This test has exact solution given by (see Platzman (1964))

$$u(x,t) = -2\sum_{n}^{\infty} \frac{J_n(-nt)}{nt}\sin(\mathrm{nx}), \tag{15}$$

where J_n is the Bessel function. In Fig. 4, it is illustrated the semi-analytical solution (convergence required, at most, 200 terms in the series Eq. (15)) and numerical results obtained with the ADBQUICKEST and TOPUS schemes (left), along with a plot of the absolute error as a function of x (right), using a mesh size of 400 computational cells, $\theta = 0.3$ and $t = 0.25$ (before the shock). One can see from this figure that the numerical results are in very good agreement with the semi-analytical solution (15).

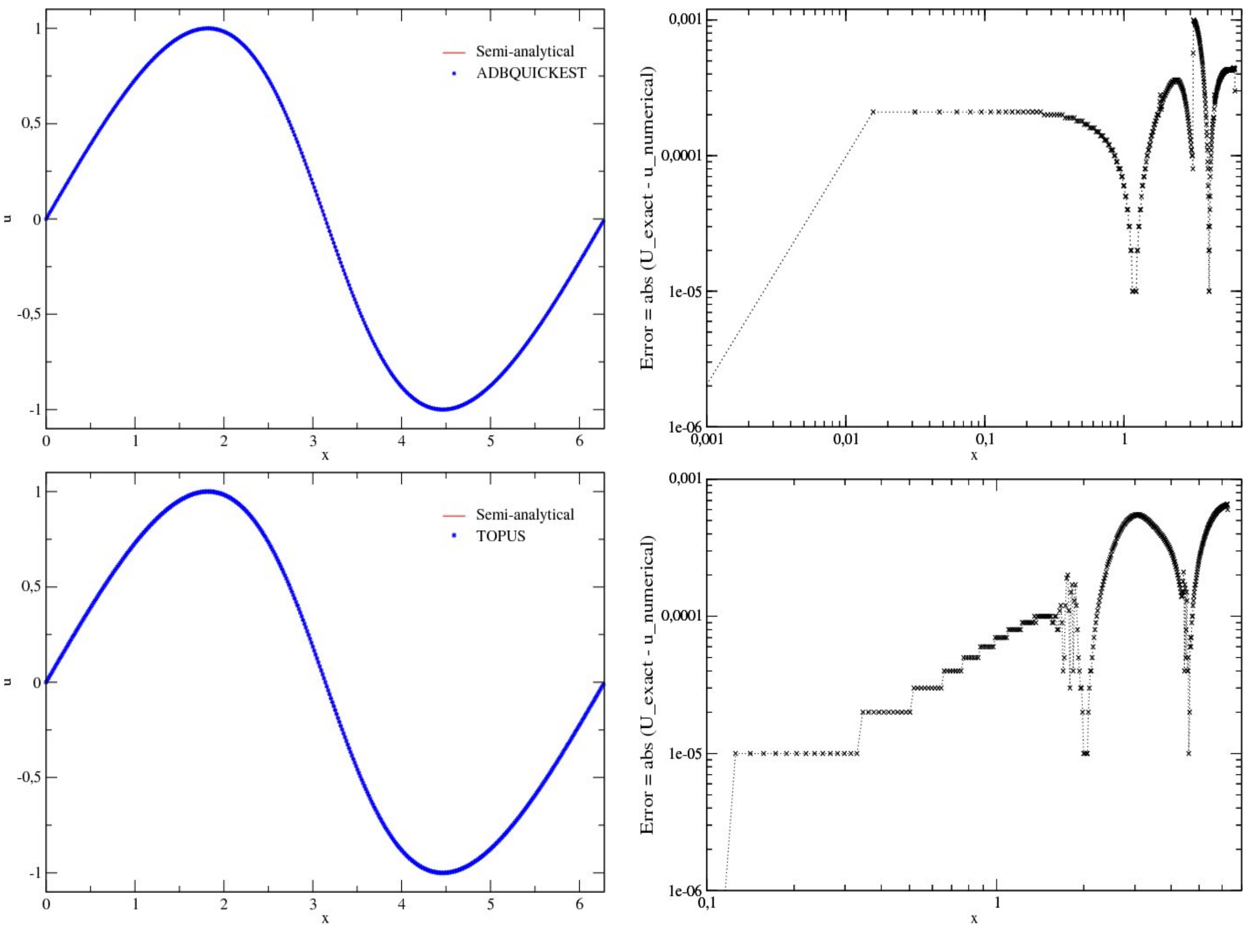


Figure 4. Comparison between the semi-analytical and numerical solutions for the non-linear Burgers equation, and the spatial distribution of the errors for ADBQUICKEST and TOPUS schemes

