SOLVING FLUID DYNAMICS PROBLEMS USING A NEW POLYNOMIAL UPWIND CONVECTION SCHEME

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Abstract: The purpose of this work is to present a new polynomial convection scheme for solving complex fluid dynamics problems. The scheme is evaluated in linear and non-linear hyperbolic conservation laws and then is applied for simulating axisymmetric flow with moving free surfaces. From the results, the scheme shows to be a good tool for CFD.

Keywords: Conservation laws, upwinding.

1. INTRODUCTION

The numerical solution of fluid flow problems has emerged as a viable alternative to both experimental and analytical studies. In order to make the simulations of these problems more acceptable and reliable, there is an increasing demand for the development, analysis and implementation of a upwinding convective scheme (in general nonlinear) for solving complex flow phenomena, which offers simplicity, accuracy, robustness and versatility. Such a scheme is particularly important when one wants to simulate transient incompressible free surface flows at high values of Reynolds number.

In this sense, we presented in this work a new high resolution polynomial convection scheme for the discretization of the linear and nonlinear convection terms. The new scheme is temporarily called of Test Scheme. This scheme is based on the normalized variable (NV) formulation of Leonard [4] and satisfies the Total Variation Diminishing (TVD) [3] and Convection Boundedness Criterion (CBC) [2] stability criteria.

A brief description of the scheme is done and then numerical results are presented for 1D and 2D hyperbolic conservation laws, namely Burgers, acoustics and Euler equations. As an application, the Test Scheme is used for the simulation of a axisymmetric incompressible free jet impinging onto a horizontal rigid wall. The numerical results show that this new upwinding scheme performs very well.

2. THEORETICAL BASE OF THE DEVELOPMENT OF A UPWIND SCHEME

In order to obtain an approximation for the convective terms, we considered the upwind strategy, in which the Test Scheme is used to interpolate a numerical flux, say \( \phi_f \), at the face \( f \). This interpolation considers three neighboring mesh points, namely \( D \) (Downstream), \( U \) (Upstream) and \( R \) (Remote-upstream), that are determined according to the convective velocity \( V_f \) at this face, as shown in Figure 1. A scheme that adopts this strategy is written in the following form (in general nonlinear):

\[
\phi_f = \phi_f(D, U, R).
\]  

Figure 1 – Position of computational nodes \( D, U \) and \( R \) according to the sign of \( V_f \) speed of a convective variable \( \phi_f \).

In order to simplify the functional relationship given by Eq. (1), linking \( \phi_D, \phi_U \) and \( \phi_R \), the original variables are transformed in NV of Leonard [4] as

\[
\hat{\phi}(i) = \frac{\phi_D(i) - \phi_R(i)}{\phi_D(0) - \phi_R(0)}.
\]  

In this context, it is possible to derive a nonlinear monotonic NV scheme by imposing the following conditions, for
0 \leq \hat{\phi}_U \leq 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). Léonard [4] also recommends that for values of \( \hat{\phi}_U \leq 0 \) or \( \hat{\phi}_U > 1 \), the scheme must be extended in a continuous manner using the FOU (First Order Upwinding) scheme, which is defined by \( \hat{\phi}_f = \hat{\phi}_U \).

Limited solution (stability) is reached by considering the CBC of Gaskell and Lau [2], namely:

\[
\begin{align*}
-\hat{\phi}_U & \leq \hat{\phi}_f(\hat{\phi}_U) \leq 1, \text{ if } \hat{\phi}_U \in [0,1]; \\
-\hat{\phi}_f & = \hat{\phi}_f(\hat{\phi}_U) = \hat{\phi}_U, \text{ if } \hat{\phi}_U \notin [0,1]; \\
-\hat{\phi}_f(0) & = 0 \text{ and } \hat{\phi}_f(1) = 1.
\end{align*}
\]

Another important stability criterion is the TVD constraint of Harten [3]. This property ensures that, in general, spurious oscillations (unphysical noises) are removed from the numerical solution. Formally, consider a sequence of discrete approximations \( \phi(t) = \phi_i(t) \in \mathbb{Z} \) 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, by definition, we say that the scheme is TVD if, for all data set \( \phi^n \), the values \( \phi^{n+1} \) calculated by numerical method satisfy

\[
TV(\phi^{n+1}) \leq TV(\phi^n), \text{ } \forall n.
\]

It is important to emphasize, from numerical point of view, that TVD schemes are very attractive, since they guarantee convergence, monotonicity and high accuracy.

