NUMERICAL SIMULATION OF NEWTONIAN AND NON-NEWTONIAN FREE SURFACE FLOWS USING THE SDPUS-C1 UPWINDING SCHEME

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Abstract. *The study deals with the numerical simulation of complex incompressible fluid flows using a new continuously differentiable bounded convection scheme (called SDPUS-C1). The scheme is based on TVD stability criteria and implemented in the context of finite difference methodology. The performance of the SDPUS-C1 scheme is assessed by solving 2D Newtonian and non-Newtonian moving free surface flows.*

Keywords: *nonlinear convective terms, upwinding, free surface flows*

1. INTRODUCTION

The appropriated modeling of convection terms is a key point for reproducing physical phenomena in fluid dynamics problems. In order to make the simulations of these phenomena more acceptable and reliable, there is an increasing demand for development, analysis and implementation of an upwinding convective scheme (in general nonlinear) which offers simplicity, accuracy, robustness and versatility. Such a scheme is particularly important when incompressible moving free surface flows at high Reynolds numbers are simulated. In addition, schemes with these characteristics have frequently been used for the approximation of the convective terms into the constitutive equations of non-Newtonian fluids (Oishi *et al.*, 2011).

In this article the continuously differentiable bounded upwinding SDPUS-C1 (Six-Degree Polynomial Upwind Scheme of C^1 Class) scheme, introduced recently by (Lima *et al.*, 2012), is employed for the numerical solution of complex incompressible free surface flows. This scheme is based on the NV (Normalized Variable) of Leonard (1988) and satisfies the TVD (Total Variation Diminishing) constraint of Harten (1983). It can achieve third-order accurate in the smooth parts of the solution, but first-order near regions with high gradients.

The objective of the study is to evaluate the performance of the SDPUS-C1 scheme in solving 2D Newtonian and non-Newtonian incompressible fluid flows with moving free surfaces. For this, the following problems are considered: i) collapse of a column of a Newtonian fluid; and ii) the fountain flow and extrudate swell of a non-Newtonian fluid. All convective terms in the governing equations are approximated by the SDPUS-C1 scheme. Results for the fountain flow problem are used to assess the order of convergence of SDPUS-C1 scheme. Other numerical results with this scheme are confronted with the solutions obtained by the well established WACEB (Weighted-Average Coefficient Ensuring Boundedness) (Song *et al.*, 2000) and CUBISTA (Convergent and Universally Bounded Interpolation Scheme for the Treatment of Advection) (Alves *et al.*, 2003) upwind schemes.

2. GOVERNING EQUATIONS AND METHOD OF SOLUTION

The dynamics of a laminar flow is modeled by two equations: the mass and momentum conservation which are, respectively, given by

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Fr^2} g_i + \frac{\partial \tau_{ij}}{\partial x_j}, \tag{2}$$

where t is the time, u_i is the component of the velocity vector, p is the pressure, and $Fr = \frac{U_0}{\sqrt{gL_0}}$ is the Froude number, being U_0 and L_0 the velocity and length scales, respectively. g_i is the acceleration of gravity and τ_{ij} the ij components of the extra-stress tensor. In the case of Newtonian fluid flows, this tensor is given by

$$\tau_{ij} = \frac{2}{Re} D_{ij}, \tag{3}$$

with $Re = \frac{U_0 L_0}{\nu_0}$ the Reynolds number; ν_0 is the viscosity of the fluid . The strain rate D_{ij} in Eq. (3) is given by

$$D_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{4}$$

In the case of non-Newtonian fluid flows, the extra-stress tensor is taken with the sum of Newtonian and non-Newtonian contributions and given by

$$\tau_{ij} = \underbrace{\frac{2\beta}{Re} D_{ij}}_{\text{Newtonian}} + \underbrace{\tau_{ij}^p,}_{\text{non-Newtonian}} \tag{5}$$

where $\beta = \nu_s/\nu_0$ is the ratio between the solvent viscosity ν_s and the solution viscosity $\nu_0 = \nu_s + \nu_p$, begin ν_p the polymeric viscosity. The non-Newtonian contribution τ_{ij}^p is defined by the Oldroyd-B model (Bird *et al.*, 1987a)

$$\tau_{ij}^p + Wi\left[\frac{\partial \tau_{ij}^p}{\partial t} + \frac{\partial (u_k \tau_{ij}^p)}{\partial x_k} - \tau_{ik}^p \frac{\partial u_j}{\partial x_k} - \tau_{jk}^p \frac{\partial u_i}{\partial x_k}\right] = 2\frac{1-\beta}{Re} D_{ij}, \tag{6}$$

where $Wi = \frac{\gamma U_0}{L_0}$ corresponds to the Weissenberg number, with the parameter γ being the relaxation time.