By using this non-linear test, we now perform a estimate for numerical convergence order. For this, the numerical solutions (with ADBQUICKEST and TOPUS) are carried out with a mesh size of 160 cells. In Tab. 1, it is shown the L_1, L_2 and L_∞ error norms, as well as the numerical order estimates p, of the computed solutions using $\theta = 0.3$ and $t = 0.25$. From this table, the numerical data indicate that, on these norms, the TOPUS converges at a rate higher than that of ADBQUICKEST.

4.1.3 Buckley-Leverett equation

The performance of the ADBQUICKEST and TOPUS schemes is now accessed when they are applied to solve non-linear conservation laws possessing non-convex flux function. For this end, the Buckley-Leverett equation is considered as a relevant example. This non-linear equation is frequently used for describing the one-dimensional flow of two incompressible fluids (water and oil) in a porous medium. The variable u in this case is the saturation of the water phase (the

Table 1. Convergence test: L_1, L_2 and L_∞ error norms and numerical order estimates using the initial condition given by Eq. (14).

Scheme	N	L_1 Error	p	L_2 Error	p	L_∞ Error	p
ADBQUICKEST	20	0.5831 e-2	—	0.7117 e-2	—	0.1205 e-1	—
	40	0.2701 e-2	1.111	0.2928 e-2	1.281	0.4572 e-2	1.398
	80	0.1335 e-2	1.016	0.1446 e-2	1.017	0.2308 e-2	0.985
	160	0.6263 e-3	1.091	0.6895 e-3	1.069	0.1681 e-2	1.079
TOPUS	20	0.4710 e-2	—	0.6263 e-2	—	0.1189 e-1	—
	40	0.1632 e-2	1.538	0.2113 e-2	1.567	0.4231 e-2	1.491
	80	0.6556 e-3	1.316	0.7875 e-3	1.424	0.2006 e-2	1.076
	160	0.3666 e-3	0.838	0.4069 e-3	0.952	0.7536 e-3	1.412

reader is referred to Ahmed (2004) for more details on this hyperbolic equation).

Test Problem 4: The Buckley-Leverett equation is solved on the domain $[-1, 1]$ and with initial condition given by

$$u_0(x) = \begin{cases} 1, & -0.5 \le x \le 0, \\ 0, & \text{otherwise.} \end{cases} \tag{16}$$

The numerical results obtained with ADBQUICKEST and TOPUS schemes on a mesh of 400 computational cells with $\theta = 0.3$ and $t = 0.3$, and the converged solution generated with the first order upwind scheme on a mesh size of 4000 computational cells (the reference solution) are presented in Fig. 5. From this figure, it can clearly be seen that the numerical results obtained with both schemes are satisfactory, with the ADBQUICKEST scheme providing a better resolution.

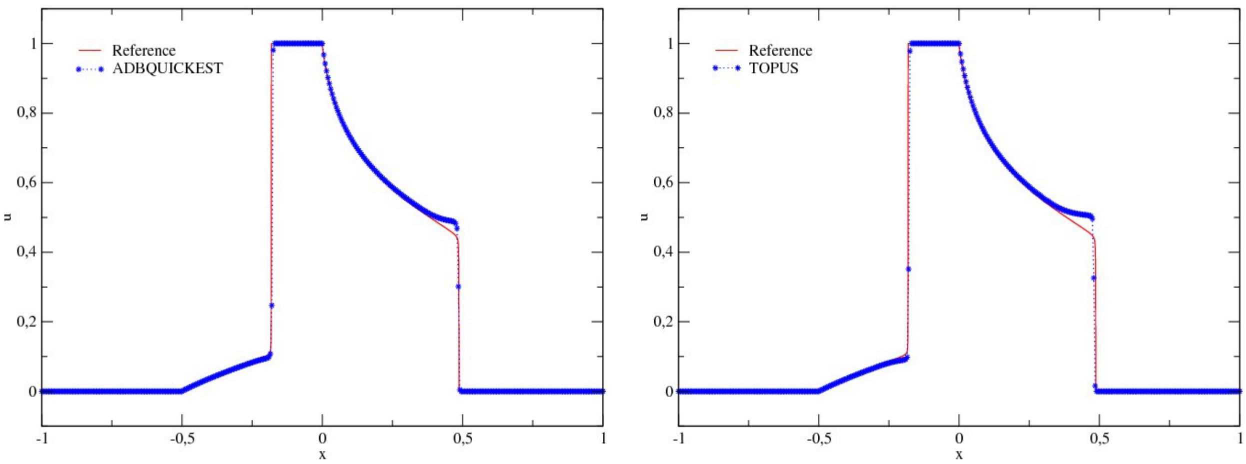


Figure 5. Numerical and reference solutions for the Buckley-Leverett equation.