3. THE TEST SCHEME

For the development of the Test Scheme, we assume that the NV at the cell interface \( f, \phi_f \), are related to \( \hat{\phi}_U \) as part of a eight-degree polynomial function

\[
\hat{\phi}_f = \sum_{k=0}^{8} a_k \hat{\phi}_U^k,
\]

for \( 0 \leq \hat{\phi}_U \leq 1 \), and the FOU scheme for \( \hat{\phi}_U < 0 \) or \( \hat{\phi}_U > 1 \). By considering the coefficient \( a_k \) as a free parameter, say \( \lambda \), the other coefficients in Eq. (8) are determined by imposing the four conditions of Leonard [4] presented above plus the condition that this polynomial function is of \( C^2 \) class (i.e., it possesses first and second derivate continuously differentiable). For this, the function is linked at the points \((0,0)\) and \((1,1)\) with the same values of the first and second derivatives. This condition of differentiability is imposed because schemes of \( C^1 \) class avoids convergence problems when coarse meshes are employed (see Lin and Chiang [6]). In this sense, we propose a new polynomial upwinding scheme (the Test Scheme), as being an original function of class \( C^2 \).

In summary, the Test Scheme having the free parameter \( \lambda \) in its formulation, in NV, is given by

\[
\psi_f = \begin{cases} 
-4(\lambda - 24)\hat{\phi}_U^5 + 16(\lambda - 23)\hat{\phi}_U^4 + & \text{if } \hat{\phi}_U \in [0,1], \\
+(528 - 25\lambda)\hat{\phi}_U^3 & \text{if } \hat{\phi}_U \notin [0,1], \\
+(80 - 7\lambda)\hat{\phi}_U^2 + 2\lambda\hat{\phi}_U + & \hat{\phi}_U, \\
\end{cases}
\]

The corresponding flux limiter function for the Test Scheme is derived rewritten the Eq. (9) (see Waterson and Deconinck [11]) as

\[
\hat{\phi}_f = \hat{\phi}_U + \frac{1}{2} \psi_f(1 - \hat{\phi}_U),
\]

where \( \psi_f = \psi(r_f) \) is the flux limiter function and \( r_f \) is the reason of two consecutive gradients (a sensor). In NV, this sensor is given by

\[
r_f = \frac{1}{1 - \hat{\phi}_U}.
\]

By combining Eqs. (9), (10) and (11), we deduce the flux limiter function for the Test Scheme. The result is

\[
\psi(r_f) = \frac{[(2\lambda - 32)r_f^3 + (160 - 4\lambda)r_f^2 + 2\lambda r_f]}{(1 + r_f)^2}, \text{ if } r_f \geq 0,
\]

or, for the computational implementation, as

\[
\psi(r_f) = \frac{0.5(|r_f| + r_f)[(2\lambda - 32)r_f^3 + (160 - 4\lambda)r_f^2 + 2\lambda r_f]}{(1 + |r_f|)^2},
\]

or still in a more widely used notation (see, e.g., Waterson and Deconinck [11]) as

\[
\psi(r_f) = \max \left\{ 0, \frac{0.5(|r_f| + r_f)[(2\lambda - 32)r_f^3 + (160 - 4\lambda)r_f^2 + 2\lambda r_f]}{(1 + |r_f|)^2} \right\}.
\]

It is important to observe that the Test Scheme is in development, and because of this, here, we have been used \( \lambda = 12 \) for Burgers equation and \( \lambda = 96 \) for other conservation laws. One can also note that, using these parameters, this scheme is TVD/CBC (see Figure 2). This choice was done because we obtained the best results in all tests.

