ON PREDICTING NON-NEWTONIAN FLOWS BY USING A STABILIZED FINITE DIFERENCE METHOD WITH PENALTY

Hernán A. González*, Nelson O. Moraga*
* Department of Mechanical Engineering
University of Santiago de Chile
Casilla 10233, Correo 2 Santiago, Chile
e-mail: nmoraga@lauca.usach.cl

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Abstract. This paper presents a numerical method to solve Navier-Stokes equations for laminar flows of non newtonian, incompressible fluids. Differential terms arising in Navier-Stokes equations are discretized by stabilized finite differences of the SUPG type (Stream Upwind Petrov-Galerkin) to calculate the convective terms. A penalty approach is used to introduce the incompressibility condition in the linear momentum equation in order to eliminate the pressure. As a result, a system of equations for the velocities arises. The aim of this paper is to describe the techniques used in the approximations to calculate each term of the discretized model. In particular, time integration techniques, solution of nonlinearities associated to convective terms and constitutive laws, stabilization procedures and discretization of Navier-Stokes equation via finite differences are explained. The method is validated by solving two standard fluid mechanics problems: the flow of a newtonian fluid in a sudden contraction and the developing non-newtonian fluid in a circular tube. Comparison with available experimental results is used to examine the accuracy of the method.
1 INTRODUCTION

Consider the general problem of a non-newtonian, incompressible fluid in laminar flow inside a pipe with a circular cross section.

The governing equations describing the unsteady flow are continuity and linear momentum

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) - 2 \nabla \cdot \left[ \mu \mathbf{e}(\mathbf{u}) \right] + \nabla p = \rho \mathbf{f} \]  \tag{1}

\[ \nabla \cdot \mathbf{u} = 0 \]  \tag{2}

that needs to be solved in \( \Omega \times (0,t_{\text{end}}) \), where \( \Omega \) is the computational domain and \([0,t_{\text{end}}]\) is the time interval. In equations (1)-(2), \( \mathbf{u} \) is the velocity field, \( p \) is the pressure and \( \rho \) is density. The dynamic viscosity \( \mu \) can depend on the invariant symmetric part of the velocity gradient \( \mathbf{e}(\mathbf{u}) \) and \( f \) are the external field forces acting on the fluid element, as for instance the gravity acceleration.

Viscous term in (1) are included on purpose in the divergence, in order to introduce the spatial variations of dynamic viscosity \( \mu \), caused by the dependence on the second invariant of \( \mathbf{e}(\mathbf{u}) \). This procedure allows to introduce into the model the constitutive nonlinear laws that allows to predict Bingham plastic or Casson fluids. This is accomplished by defining the apparent dynamic viscosity as follows,

\[ \mu(x,t) = \mu\left(I,\mathbf{e}(\mathbf{u})\right) \]  \tag{3}

As a result, a new nonlinearity arises in the mathematical model, which will be examined later.

Figure 1 shows the physical situation for the fluid flow inside an axi-symmetric pipe with a sudden contraction. Inlet velocity is assumed to be defined with a known spatial distribution. On the interval walls the no-slip condition is applied. Denote \( \Gamma_{\text{inp}}, \Gamma_{\text{out}} \) y \( \Gamma_{\text{wall}} \) as the three parts of the contour describing inlet, outlet and lateral walls. Let \( \mathbf{\sigma} \) be the Cauchy stress tensor, defined as \( \mathbf{\sigma} = -p\mathbf{I} + 2\mu \mathbf{e}(\mathbf{u}) \) and be \( n \) the normal to the external surface of \( \Omega \). When prescribed values are defined with a bar on top, the boundary conditions for velocity are:

\[ u(x,t) = \bar{u}(x,t) \quad \text{in} \quad \Gamma_{\text{inp}} \]  \tag{4}

\[ u(x,t) = \mathbf{0} \quad \text{in} \quad \Gamma_{\text{wall}} \]  \tag{5}

\[ n \cdot \mathbf{\sigma}(x,t) = 0 \quad \text{in} \quad \Gamma_{\text{out}} \]  \tag{6}

for times \( t \in (0,t_{\text{end}}) \).

