A new type of TVD/CBC polynomial upwind scheme for hyperbolic conservation laws and fluid dynamics problems

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Abstract. *A new high-resolution polynomial TVD/CBC-based upwind scheme is developed for numerical solution of hyperbolic conservation laws and related fluid dynamic problems. The scheme, called TDPUS-C3, is implemented into the CLAWPACK software. Unsteady simulation of nonlinear problems demonstrates that the scheme is capable of stably reproducing shocks, discontinuities and complex structures in flows.*

Keywords: *convective terms, simulation of hyperbolic conservation laws, upwinding, TVD/CBC*

1. INTRODUCTION

Modeling of the nonlinear convective terms in conservation equations of the fluid dynamics continues to be a challenge. On the one hand, classical methodologies, such as first order upwind (FOU) and centered difference (CD) schemes, are prone to produce errors during the computational process. Numerical solutions computed with the FOU scheme present smearing, compromising the accuracy; computations with CD schemes introduce spurious oscillations, leading to instabilities. On the other hand, the sophisticated ENO and WENO schemes provide high accuracy and are free from oscillations, but their computational costs are very high, specially on irregular meshes. An intermediate approach that satisfies the total variation diminishing (TVD) and convection boundedness criterion (CBC) stability criteria constitutes another useful manner of approximating convective terms. In this article, a new high-resolution polynomial TVD/CBC-based upwind scheme is developed for numerical solution of hyperbolic conservation laws and related fluid dynamic problems. The scheme, called tenth degree polynomial upwind scheme (TDPUS-C3), is implemented into the CLAWPACK software for solving these problems. Unsteady simulation of nonlinear equations demonstrates that TDPUS-C3 scheme is capable of stably reproducing shocks, discontinuities and complex structures in flows.

2. MATHEMATICAL FRAMEWORK

In this section we present the fundamental concepts of upwind schemes based on TVD/CBC limited constraints.

2.1 The TVD/CBC criteria

As usual, we consider the 1D scalar advection equation to study the numerical discretization defined by Eq. (1) (further extension for 2D/3D cases are straightforward),

$$\begin{cases} u_t + au_x = 0, \quad a = \text{const.} \\ u(x,0) = u_0(x), \quad x \in \mathbb{R}, \end{cases} \tag{1}$$

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

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

where u_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. $u_{i+1/2}^n$ and $u_{i-1/2}^n$ are the numerical flux functions, which depend on the following three selected points: **D**ownstream, **U**pstream and **R**emote-upstream (see Fig. 1). These locations are previously defined according to the convection velocities V_f and V_g at the faces $i+1/2$ and $i-1/2$ (upwinding). The general variable u is transformed into a new variables called normalized variable (NV) of Leonard (1988) by $\hat{u}_{()} = \dfrac{u_{()} - u_{(R)}}{u_{(D)} - u_{(R)}}$. Following Leonard's formulation, the interface value $\hat{u}_f$ depends on $\hat{u}_U$ only, since $\hat{u}_D = 1$ and $\hat{u}_R = 0$.