Note that the Test Scheme is monotone and reaches second order accuracy, since its flux limiter function, for \( r_f \geq 0 \), satisfies the condition introduced by Waterson and Deconinck [11], namely a scheme must respect the linear variation of the solution, satisfying \( \psi(1) = 1 \), which is also a necessary condition for achieving second order accuracy on uniform meshes. In addition, the Test Scheme can achieve third order accuracy, since its flux limiter function, for \( r_f \geq 0 \), satisfies \( \psi'(1) = \frac{1}{2} \) (see Zijlema [14]), which is a necessary and sufficient condition for obtaining third order accuracy.
4. NUMERICAL RESULTS

In order to evaluate the Test Scheme, from now on we solve various linear and nonlinear conservation laws, such as 1D Burgers, 1D/2D Euler and 2D acoustics equations. For this, we have used the well recognized CLAWPACK (Conservation LAW PACKage) software of LeVeque [5]. This package uses the Godunov method with a correction term equipped with a flux limiter (see LeVeque [5]), for instance with the monotonized central-difference (MC) of van Leer [10] or with the Test Scheme. For solving 1D Burgers equation, we have used an in-house program (in C language). And as application, the Test Scheme is used for simulating an incompressible free jet impinging onto a rigid surface modeled by axisymmetric Navier-Stokes equations. In this case, we have employed the genuinely Brazilian Freeflow code of Castelo et al. [1] equipped with Test Scheme.

4.1. 1D Conservation laws

Many problems in fluid dynamics that involve conservation of quantities are modeled by hyperbolic conservation laws. In particular, in 1D case, these equations are given by

\[ \phi_t + F(\phi)_x = 0, \]

where \( \phi = \phi(x, t) \) represents the conserved variable vector and \( F(\phi) = F(\phi(x, t)) \) is the flux function vector.

**– Burgers equation**

The nonlinear Burgers equation is one of the simplest PDEs that models a variety of problems. It is given by Eq. (15) with \( \phi = u \) and \( F(\phi) = \frac{1}{2}u^2 \). Here, this equation is defined in \( \Omega = [1, 3.5] \) and supplemented with prescribed boundary condition and with the initial condition

\[ u_0(x) = \begin{cases} 
1, & \text{if } x \leq 1.5, \\
2.5 - x, & \text{if } 1.5 < x \leq 2.5, \\
0, & \text{if } x > 2.5,
\end{cases} \]

whose exact solution is (see Shin et al. [9]):

- For \( t < 1 \):
  \[ u(x, t) = \begin{cases} 
1, & \text{if } x \leq 1.5 + t, \\
2.5 - x, & \text{if } 1.5 + t < x \leq 2.5, \\
0, & \text{if } x > 2.5,
\end{cases} \]

- For \( t > 1 \):
  \[ u(x, t) = \begin{cases} 
1, & \text{if } x \leq 2 + 0.5t, \\
0, & \text{if } x > 2 + 0.5t.
\end{cases} \]

For the simulation of this nonlinear problem, we used a mesh size of 500 computational cells and CFL number \( \theta = 0.5 \).

Figures 3 and 4 show the analytical and numerical (with the Test Scheme) results for transient \( u \) profile as a function of \( x \). One can observe from these figures that, in general, the numerical results with the Test Scheme are of good quality in all domain and better than those provided by the scheme MQUICK (Modified QUICK) of Shin et al. [9].

**– Euler equations**

The 1D Euler equations of gas dynamics are given by Eq. (15), where \( \phi = [\rho, \rho u, E]^T \) and \( F(\phi) = [\rho u, \rho u^2 + p, (E + p)u]^T \), being \( \rho \) the density, \( p \) the pressure, \( \rho u \) the momentum...
and $E$ is the total energy. To close the system formed by $\phi$ and $F(\phi)$, it was considered the ideal gas equation

$$p = (\gamma - 1)(E - \frac{1}{2}\rho u^2),$$

(19)

where $\gamma = 1.4$ is the reason of specific heat. The problem to be simulated here is a challenger Riemann problem proposed by Wood and Collela [13], which involves multiple interactions of strong shocks. Its initial condition is given by

$$(\rho_0, \text{u}_0, p_0)^T = \begin{cases} (1, 0, 1000)^T, & \text{if } 0 \leq x \leq 0.1, \\ (1, 0, 0.01)^T, & \text{if } 0.1 < x \leq 0.9, \\ (1, 0, 100)^T, & \text{if } 0.9 < x \leq 1.0. \end{cases}$$