4.1.4 Shallow water equations

The shallow water equations model the incompressible hydrostatic motion of a fluid with free surface. In order to simulate this non-linear system, we consider a fluid in a channel of unit width and assume that the vertical velocity of the fluid is negligible and the horizontal velocity v is roughly constant throughout any cross section of the channel. Next, this problem is solved by using the ADBQUICKEST and TOPUS schemes.

Test Problem 5: The one-dimensional shallow water equations is solved in the domain $[-5, 5]$. At the beginning of the simulation, the dam divides the domain in two parts, namely the reservoir at the left and the tailwater at the right. The initial conditions consist of piecewise-constant data (the reservoir and the tailwater separated by a discontinuity at $x = 0$) given by

$$v_0(x) = 0, \quad h_0(x) = \begin{cases} 3, & \text{se} \quad x \le 0, \\ 1, & \text{se} \quad x > 0. \end{cases} \tag{17}$$

On the boundaries, we used the Neumann condition (see LeVeque (2004)). The dam is instantaneously removed and the solution is computed. The reference solution is given by the Godunov method (see LeVeque (2004)) using 1000 computational cells. The numerical solutions were obtained on a mesh size of 200 computational cells. In the computational simulation, the conservation law package (CLAWPACK) of LeVeque (2003), equipped with ADBQUICKEST ($\theta = 0.5$) and TOPUS schemes, was employed. CLAWPACK is a general purpose and open-source software developed at the University of Washington, Seattle, by LeVeque (2004). Figures 6 and 7 show the comparison between numerical and reference solutions at time $t = 2$ for the h and hv (the discharge). From these figures, it can be seen that the discontinuity was correctly captured by both schemes, being that in this case the TOPUS scheme provided the better result.

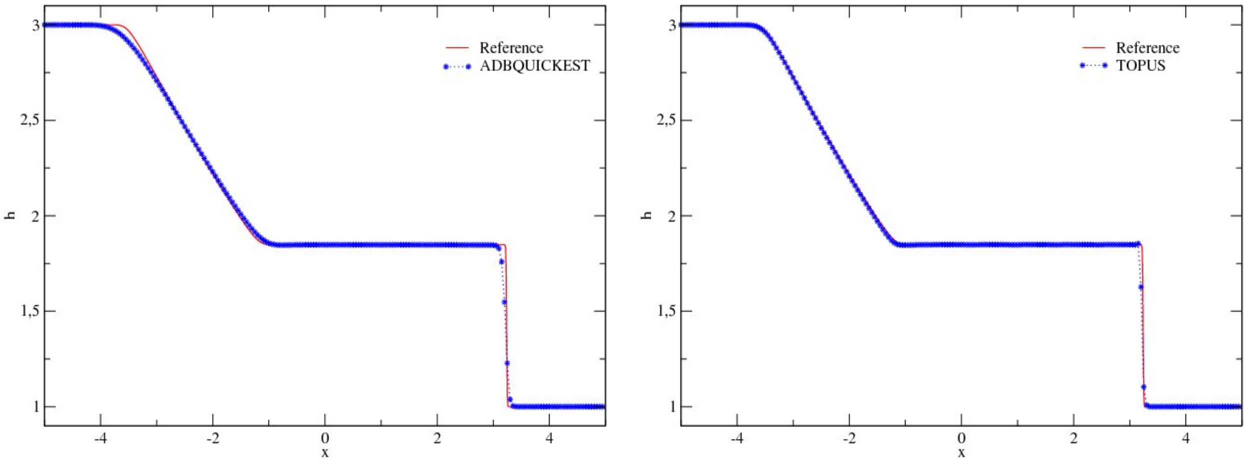


Figure 6. Numerical and reference solutions for the dam break problem.