Velocity distribution \( \bar{u}(x,t) \) must be defined from existing experimental data. The full description of the mathematical model is completed after an initial condition is specified as a known initial velocity distribution \( u^0(x) \) is defined in the domain.

\[ u(x,0) = \mathbf{u}^0(x) \quad x \in \Omega \]  \tag{7}

The computational domain and boundary conditions are described in Fig. 1. Dimensions used are those defined in a previous paper that reports experimental laser Doppler measurements for the
velocity at different locations for a flow in a pipe with a sudden contraction, that are going to be used as a validation procedure.

\[
\begin{align*}
\Gamma_{\text{in}} & \quad 25\text{mm} \\
9.5\text{mm} & \\
\Gamma_{\text{wall}} & \quad 5.1\text{mm} \\
25\text{mm} & \quad \Gamma_{\text{out}}
\end{align*}
\]

Fig. 1. Computational domain and boundary condition for flow in sudden contraction

2 FINITE DIFFERENCE METHOD

The description of the finite differences method used and the algorithm developed to solve the general problem of fluid dynamics for laminar, non-newtonian, incompressible, unsteady flows is described here.

Two overlapping grids are defined after finite differences have been applied to a Cartesian system with base \( \{e_1, e_2\} \) for a two dimensional flow. Overlapping results in a consistent method due to the use of conservative equations as discussed previously.

2.1 Time discretization

Use the Crank-Nicholson method to obtain the time discretization of equations (1)-(2). Let define \( 0=t^0 < t^1 \ldots < t^n = t_{\text{end}} \) as a partition of the time interval, with the following notation:

\[
\delta f_i^n := f_i^{n+1} - f_i^n, \quad f_i^{n+1/2} = \frac{f_i^{n+1} + f_i^n}{2}
\]

where \( f_i \) is a generic time function and \( f_i^n \) denotes the value of \( f_i \) in time \( t^n \). The Crank-Nicholson method is implemented in terms of \( u_i^{n+1/2} \), instead of \( u_i^{n+1} \), and hence that the local acceleration is evaluated in the following way:

\[
\frac{\delta u_i^n}{\delta t} = 2\frac{u_i^{n+1/2} - u_i^n}{t^{n+1} - t^n}
\]

Let assume that the force vector \( f_i \) is continuous in time, the Crank-Nicholson scheme applied to eqs. (1)-(2) generates the following model discretized in time, where \( u_i^n \) is known and \( u_i^{n+1} \) and \( p_i^{n+1} \) must be found by the following way:

\[
\rho \left[ \frac{\delta u_i^n}{\delta t} + u_i^{n+1/2} \cdot \left( \frac{\partial u_i^{n+1/2}}{\partial x_j} \right) \right] - \mu \left( \frac{\partial^2 u_i^{n+1/2}}{\partial x_j^2} \right) = \frac{\partial p_i^{n+1}}{\partial x_i} + \delta f_i^{n+1/2}
\]

(10)
\[ \frac{\partial u_{j}^{n+1}}{\partial x_j} = 0 \]  

where sub-indexes \( i \) and \( j \) are 1, 2, 3 in a general 3D problem.

Equations (10) and (11) must satisfy the boundary conditions:

\[ u_i^{n+\mathcal{K}} = \overline{u}_i^{n+\mathcal{K}} = \frac{\overline{u}(x,t^{n}) + \overline{u}(x,t^{n-1})}{2} \quad \text{in } \Gamma_{\text{out}} \]

\[ u_i^{n+\mathcal{K}}(x) = 0 \quad \text{in } \Gamma_{\text{ent}} \]

\[ n_j \left( - p \delta_{ij} + \mu \left( \frac{\partial u_i^{n+\mathcal{K}}}{\partial x_j} + \frac{\partial u_j^{n+\mathcal{K}}}{\partial x_i} \right) \right) = 0 \quad \text{in } \Gamma_{\text{sal}} \]

where \( \delta_{ij} \) is the Kronecker delta and \( n_j \) is the unit vector normal to surface \( \Gamma_{\text{out}} \).

### 2.2 Linearization of equations

The last step in the discretization process is the linearization of problem (10). The two sources of non-linearities are: convective terms and the non linear nature of the apparent viscosity.