(20)

The numerical solution was obtained by CLAWPACK software equipped with the Test Scheme flux limiter in a mesh size of 1000 computational cells, at $\theta = 0.9$ and final time $t = 0.38$. The reference solution was generated by the MC limiter in a mesh size of 2000 computational cells, at $\theta = 0.9$ and final time $t = 0.38$. Figures 5-7 show a comparison between the reference and numerical solutions, where it can be seen that the Test Scheme provides solutions in good agreement with the reference one, although introducing numerical viscosity in some regions (see Figure 6 - Zoom 1 and Figure 7 - Zoom 2).
4.2. 2D Conservation laws

For the 2D case, the conservation laws are given by

\[ \phi_t + F(\phi)_x + G(\phi)_y = 0, \]  

(21)

where \( \phi = \phi(x, y, t) \) is the conserved variable vector, and \( F(\phi) = F(\phi(x, y, t)) \) and \( G(\phi) = G(\phi(x, y, t)) \) are the flux function vectors.

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**Acoustics equations**

We solve now the 2D linear hyperbolic system with variable coefficients given by Eq. (21), which models acoustic waves in a heterogeneous (piecewise constant) medium. In this system, \( \phi = [p, u, v]^T \), \( F(\phi) = [Ku, p/\rho, 0]^T \) and \( G(\phi) = [Kv, 0, p/\rho]^T \), being \([u, v]^T\) the velocity vector, and \( K \) bulk modulus of compressibility of the material (for details, the reader is referred to LeVeque [5]). These equations are solved in the domain \( \Omega = [0, 1] \times [0, 1] \), where the interface \( x = 0.5 \) separates two materials (one on the left and another on the right) with different densities and sound speeds \((\rho_L = 1, c_L = 1, \text{and } \rho_R = 4, c_R = 0.5)\). Another important datum for the simulation is a pulse for the pressure, which leads to a radially-symmetric pressure disturbance, namely

\[ r = \sqrt{(x - 0.25)^2 + (y - 0.4)^2}. \]  

(22)

This hyperbolic system is supplemented with the following initial conditions:

\[ p_0 = \begin{cases} 1 + 0.5 \left[ \cos \left( \frac{2\pi r}{0.7} \right) - 1 \right], & \text{if } r < 0.1, \\ 0, & \text{otherwise}, \end{cases} \]  

(23)

\[ u_0 = 0 \quad \text{and} \quad v_0 = 0. \]

For the simulation of this problem, we have used the CLAWPACK software equipped with the Test Scheme flux limiter and the MC limiter for obtaining the reference solution. The numerical solution was obtained in a mesh size of \( 200 \times 200 \) computational cells and Courant number \( \theta = 0.8 \), while the reference solution was calculated in a mesh size of \( 400 \times 400 \) computational cells and Courant number \( \theta = 0.8 \). Figures 8-10 show the cross-sections for the pressure at time \( t = 0.1, 0.4 \) and \( 0.8 \), for both the reference (a) and numerical (b) solutions. Note from these figures that the Test Scheme provides similar results as those derived by reference solutions. In particular, one can also observe that when the numerical pressure pulse hits the interface (see Figure 9 - case (b), it is partially reflected and partially transmitted, in perfect according to the physical phenomenon simulated by the reference solution. In order to complete the analysis, we calculated the pressure variation along of \( y = x \), as shown in Figures 11-13. From this figures, the Test Scheme compares favorable with the reference solution.
The 2D Euler equations of gas dynamics are given by Eq. (21), where \( \phi = [\rho, \rho u, \rho v, E]^T \), \( F(\phi) = [\rho u, \rho u^2 + p, \rho u v, (E + p)u]^T \) and \( G(\phi) = [\rho v, \rho u v, \rho v^2 + p, (E + p)v]^T \), being \([\rho u, \rho v]^T\) the momentum vector and \( E \) is the total energy. To close the system formed by \( \phi \), \( F(\phi) \) and \( G(\phi) \), it was considered the ideal gas equation