In both Newtonian and non-Newtonian cases, the equations are supplemented with prescribed initial and boundary conditions. At the inflow, the normal and tangential velocities are, respectively, given by $u_{\vec{n}} = U_0$ and $u_{\vec{t}} = 0$, and $\tau_{ij}^p = 0$. At the outflow, the conditions are $\frac{\partial u_i}{\partial x_{\vec{n}}} = \frac{\partial \tau_{ij}^p}{\partial x_{\vec{n}}} = 0$. On rigid boundaries, the no-slip condition is assumed for the velocity, and the conditions for τ_{ij}^p on this boundary can be found in Martins (2009). On a moving free surface, the imposed conditions are $\vec{n} \cdot (\sigma_{ij} \cdot \vec{n}) = 0$ and $\vec{t} \cdot (\sigma_{ij} \cdot \vec{n}) = 0$, with $\sigma_{ij} = -p\delta_{ij} + \tau_{ij}$.

In the solution procedure, the finite difference methodology is employed and the GENSMAC (GENeralized Simplified Marker-And-Cell) method of Tomé and Mckee (1994) is used. This method, defined on a staggered grid, is incorporated into the 2D version of the Freeflow code (Castelo *et al.*, 2000). Time derivatives are discretized (for simplicity) by the explicit Euler method, while the spatial derivatives are approximated by the second-order central differences, except the nonlinear convection terms which are approximated by the SDPUS-C1 scheme.

3. THE SDPUS-C1 SCHEME

The SDPUS-C1 scheme approximates the numerical flux ϕ_f at a cell interface f between two control volumes by using three neighboring grid points, namely the Downstream (D), the Upstream (U) and the Remote-upstream (R), plus the average convective velocity V_f at this face (see Fig. 1). The SDPUS-C1 scheme can then be represented by the (non-normalized) relationship of the form $\phi_f = \phi_f(\phi_D, \phi_U, \phi_R)$. The original variables $\phi_{[\ ]}$ are transformed in NV of

Leonard (1988) as

$$\hat{\phi}_{[\ ]} = \frac{\phi_{[\ ]} - \phi_R}{\phi_D - \phi_R}. \tag{7}$$

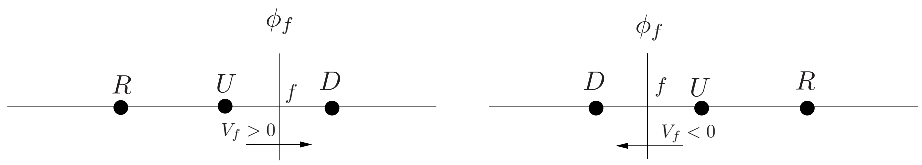

Figure 1. Interface f and related grid points and convection velocity for upwinding.

The advantage of this NV formulation is that $\hat{\phi}_f$ depends on $\hat{\phi}_U$ only, since $\hat{\phi}_D = 1$ and $\hat{\phi}_R = 0$. Thus, the SDPUS-C1 scheme is rewritten as a normalized functional relationship given by $\hat{\phi}_f = \hat{\phi}_f(\hat{\phi}_U)$. The derivation of the SDPUS-C1 scheme is summarized in the following.

It is assumed that $\hat{\phi}_f = \hat{\phi}_f(\hat{\phi}_U)$ is a six-degree polynomial function for $\hat{\phi}_U \in [0,\ 1]$ and a linear function (the first order upwind scheme (Spalding, 1972)) given by $\hat{\phi}_f = \hat{\phi}_U$ for $\hat{\phi}_U \notin [0,\ 1]$. The coefficients of the polynomial are calculated by imposing the following necessary and sufficient conditions of Leonard (1988) for a nonlinear monotonic third-order NV scheme

$$\hat{\phi}_f(1) = 1, \quad \hat{\phi}_f(0) = 0 \quad \text{(necessary conditions for monotonicity)} \tag{8}$$

and

$$\hat{\phi}_f(0.5) = \hat{\phi}'_f(0.5) = 0.75 \quad \text{(necessary and sufficient conditions for third-order),} \tag{9}$$

plus, in order to avoid problems with convergence on coarse meshes (Lin and Chieng, 1991), the condition that the scheme is a continuously differentiable, namely $\phi'_f(0) = \phi'_f(1) = 1$. A free parameter (say λ) is imposed to close the system of equations. In summary, the SDPUS-C1 scheme is given by

$$\hat{\phi}_f = \begin{cases} (-24+4\lambda)\hat{\phi}_U^6 + (68-12\lambda)\hat{\phi}_U^5 + (-64+13\lambda)\hat{\phi}_U^4 + (20-6\lambda)\hat{\phi}_U^3 + \lambda\hat{\phi}_U^2 + \hat{\phi}_U, & \hat{\phi}_U \in [0,1], \\ \hat{\phi}_U, & \hat{\phi}_U \notin [0,1]. \end{cases} \tag{10}$$