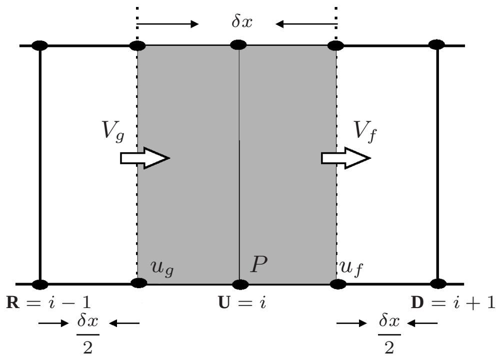


Figure 1. Sketch of upwind-biased stencil at point P

Therefore it is possible to derive a nonlinear monotonic NV scheme by imposing the following conditions for $0 \le \hat{u}_U \le 1$: $\hat{u}_f(0) = 0$ (a necessary condition), $\hat{u}_f(1) = 1$ (a necessary condition), $\hat{u}_f(0.5) = 0.75$ (a necessary and sufficient condition to reach second order of accuracy) and $\hat{u}_f'(0.5) = 0.75$ (a necessary and sufficient condition to reach third order of accuracy). Leonard (1988) also recommends that for values of $\hat{u}_U < 0$ or $\hat{u}_U > 1$, the scheme must be extended using FOU scheme, then $\hat{u}_f = \hat{u}_U$. Schemes define in NV can be rewritten in flux limiter form by using the relationship $\hat{u}_f = \hat{u}_U + \frac{1}{2}\Psi(r)(1-\hat{u}_U)$, where $\Psi(r)$ is the flux limiter function and r is the ratio of successive gradients (a sensor), given by $r_f = \frac{1}{1-\hat{\phi}_U}$ (Waterson and Deconinck, 2007). The aim idea of the flux limiter is to control the process of generation of over/undershoots by preventing gradients to exceed certain limits, or to change sign between adjacent points (Hirsch, 2007). For stability reasons we ensure limited solution implementing the CBC criterion of Gaskell and Lau (1988), as follows: $\hat{\phi}_U \le \hat{\phi}_f(\hat{\phi}_U) \le 1$, if $\hat{\phi}_U \in [0,1]$; $\hat{\phi}_f = \hat{\phi}_f(\hat{\phi}_U) = \hat{\phi}_U$, if $\hat{\phi}_U \notin [0,1]$; $\hat{\phi}_f(0) = 0$ and $\hat{\phi}_f(1) = 1$. The TVD criterion constraint of Harten (1983) ensures that, in general, spurious oscillations (unphysical noises) are removed from the numerical solution. Formally, we consider a sequence of discrete approximations $u(t) = u(t)_{i\in\mathbb{Z}}$ for a scalar quantity. The total variation (TV) at time t of this sequence is defined by $TV(u(t)) = \sum\limits_{i\in\mathbb{Z}} |u_{i+1}(t) - u_i(t)|$, a scheme satisfies the TVD condition if, for all data set u^n, it is truth that $TV(u^{n+1}) \le TV(u^n),\ \forall n$. The schemes that satisfy TVD criterion guarantee convergence, monotonicity and high accuracy.

3. THE NEW UPWIND SCHEME TDPUS-C3

We present a new high resolution polynomial upwind scheme by using the Leonard's formulation above defined, based on TVD/CBC conditions called tenth degree polynomial upwind scheme (TDPUS-C3), defined by $\hat{u}_f(\hat{u}_U) = \sum_{i=0}^{10} \alpha_i \hat{u}_U^i$. This new upwind scheme is developed satisfying the second and third order of accuracy conditions from Leonard, plus the following conditions: $\hat{u}_f'(0.5) = 0.75$ to reach third order of accuracy; $\hat{u}_f'(0) = 1$ and $\hat{u}_f'(1) = 1$ to avoid convergence problem in coarse grids (Lin and Chieng, 1991); $\hat{u}_f''(1) = 0$ and $\hat{u}_f'''(0) = 0$ to impose smoothness on the solutions (Zijlema, 1996); $\hat{u}_f'''(0) = 0$ and $\hat{u}_f'''(1) = 0$ these conditions are impose for the authors to reach that curvature varies slowly (a few abrupt changes). With these conditions and fixing a constant, e.g. α_4, we find the others coefficients: $\alpha = [0, 1, 0, 0, 320 - 8\beta, 26\beta - 1664, 3456 - 44, 41\beta - 3584, 1856 - 20\beta, 4\beta - 384]^T$. After solving a benchmark test problem, the advection equation with Zalesak (1987) initial conditions, we find that the ideal parameter is $\beta = 567.25$. The new upwind scheme in not normalized variables (for easy computational implementation) is defined by

$$u_f = \begin{cases} u_R + (u_D - u_R) * (\hat{u}_U + \hat{u}_U^4(\alpha_4 + \hat{u}_U(\alpha_5 + \hat{u}_U(\alpha_6 + \hat{u}_U(\alpha_7 + \hat{u}_U(\alpha_8 + \hat{u}_U(\alpha_9 + \hat{u}_U\alpha_{10}))))))), & \hat{u}_U \in [0,1]; \\ \hat{u}_U, & \hat{u}_U \notin [0,1], \end{cases} \tag{3}$$

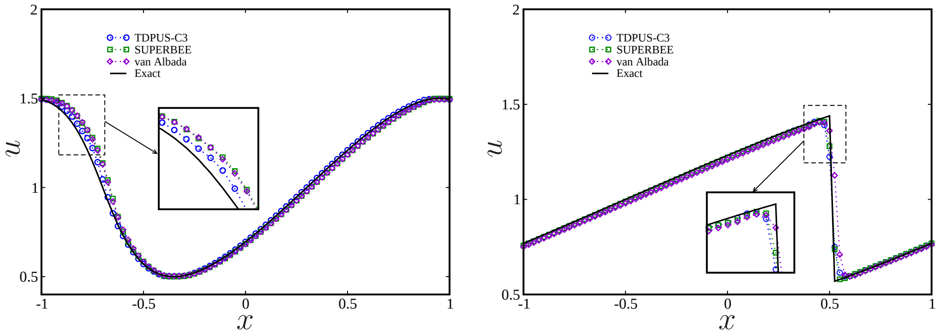
4. NUMERICAL RESULTS

In this section, we numerically study the results obtained by using TDPUS-C3 with the aim of evaluating his performance, e.g. second order of accuracy and absence of spurious oscillations at discontinuities and sharp gradients.