\[
p = (\gamma - 1)(E - \frac{1}{2}\rho(u^2 + v^2)),
\]

with \( \gamma = 1.4 \). The problem to be simulated here is the shock-shock interaction described by Ricchiuto et al. [8], which consists in the interaction of two oblique shocks (states a and c) with two normal shocks (states b and d). The considered domain is \( \Omega = [0, 1] \times [0, 1] \) and the Euler equations are supplemented with the initial conditions

\[
[p_0, u_0, v_0]^T = \begin{cases} [1.5, 0, 0, 1.5]^T, & \text{state a,} \\ [0.13799, 1.2060454, 1.2060454, 0.0290323]^T, & \text{state b,} \\ [0.5322581, 1.2060454, 0, 0.3]^T, & \text{state c,} \\ [0.5322581, 0, 1.2060454, 0.3]^T, & \text{state d.} \end{cases}
\]
For the simulation, we used the CLAWPACK software equipped with the Test Scheme flux limiter for the numerical solution (the MC limiter was used for obtaining the reference solution). The numerical solution was obtained in a mesh size of 200 × 200 computational cells at Courant number $\theta = 0.8$, while the reference solution was calculated in a mesh size of 200 × 200 computational cells at Courant number $\theta = 0.5$. The solutions can be seen in Figures 14 and 16, where it is shown contours for the density and pressure, respectively, both at time $t = 0.8$. From these figures, the Test Scheme provides results in good agreement with the reference solution. The analysis is completed by calculating the density and pressure variation on $y = x$, as shown in Figures 15 and 17, respectively. Once more, it can clearly seen that the Test Scheme compares favorable with the reference solution.

4.3. Axisymmetric Navier-Stokes equations

In this section, as an application, we evaluate the Test Scheme in solving laminar incompressible fluid flows involving a moving free surface, modeled by the axisymmetric Navier-Stokes equations. For this, we considered a vertical free jet impinging perpendicularly onto an impermeable rigid surface (under the gravitational field), leading to the formation of a curious phenomenon, observable in everyday life, known as circular hydraulic jump (see Figure 18). For the simulation this phenomenon, we used the axisymmetric version of the Freeflow code of Castelo et al. [1] equipped with the Test Scheme. The instantaneous model equations are

$$\frac{\partial u}{\partial t} + \frac{1}{r} \frac{\partial (ruu)}{\partial r} + \frac{\partial (uv)}{\partial z} = -\frac{\partial P}{\partial r} + \frac{1}{Re} \frac{\partial}{\partial z} \left( \frac{\partial u}{\partial z} - \frac{\partial v}{\partial r} \right) + \frac{g_r}{Fr^2},$$  

(26)

$$\frac{\partial v}{\partial t} + \frac{1}{r} \frac{\partial (vuu)}{\partial r} + \frac{\partial (vv)}{\partial z} = -\frac{\partial P}{\partial z} + \frac{1}{Re} \frac{\partial}{\partial r} \left( \frac{\partial u}{\partial r} - \frac{\partial v}{\partial z} \right) + \frac{g_z}{Fr^2},$$  

(27)

$$\frac{1}{r} \frac{\partial (ru)}{\partial r} + \frac{\partial (rv)}{\partial z} = 0,$$  

(28)

where $t$ is time, $u = u(r, z, t)$ and $v = v(r, z, t)$ are, respectively, the components of velocity vector in the $r$ and $z$ directions and $g = (g_r, g_z)^T$ is the acceleration due to gravity, with $g_r = 0m/s^2$ and $g_z = 9.81m/s^2$. The dimensionless parameters $Re = U_0L_0/\nu$ and $Fr = U_0/\sqrt{L_0g}$ represent, respectively, the Reynolds and Froud numbers, with $\nu$ being the coefficient of kinematic viscosity given by $\nu = \frac{\mu}{\rho}$, where $\mu$ is the dynamic viscosity. Finally, $U_0$ and $L_0$ are characteristic scales for velocity and length, respectively.