It can be showed (see (Lima *et al.*, 2012)) that this scheme satisfies the TVD constraint for $\lambda \in [4, 12]$. It worth noting that a scheme that satisfies the TVD criterion is bounded and presents physically acceptable solutions (Harten, 1983). In this study, the value of $\lambda = 12$ will be used in all simulations, since with this value the scheme generates better solutions than those obtained by using other values of $\lambda \in [4, 12]$ (Lima *et al.*, 2012).

4. NUMERICAL RESULTS

Numerical results for moving free surface flow problems using the SDPUS-C1 scheme are now presented. These results are compared with experimental data and analytical solutions of the literature. In addition, results for Newtonian and non-Newtonian fluid flows are confronted with those generated by WACEB and CUBISTA schemes, respectively. For this, three benchmark problems are considered, namely: i) the collapse of a (Newtonian fluid) column onto a horizontal impermeable wall; and ii) the (non-Newtonian fluid) fountain flow and time-dependent extrudate swell.

4.1 Newtonian fluid flow case

In the numerical results for a Newtonian fluid flow, the geometry considered is a rectangular column where a specified Newtonian fluid is in hydrostatic equilibrium and confined between walls. A wall is instantaneously removed and the fluid, under action of gravity, is free to flow out along the rigid horizontal wall (see Fig. 2). The domain $0.3\,m \times 0.15\,m$ is discretized by 600×300 computation cells, with the length and velocity scales given by $L_0 = a = 0.05\,m$ and $U_0 = 0.74778\,m/s$, respectively. The dimensionless parameters used in the simulation are $Re = 426323.27$ and $Fr = 1$ ($g = 9.81 m/s^2$). Figure 3 depicts the experimental data of Martin and Moyce (1952) and the numerical results with SDPUS-C1 and WACEB schemes, for the position of the fluid front $x_{\max}$ versus time (see Fig. 2). It can be seen, from this figure, that the numerical results agree fairly well with the experimental data. It can be also observed that the solution with the SDPUS-C1 scheme competes very well with the solution generated by the WACEB scheme.

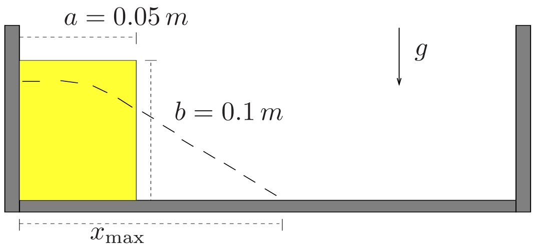

Figure 2. Schematic diagram of the collapse of a fluid column.

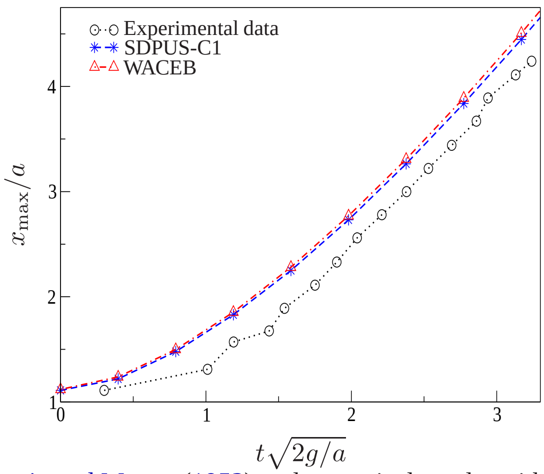

Figure 3. Experimental data of Martin and Moyce (1952) and numerical results with SDPUS-C1 and WACEB schemes for collapse of a Newtonian fluid column.