Scalar equation: the new high-resolution upwind scheme is studied solving the nonlinear inviscid Burgers equation 1D defined by Eq. (4) for evaluating the ability for capturing the wave before ($t \approx 0.33$) and after ($t \approx 1.5$) the shock; the shock is developed at $t \approx 2/\pi$. The numerical solutions are computed with $N = 80$ and $\theta = 0.5$ on a domain $[-1, 1]$. Periodic boundary conditions are implemented. The "exact" solution is computed using the algorithm of Teng (2010). We implement for this problem a TVD Runge-Kutta scheme of third order (RK3) for time integration (Gottlieb and Chi-Wang-Shu, 1998). The initial conditions is $u(x, 0) = 1 + \frac{1}{2} + \sin(\pi x)$. The solutions obtained with TDPUS-C3 are compared with two well known schemes from litearure: SUPERBEE by Roe (1986) and Van Albada by van Albada *et al.* (1982)

$$u_t + \left(\frac{u^2}{2}\right)_x = 0, \tag{4}$$

It is clearly seen from Fig. 2 that TDPUS-C3 models well the wave before and after the shock. These solutions are in



$t \approx 0.33$ $t \approx 1.5$

Figure 2. 1D Burgers equation. Before ($t =\approx 0.33$) and after ($t \approx 1.5$) the shock. $CFL = 0.5, N = 80$.

good agreement with the "exact" ones.

The Buckley-Leverett equation: we test TDPUS-C3 scheme for the nonlinear nonconvex Buckley-Leverett problem defined by

$$u_t + \left(\frac{4u^2}{4u^2 + (1-u)^2}\right) = 0. \tag{5}$$

The numerical solutions are computed at $t = 0.4$ with $N = 400$ and $\theta = 0.4$ on a domain $x \in [-1, 1]$. Periodic boundary conditions are implemented. The "exact" solution is a shock rarefaction-contact discontinuity mixture and is computed by using van Leer scheme (van Leer, 1974) with $N = 2000$ computational cells. RK3 at time is implemented. The initial conditions are $u(x, 0) = 1$ if $-0.5 \leq x \leq 0$ and 0, otherwise. In Fig. 3, the numerical solutions free of oscillations obtained with TDPUS-C3 are well comparable with the "exact" ones. It can be seen from this figure that, in particular, TDPUS-C3 is more accurate than other schemes, while SUPERBEE and van Albada schemes shown to be more dissipative before the shock and the contact discontinuity.

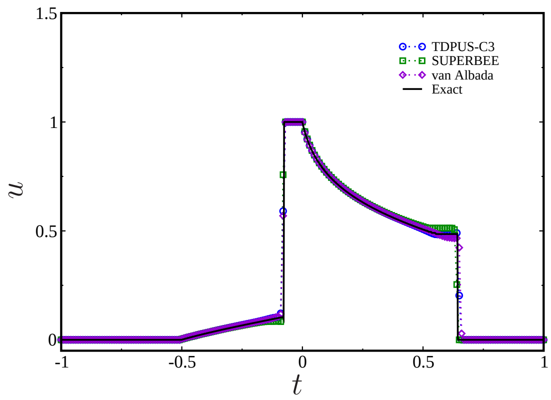


Figure 3. The Buckley-Leverett equation. $CFL = 0.4$, $N = 200$ and $t = 0.4$.

It is important comment that some high-resolution schemes fail to converge to the correct entropy solutions for this problem (Qiu and Shu, 2002).

System of equations. (Euler equations): we solve the nonlinear systems of Euler equations in an accuracy test for the 2D Euler equations. The Euler equations are defined by

$$\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(E+p) \end{pmatrix}_x + \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(E+p) \end{pmatrix}_y = \mathbf{0}, \qquad (6)$$

where ρ is the density, u and v are the component of the velocity vectors. p is the pressure and $E = p/(\gamma-1)+\frac{1}{2}\rho(u^2+v^2)$ is the total energy. γ is a constant, the ratio of specific heat.