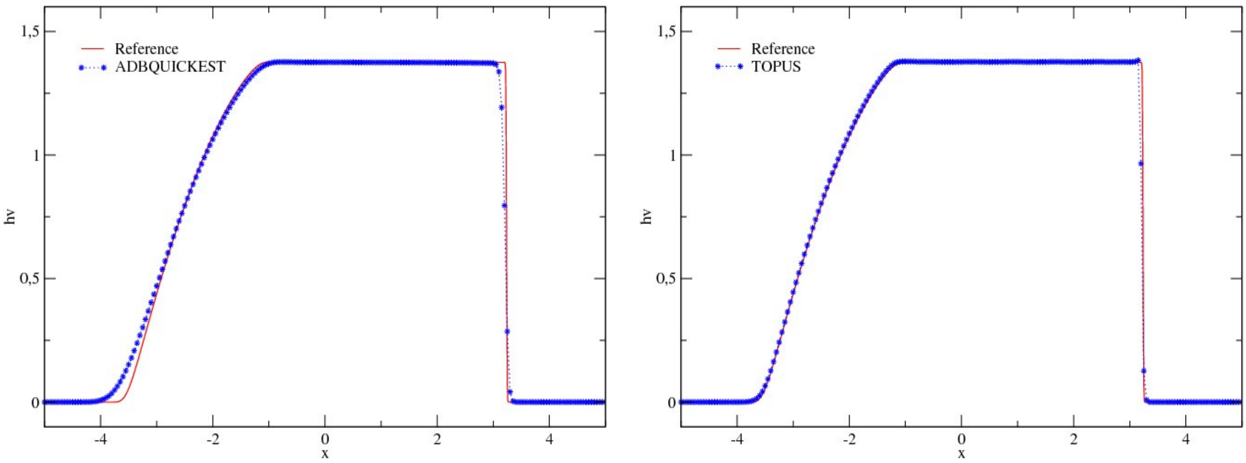


Figure 7. Numerical and reference solutions for the dam break problem.

4.1.5 Euler equations

The Euler equations with colliding blast waves is called the "bang-bang problem" (see LeVeque (2003)). This problem involves multiple interactions of strong shock and is a very challenging one. It was used by Woodward and Colella (1984) to compare Eulerian schemes. In the following, the ADBQUICKEST and TOPUS schemes are applied to simulate this complex problem.

Test Problem 6 (Interaction of two blast waves): In this test, the Euler equations with colliding blast waves, on domain $[0, 1]$ and $t = 0.38$, are solved. The initial conditions consist of two parallel, planar flow discontinuities. The density is unity, the velocity is zero everywhere and the pressure is given by

$$P_0(x) = \begin{cases} 1000, & \text{se} \quad 0 \leq x \leq 0.1, \\ 0.01, & \text{se} \quad 0.1 \leq x \leq 0.9, \\ 100, & \text{se} \quad 0.9 \leq x \leq 1.0. \end{cases} \tag{18}$$

The boundary conditions at $x = 0$ and $x = 1$ are set to solid reflecting walls. The reference solution for this problem is calculated on a mesh size of 2000 computational cells using the Godunov method with term correction. The basic form of these correction terms is motivated by the Lax-Wendroff method (the reader is referred to LeVeque (2004) for more details). The numerical solutions were obtained on a mesh size of 1000 computational cells. For this, the CLAWPACK software (see LeVeque (2003)), equipped with ADBQUICKEST ($\theta = 0.5$) and TOPUS schemes, was employed. Figure 8 shows the reference solution and numerical results for the pressure and density, respectively. It can be seen from this figure that the discontinuity is correctly captured by both scheme. However, the ADBQUICKEST scheme solves these equation with a better satisfactory resolution than the TOPUS scheme.