4.2 Non-Newtonian fluid flow case

In this case, simulations are performed for two complex flows: i) the fountain flow; and ii) the time-dependent extrudate swell.

i) Fountain flow: in this case, a non-Newtonian fluid is injected at the inflow of the a channel with a parabolic velocity profile. Initially, there is a moving free surface along the channel. The problem has a steady state analytical solution (Bird *et al.*, 1987b) which is used for assessing the accuracy of the numerical method equipped with the SDPUS-C1 scheme. Analytical profiles for components u and τ^p_{xx} are

$$u(y) = 4U_0 \left(\frac{y}{L_0}\right)\left(1 - \frac{y}{L_0}\right), \tag{11}$$

$$\tau^p_{xx} = 2\frac{Wi}{Re}(1-\beta)\left(\frac{\partial U}{\partial y}\right)^2. \tag{12}$$

For the simulations, a channel of dimensions $2m \times 10m$ is considered. The length and velocity scales are $L_0 = 1m$ and $U_0 = 1m/s$, respectively, and the dimensionless parameters are $Re = 0.1$, $\beta = 0.5$ and $Wi = 2$. The domain is discretized by using three meshes with 25×5 , 50×10 and 100×20 computacional cells. The relative errors E_h in a mesh with spacing h is calculated in the l_2-norm as

$$||E_h||_2 = \sqrt{\frac{\Sigma(E_S - N_S)^2}{E_S}}, \tag{13}$$

where E_S and N_S denote the exact and numerical solutions, respectively. The order of convergence q is calculated of usual way as

$$q = \frac{\log\left(\frac{||E_h||_2}{||E_{\frac{h}{2}}||_2}\right)}{\log 2}. \tag{14}$$

The fountain flow problem is simulated until final time of $50s$, since at this time the flow reaches the steady state regime. Table 1 shows the errors and the order of convergence of the numerical method with the SDPUS-C1 scheme. From this table it can be seen that, as the mesh is refined, the errors decrease indicating convergence. In addition, one can clearly noted that the scheme provides a convergence rate greater than 2 for the non-Newtonian contribution of the stress-tensor and 2 for u-component of the velocity field.

Table 1. Errors and the order of convergence for the numerical method equipped with SDPUS-C1 scheme. Results for the fountain flow problem.

Variable	Mesh	l_2-Error	q
u	25×5	0.54611×10^{-1}	—
	50×10	0.14954×10^{-1}	1.8686
	100×20	0.36004×10^{-2}	2.0543
τ^p_{xx}	25×5	0.94033×10^{-1}	—
	50×10	0.15752×10^{-1}	2.5776
	100×20	0.69010×10^{-2}	1.1907

ii) Time-dependent extrudate swell: in this case, the problem consists of a jet of fluid exiting of a capillary of width L; depending on the viscosity of the fluid, it swells and its width expands (see Martins (2009) for more details). For the simulation of this problem, the geometry is shown in Fig. 4. It is well known (see, for instance, Tanner (2000)) that the swelling rate S_r is

$$S_r = 0.1 + [1 + 18(Wi)^2]^{\frac{1}{6}} \tag{15}$$

and, at the wall of the domain in Fig. 4, it can be measured whose result is (see Bird *et al.* (1987b))

$$Sr = 0.1 + \left[1 + \frac{1}{2}\left(\frac{\tau^p_{xx} - \tau^p_{yy}}{\tau^p_{xy}}\right)\right]. \tag{16}$$

The numerical results for S_r obtained with the use of the SDPUS-C1 and CUBISTA schemes via Eq. (16) are compared with those of Tanner given by Eq. (15). For the simulation, the domain of $10m \times 1m$ is discretized by 80×20 computational cells; the length and velocity scales are taken as $L_0 = 1m$ and $U_0 = 1m/s$, respectively. The dimensionless parameters $Re = 0.1$, $Fr = 1$ ($g = 9.81m/s^2$) and $\beta = 0.64$, and several Weissemberg numbers, namely $Wi = 0.2, 0.4, 0.6, 0.8,$

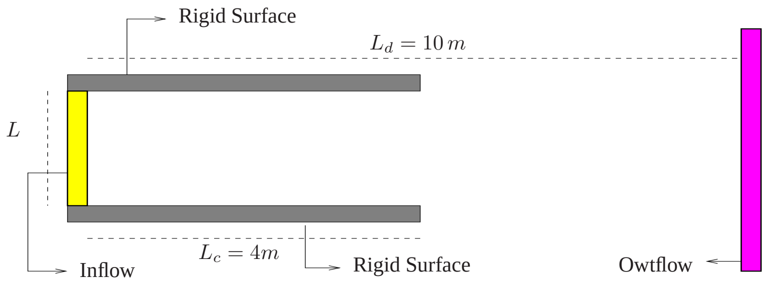

Figure 4. Schematic diagram for the extrudate swell problem.

1.0 and 1.2, are adopted in the computation of Sr.