Accuracy test: the TDPUS-C3 scheme is evaluated in an accuracy test by using Eq. (6) with initial conditions $(\rho, u, v, p)^T = (1 + 0.2\sin(\pi(x + y)), 0.7, 0.3, 1)$ at final time $t = 2$ on a domain $[0, 1] \times [0, 1]$. $\theta = 0.475$ and $\gamma = 1.4$. The exact solution is $\rho(x, y, t) = 1 + 0.2\sin(\pi(x + y - (u + v)t))$. Periodic boundary conditions are implemented. In Tab.1 we show the L_1 errors and numerical orders of convergence p (LeVeque, 2007) on four meshes: $20\times20, 40\times40, 80\times80, 160\times160$ and 320×320. For comparisons, we compute the numerical errors and orders of convergence for this problem by using SUPERBEE scheme of Roe (1986). We can see from Tab.1 that TDPUS-C3 achieves the designed order of convergence. In the first mesh sizes the order of convergence computed with TDPUS-C3 are slightly superior that those produced by SUPERBEE scheme but slightly inferior to those ones produced by van Albada scheme.

Table 1. L_1 errors of the density ρ for the 2D Euler equations at $t = 2$ and $\theta = 0.475$.

Mesh	TDPUS-C3		SUPERBEE		VAN ALBADA	
	L_1	p	L_1	p	L_1	p
20×20	$9.03E-03$	—	$8.311E-03$	—	$9.034E-03$	—
40×40	$2.13E-03$	2.08	$2.074E-03$	2.00	$2.157E-03$	2.07
80×80	$5.17E-04$	2.04	$5.173E-04$	2.00	$5.203E-04$	2.05
160×160	$1.27E-04$	2.02	$1.283E-04$	2.01	$1.277E-04$	2.03
320×320	$3.16E-05$	2.01	$3.176E-05$	2.01	$3.158E-05$	2.02

The shock-entropy wave problem: The Shu-Osher shock's tube is a 1D moving Mach 3 shock with sine waves interacting with a turbulent field Shu and Osher (1989) and defined by Eq. (6). with initial condition given by

$$\begin{cases} \rho = 3.857143; & u = 2.629369; \; p = 10.33333, \quad x < 0.4; \\ \rho = 1 + 0.2\sin(5x); & u = 0; \qquad p = 1, \qquad x \geq 0.4. \end{cases} \tag{7}$$

The computational domain is defined on $-5 \leq x \leq 5$. The boundary conditions are inflow/outflow. The CFL number is $\theta = 0.5$. $\gamma = 1.4$. We present a spatial evolution with meshes size $125, 250, 500$ and 1000 of the numerical solutions for density ρ computed by TDPUS-C3 at final $t = 1.8$. The reference solution is computed with SUPERBEE (Roe, 1986) with $N = 2000$ mesh points. In Fig.4 are depicted the numerical solutions for density ρ computed with TDPUS-C3. We

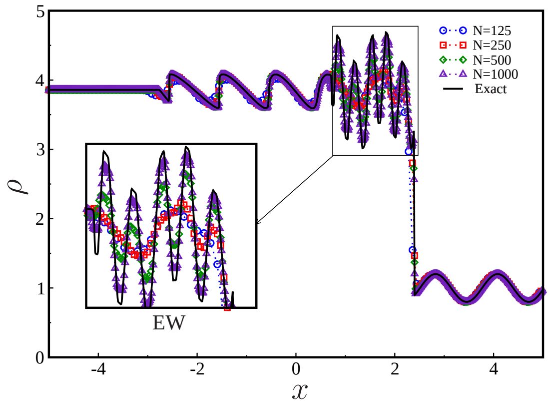


Figure 4. Spatial evolution for density ρ for Shu-Osher problem computed with TDPUS-C3 $N = 500, \theta = 0.5, t = 1.8$.

zoom-in on the more complicated regions of the problem, the entropy wave (EW) region, and show that for finest grids the numerical solutions computed with TDPUS-C3 is more approximated to the reference solutions.