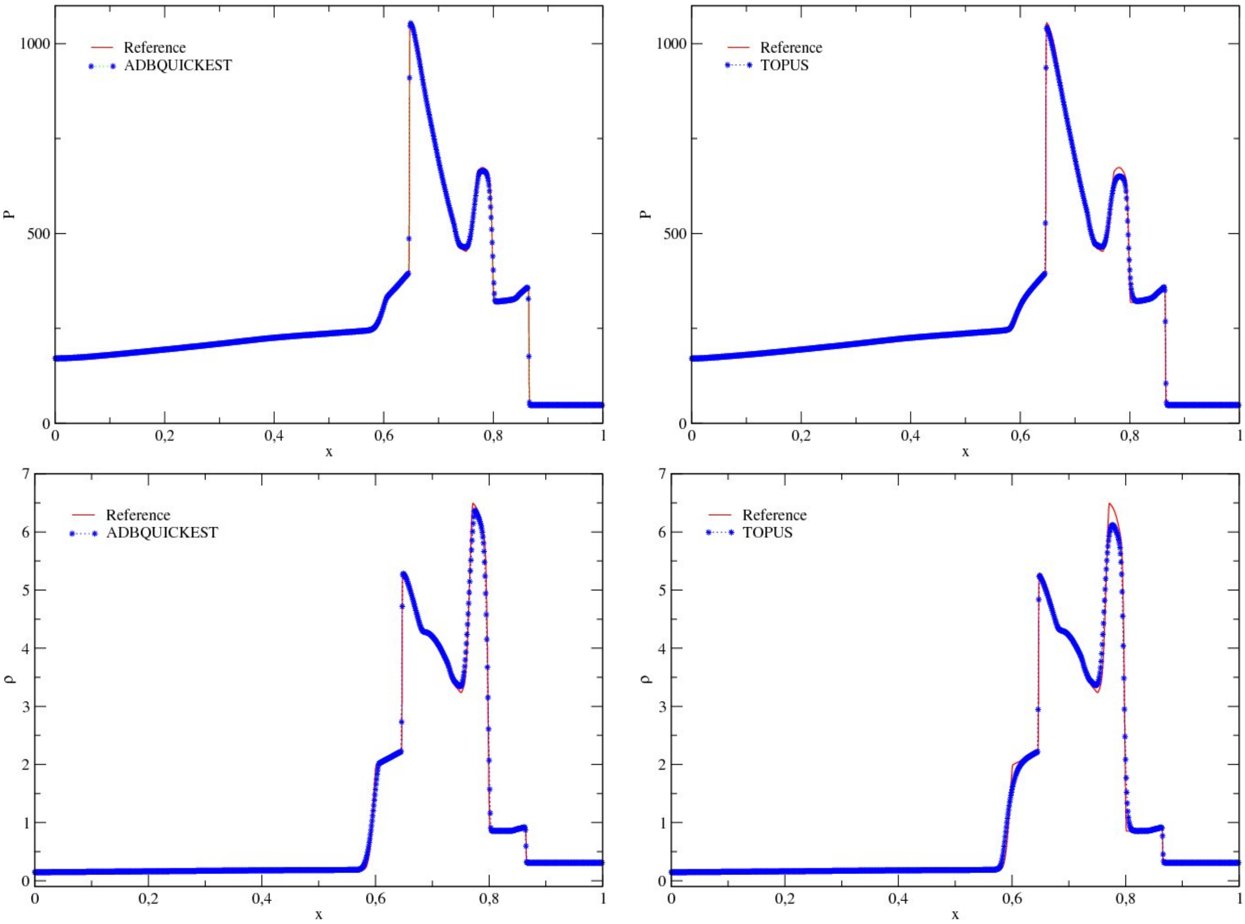


Figure 8. Numerical and reference solutions for the Euler equations with colliding blast wave.

4.2 Three-dimensional incompressible Navier-Stokes equations

From now on, we examine the capability of the ADBQUICKEST and TOPUS schemes for solving complex flow problems involving moving free surface. We have choose, as a difficult test, the well know circular hydraulic jump (see reference Ellegaard et al. (1998) for more details on the phenomenon). For the simulation of this free surface flow, we have used the 3D version Freeflow code of Castelo et al. (2000) equipped with both ADBQUICKEST and TOPUS schemes. The governing equations are Navier-Stokes and mass conservation equations given, respectively, by

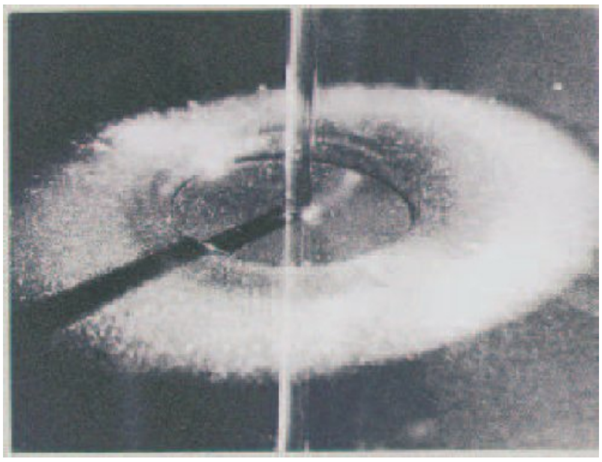
$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{g}, \qquad (19)$$