A viscous analytical solution for this problem was calculated by Watson [12], for the total thickness of the fluid layer, $h$, flowing on a rigid surface. For this, Watson divided the fluid flow in four regions (see [12]): (i) when $r = O(a)$, the speed outside the boundary layer rises rapidly from 0 at the stagnation point to $U_0$ and the boundary layer thickness is $\delta = O(va/U_0)^{1/2}$, with $a$ being the
impinging jet radius; (ii) for $r \gg a$, where the conditions in region (i) do not affect the flow and the boundary layer remains almost constant (equal to $U_0$), also the velocity distribution has the Blasius profile and the boundary layer thickness is $O(\nu a/U_0)^{1/2}$; (iii) from the point where the boundary layer absorbs the layer of fluid to the point where the velocity profile becomes self-similar; (iv) at large distances from the stagnation point where the final similarity solution is valid. According to Watson [12], the viscous analytical solution is valid only in (ii) and (iv) regions for the Reynolds number $Re = Q/\nu a \gg 1$, with $Q = \pi a^2 U_0$ being the discharge of flow. It is worth adding that his approximate solution is not applicable in the neighborhoods of the stagnation point. Considering the boundary layer thickness being $\delta$, this viscous analytical solution is given by:

- For $r < r_0$:
  \[ h(r) = \left(\frac{a^2}{2r}\right) + \left(1 - \frac{2\pi}{3\sqrt{3}c^2}\right)\delta, \]  
  \[ (29) \]

- For $r \geq r_0$:
  \[ h(r) = \frac{2\pi^2 \nu (r^3 + l^2)}{3\sqrt{3}Qr}, \]  
  \[ (30) \]

where $c = 1.402$, $r_0 = 0.3155aRe^{1/4}$ and $l$ is an arbitrary constant which was estimated by considering the initial development of the boundary layer to be $l = 0.567aRe^{1/4}$.

For the simulation, we considered the following data:
- Mesh-I: $200 \times 126$ computational cells;
- Mesh-II: $400 \times 252$ computational cells;
- Mesh-III: $800 \times 504$ computational cells;
- Domain: $0.050 \times 0.0315m$;
- Length scale: $0.008m$;
- Velocity scale: $0.375m/s$;
- Coefficient of kinematic viscosity: $1.2 \cdot 10^{-5}m^2/s$;
- Reynolds number: $Re = 250$.

Figure 19 shows the comparison between the viscous analytical solution of Watson and the numerical solutions obtained by the Test Scheme, in the meshes Mesh-I, Mesh-II and Mesh-III. This figure also depicts, simple comparison, the boundary layer thickness $\delta$ of Watson. From this figure, one can conclude that the solution obtained by Test Scheme is in agreement with the Watson solution (in the region where it is valid). This simulation shows that the Test Scheme constitutes in a good tool for solving incompressible fluid flows
involving moving free surfaces. As illustration, Figure 20 (see [7]) presents an experiment of the phenomenon. This three dimensional figure is used for comparison with the 3D result obtained by the new scheme.

5. CONCLUSION

In this work we presented a new polynomial upwind scheme for numerical solution of conservation laws and related fluid dynamics problems. For evaluate the performance of the Test Scheme, it was applied for solving Burgers, acoustic and Euler equations. In these linear and nonlin-
ear test cases, the Test Scheme showed good performance. Then, as application, we used the new scheme for simulating a vertical free jet impinging perpendicularly onto a rigid surface, whose numerical solutions showed to be in accordance with the analytical solution of Watson. For the future, we are considering to simulate the circular hydraulic jump in generalized-Newtonian fluids.

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