Double Mach reflection (DMR): This problem was originally studied by Woodward and Colella (1984) and it is given by Eq. (6) defined in a rectangular region $[0, 4] \times [0, 1]$ where, initially, a shock moves diagonally with a Mach 10 forming an angle of $\alpha = \frac{\pi}{3}$ with the $x-$axis. The initial conditions are

$$(\rho, u, v, p) = \begin{cases} (8, 8.25 \cdot \cos\frac{\pi}{6}, -8.25 \cdot \sin\frac{\pi}{6}, 116.5), & x < x_0 + \frac{y}{\sqrt{3}}; \\ (1.4, 0, 0, 1.0), & x \geq x_0 + \frac{y}{\sqrt{3}}, \end{cases} \tag{8}$$

where $x_0 = \frac{1}{6}$. The boundary conditions are as follows. At the left, $x = 0$ (the inflow boundary), it is imposed post-shock values (Eq. (8)); at the right (the outflow boundary) the imposed conditions at the bottom, $y = 0$, are reflecting boundary conditions on $[x_0, 4]$ and exact post-shock conditions otherwise. The exact position of the shockwave at time t and at $y = 1$ is given by $s(t) = x_0 + \dfrac{(1+20t)}{\sqrt{3}}$. We set the pre- and post-shock conditions at $y = 1$, before and after of shockwave position at instant t

$$(\rho, u, v, p) = \begin{cases} (8, 8.25\cos\frac{\pi}{6}, -8.25\sin\frac{\pi}{6}, 116.5), & 0 < x < s(t); \\ (1.4, 0, 0, 1.0), & s(t) \leq x \leq 4. \end{cases} \tag{9}$$

Fig. 5 depicted the numerical solutions of density ρ for the DMR problem on a domain $[0, 3] \times [0, 1]$. In Fig. 6 it is seen how the TDPUS-C3 models this shock problem describing the small viscosities at the "blown-up" region approximately on the interval $[2, 3] \times [0, 0.5]$. We can see from this figure that TDPUS-C3 combined with a first order in time Godunov scheme captures some vortical structures like those ones obtained with WENO5- 5th order in space and 3rd order in time These results are in agreement with numerical results found in literature (see Woodward and Colella (1984)).

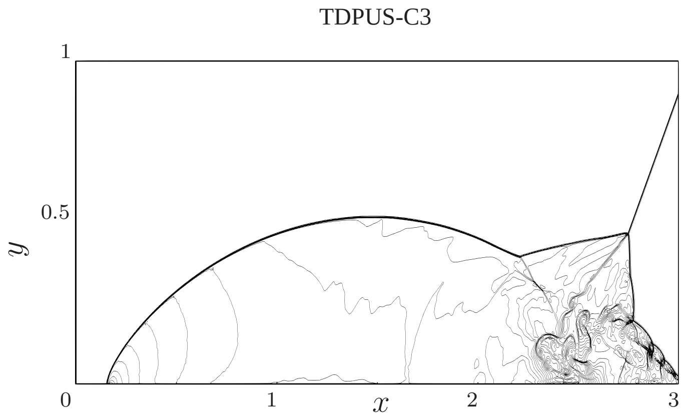


Figure 5. Density contours for double Mach reflection problem at time $t = 0.2$, computed with TDPUS-C3 on a mesh 1600×400. 30 contour lines from $\rho = 1.5$ to $\rho = 22.97$. $(x, y) \in [0, 3] \times [0, 1]$.

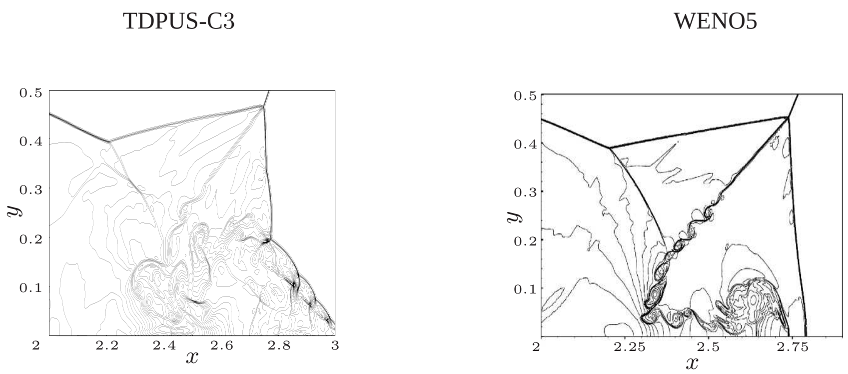


Figure 6. "Blown up" region for density ρ computed with TDPUS-C3 on a mesh 1600×400 and WENO5 of (Jiang and Shu, 1996) on a mesh 3840×960 at time $t = 0.2$. 30 contour lines from $\rho = 1.5$ to $\rho = 22.97$ and $CFL = 0.6$.