$$\nabla \cdot \mathbf{u} = 0, \qquad (20)$$

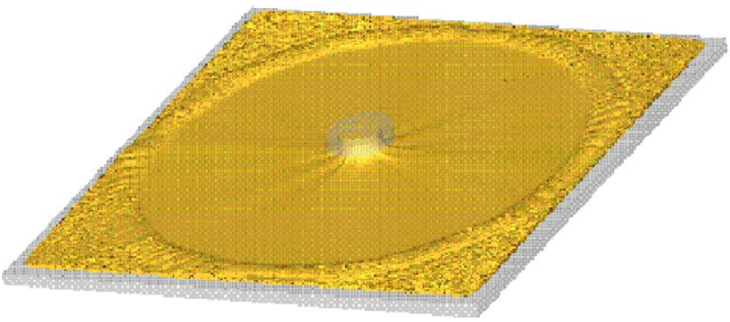
where $\mathbf{u}$ is the velocity vector field, P is the pressure, $\mathbf{g}$ gravitational field and ν is the viscosity coefficient.

Test Problem 7: The circular hydraulic jump may arise when a free jet of water falling vertically at moderate Reynolds number strikes a horizontal rigid surface. Fluid is spread radially in a thin layer, until it reaches a critical radius (sudden discontinuity) at which the layer depth increases abruptly (as example, see an experimental visualization at high Reynolds number in Fig. 9(a)). A better understanding of the phenomenon and the instabilities, at least in its turbulent form, is of commercial interest, since jet impingement is often used in cooling systems and the flow of the fluid beyond the jump can degrade the efficiency of the system. Probably, the first author to study the influence of fluid viscosity on the jump radius was Watson (1964). A 3D turbulent hydraulic jump constitutes an excellent test for validating codes based on front tracking techniques. In order to simulate this complex free surface flow, the Reynolds number, based on the maximum velocity $U_0 = U_{max} = 1.0$ m/s and diameter of the inlet ($D = 0.05$m), was 1.0×10^3. The mesh used was 120×120×10 computational cells. Figure 9 shows a qualitative comparison between the experimental results of Ellegaard et al. (1996) (Fig. 9(a)) and the results obtained with our numerical methods combined with ADBQUICKEST and TOPUS schemes (Fig. 9(b)-(c)). One can clearly see from this figure that our numerical methods captured the complete physical mechanism of this complex free surface flow.

(a) Experimental result of Ellegaard et al. (1996)



(b) Numerical result obtained with ADBQUICKEST



(c) Numerical result obtained with TOPUS

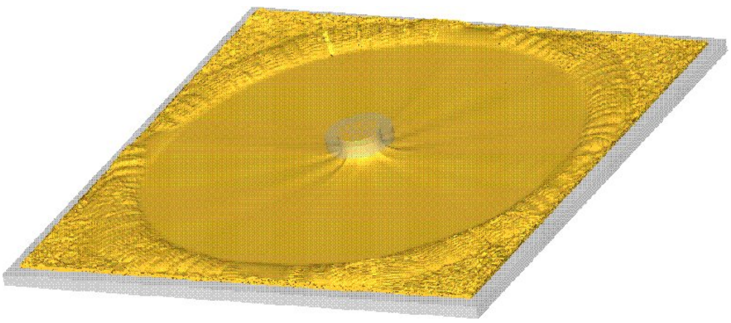


Figure 9. 3D qualitative comparison between the experimental and numerical results for a turbulent hydraulic jump using ADBQUICKEST and TOPUS schemes.

5. CONCLUSIONS

In this paper, the performance of the ADBQUICKEST and TOPUS schemes was evaluated with respect to various test problems, namely advection of scalars, Riemann problems for Burgers, Buckley-Leverett, shallow water, and Euler equations and a 3D circular hydraulic jump (an incompressible flow with moving free surface).

From 1D numerical results, one can conclude that the ADBQUICKEST and TOPUS schemes are robust strategy for capturing shocks, when compared with a reference solution. These results confirm the capability of these schemes to control the generation of unphysical oscillations in the vicinity of discontinuities. The results obtained in the 3D case demonstrated that these upwinding schemes are effective tools for studying 3D complex flow problems.

For the future, the authors are planning to apply the ADBQUICKEST and TOPUS schemes to the solution of three-dimensional turbulent and viscoelastic free surface flows.

6. ACKNOWLEDGMENTS

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