In Tab. 2 and Fig. 5, it is shown a comparison between Tanner'solution and numerical results at steady state ($t = 80s$) for Sr. It can be observed that there is a good agreement between the numerical results with both CUBISTA and SDPUS-C1 schemes and the analytical solution. However, for $Wi = 0.4$, 0.6, 0.8 and 1.2 the numerical solutions with the SDPUS-C1 scheme are better than that provided by CUBISTA scheme.

Table 2. Swelling rate of an Oldroyd-B fluid as a function of Wi.

Wi	Tanner[1]	SDPUS-C1[2]	CUBISTA[2]
0.2	1.1946	1.3137	1.3097
0.4	1.3535	1.3738	1.3833
0.6	1.4985	1.4981	1.4811
0.8	1.6238	1.6243	1.6076
1.0	1.7335	1.7860	1.7687
1.2	1.8312	1.8627	1.8676

[1] Tanner'solution given by Eq. (15)
[2] Numerical results measured by Eq. (16)

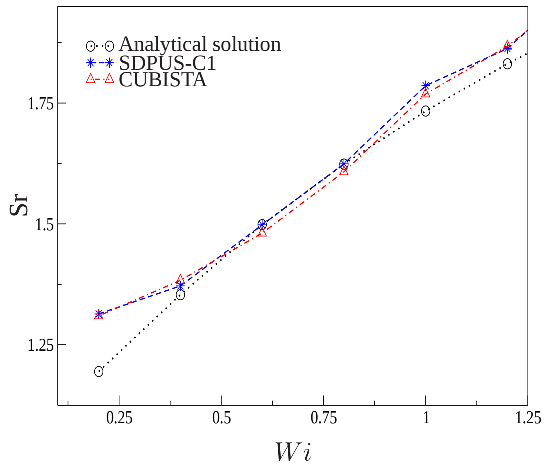

Figure 5. Analytical solution (Tanner, 2000) and the numerical results with SDPUS-C1 and CUBISTA schemes for the extrudate swell problem.

As illustration, Fig. 6 depicts the numerical solutions for velocity field, at time $0.13s$ and at steady state regime, obtained with the SDPUS-C1 scheme for the swelling extruded from an Oldroyd-B fluid.

5. CONCLUSION

A TVD-based upwinding polynomial approximation for the convection term discretization (called SDPUS-C1) has been applied for the solution of complex free surface flows (in cases of Newtonian and non-Newtonian fluids). The

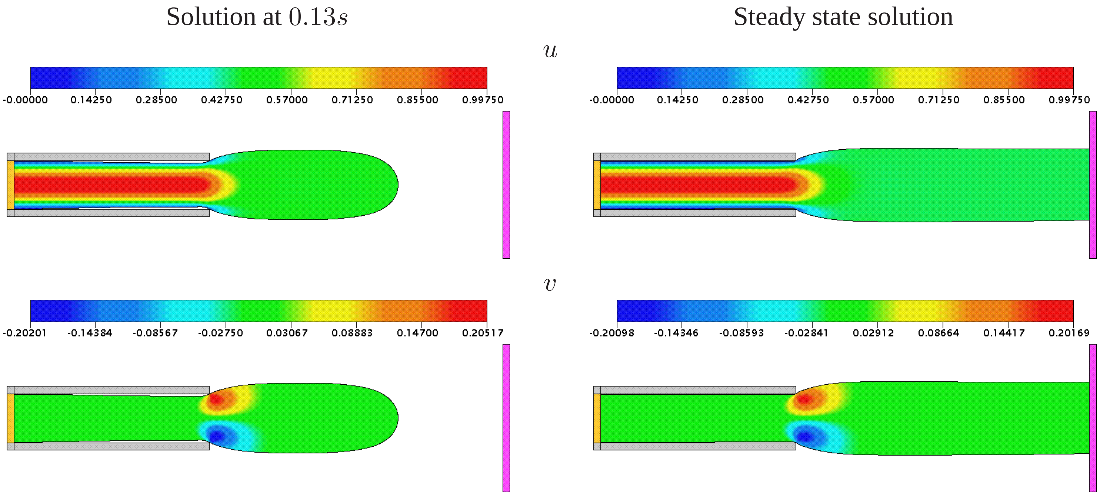

Figure 6. Numerical solutions with the SDPUS-C1 scheme, u and v, for the extrudate swell problem of a non-Newtonian fluid at $Wi = 0.6$.

numerical results show that the scheme is an effective tool for studying these complicated flows and competitive with the well established WACEB and CUBISTA schemes. For the future, the authors are planning to apply the SDPUS-C1 scheme to the numerical solution of turbulent flow of viscoelastic fluids.

6. ACKNOWLEDGMENTS

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