5. CONCLUSIONS

A new upwind biased scheme, based on TVD and CBC stability criteria called TDPUS-C3, has been presented. The performance of the scheme was assessed by solving 1D/2D complex hyperbolic conservation laws involving shocks and sharp gradients. An accuracy test has shown that the scheme can achieve (at a minimum) second order of accuracy. In summary, the TDPUS-C3 upwind scheme can be considered as an innovate and useful tool for modeling convective terms of the general conservation equations. For the future, the authors are planning to apply the TDPUS-C3 upwind scheme to complex incompressible turbulent free surface flows.

6. ACKNOWLEDGEMENTS

We are grateful to CAPES/CNPq IEL Nacional-Brasil(PECPG1462/08-3), CAPES: grant BEX 5458/11-0, FAPESP: grant 2009/16954-8, CNPq: grants 300479/2008-2(INCT-MACC) and FAPERJ (E-26/170.030/2008(INCT-MACC)) for supporting this study.

7. REFERENCES

Gaskell, P.H. and Lau, A.K.C., 1988. "Curvature-compensated convective transport: SMART, a new boundedness-preserving transport algorithm". *Int. J. Numer. Methods Fluids*, Vol. 8, pp. 617–641.

Gottlieb, S. and Chi-Wang-Shu, 1998. "Total variation diminishing Runge-Kutta schemes". *Math. Comput.*, Vol. 67, pp. 73–85.

Harten, A., 1983. "High resolution schemes for hyperbolic conservation laws". *J. Comput. Phys.*, Vol. 49, pp. 357–393.

Hirsch, C., 2007. *Numerical Computation of Internal and External Flows, Volume 1, The Fundamentals of Computational Fluid Dynamics*. Butterworth-Heinemann. ELSEVIER, 2nd edition.

Jiang, G. and Shu, C.W., 1996. "Efficient implementation of weighted ENO schemes". *J. Comput. Phys.*, Vol. 126, pp. 206–228.

Leonard, B., 1988. "Simple high-accuracy program for convective modeling of discontinuities". *Int. J. Numer. Methods Fluids*, Vol. 8, pp. 1291–1318.

LeVeque, R.J., 2007. *Finite Difference Methods for Ordinary Partial Differential Equations. Steady State and Time Dependent Problems*. Society for Industrial and Applied Mathematics (SIAM).

Lin, C.H. and Chieng, C.C., 1991. "Characteristic-based flux limiters of an essentially third-order flux-splitting method for hyperbolic conservation laws". *Int. J. Numer. Methods Fluids*, Vol. 13, pp. 287–307.

Qiu, J. and Shu, C.W., 2002. "On the construction, comparison, and local characteristic decomposition for high-order central weno schemes". *J. Comput. Phys.*, Vol. 183, pp. 187–209.

Roe, P., 1986. "Characteristic-based schemes for the Euler equations". *Ann. Rev. Fluid. Mech.*, Vol. 18, pp. 337–365.

Shu, C.W. and Osher, S., 1989. "Efficient implementation of essentially non-oscillatory shock-capturing schemes, II". *J. Comput. Phys.*, Vol. 83, pp. 32–78.

Teng, Z.H., 2010. "Exact boundary conditions for the initial value problem of convex conservation laws". *J. Comput. Phys.*, Vol. 229, pp. 3792–3801.

van Albada, G.D., van Leer, B. and Roberts, W.W., 1982. "A comparative study of computational methods in cosmic gas dynamics". *Astron. Astrophys.*, Vol. 108 No. 1, pp. 76–84.

van Leer, B., 1974. "Towards the ultimate conservative difference scheme II. Monotonicity and conservation combined in a second-order scheme". *J. Comput. Phys.*, Vol. 14, pp. 361–370.

Waterson, N.P. and Deconinck, H., 2007. "Design principles for bounded higher-order convection schemes - a unified approach". *J. Comput. Phys.*, Vol. 224, pp. 182–207.

Woodward, P. and Colella, P., 1984. "The numerical simulation of two-dimensional fluids flow with strong shocks". *J. Comput. Phys.*, Vol. 54, pp. 115–173.

Zalesak, S., 1987. "A preliminary comparison of modern shock-capturing schemes:linear advection". In *Advances in Computer Methods for Partial Differential Equation VI. Vichnevetsky R. Stepleman RS(eds) IMACS: New Brunswick, NJ.*

Zijlema, M., 1996. "On the construction of a third-order accurate monotone convection scheme with application to turbulent flows in general domains". *Int. J. Numer. Methods Fluids*, Vol. 22, pp. 619–641.