The conservative terms can be calculated by using an iterative technique. In the present method the Picard fixed point scheme has been used. Let define super-index \( k \) as the iteration index, then an approximation \( u_i^{n+\mathcal{K},k} \) of \( u_i^{n+\mathcal{K}} \) can be calculated by the following approximation:

\[ \left( u_i^{n+\mathcal{K},k+1} \cdot \nabla \right) u_i^{n+\mathcal{K},k+1} \approx \left( u_i^{n+\mathcal{K},k} \cdot \nabla \right) u_i^{n+\mathcal{K},k+1} \]

Therefore, in order to linearize problem (10) the following procedure was used: for an approximation of \( u_i^{n+\mathcal{K},k} \) of \( u_i^{n+\mathcal{K}} \), find \( u_i^{n+\mathcal{K},k+1} \) as the solution to the problem:

\[ \rho \left[ \frac{\partial u_i^{n+\mathcal{K},k+1}}{\partial t} + u_j^{n+\mathcal{K},k} \cdot \left( \frac{\partial u_i^{n+\mathcal{K},k+1}}{\partial x_j} \right) \right] = - \frac{\partial \mu^{n+\mathcal{K},k}}{\partial x_j} \left( \frac{\partial u_i^{n+\mathcal{K},k+1}}{\partial x_j} \right) + \frac{\partial p^{n+\mathcal{K},k+1}}{\partial x_j} = \rho f_i^{n+\mathcal{K}} \]

where \( \mu^{n+\mathcal{K},k} \) denotes the viscosity calculated with \( u_i^{n+\mathcal{K},k} \). After solving equation (16), convergence must be verified iteratively until to reach the required requirement, make \( k \leftarrow k+1 \) and solve again (16).

### 2.3 Penalization for Navier-Stokes equations

Numerical solution of equations (10) and (11) is obtained by penalization. The main idea is to
produce a perturbated version of the incompressibility equation, by introducing the pressure multiplied by a penalty factor

$$\varepsilon \ p + \frac{\partial u_j}{\partial x_j} = 0$$

(17)

where $\varepsilon$ is an small constant parameter$^3$. The discrete representation of the linearized penalized version of Navier-Stokes equations is:

$$\rho \left[ \frac{\partial u_j^{n+1,k}}{\partial t} + u^+_i \partial_j \left( \frac{\partial u_j^{n+1}}{\partial x_j} \right) \right] - \mu \partial_j \left( \frac{\partial u_j^{n+1,k+1}}{\partial x_j} \right) = \frac{\partial p^{n+1,k+1}}{\partial x_j}$$

(18)

$$\varepsilon \ p^{n+1,k+1} + \frac{\partial u_j^{n+1,k+1}}{\partial x_j} = 0$$

(19)

2.4 Finite difference Approximation

A two dimensional representation of problem (18), (19) is defined in terms of the super-index $l$ and $m$. Let define a grid with a discrete set of points $x = l_1 \ h_1$, $y = m_2 \ h_2$ and denote $f^{l,m} = f(lh_1, mh_2)$. The factors $h_1$ and $h_2$ are the grid sizes used to discretize the physical domain in $x$ and $y$. When this two factors are equal to a constant $h$ value, the operators acting on the grid $f = \{ f^{l,m} \}$ used are described in table 1.

<table>
<thead>
<tr>
<th>Table 1. Finite difference operators.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{1+}f^{l,m} = \frac{f^{l+1,m} - f^{l,m}}{h}$, $D_{2+}f^{l,m} = \frac{f^{l,m+1} - f^{l,m}}{h}$</td>
</tr>
<tr>
<td>$D_{1-}f^{l,m} = \frac{f^{l,m} - f^{l,m-1}}{h}$, $D_{2-}f^{l,m} = \frac{f^{l+1,m} - f^{l,m-1}}{h}$</td>
</tr>
<tr>
<td>$D_{10}f^{l,m} = \frac{f^{l+1,m} - f^{l-1,m}}{2h}$, $D_{20}f^{l,m} = \frac{f^{l,m+1} - f^{l,m-1}}{2h}$</td>
</tr>
</tbody>
</table>

The standard formulation in finite differences, obtained by using the operators defined in Table 1, when applied to equation (18) has a major drawback when convective terms are important, as is usual near a region with a sudden change in cross section. Using artificial diffusion can reduce numerical induced oscillation arising in these cases.
2.5 Staggered grids

Figure 2a shows the finite difference discretization of the flow domain in terms of the base \{e_1, e_2\}. The finite volume that results of the overlapping is shown in gray. Pressure and all scalar variables such as density, viscosity and temperature are evaluated at the nodal points located in the center of the volume. Velocity components and heat fluxes are calculated at the cell faces, as it is shown in Fig. 2b.

The choice of the center of the volume to calculate pressure, allows that the approximation scheme selected for velocity be one order higher than the scheme used to evaluate the pressure. This is similar to the situation in the finite element formulation, where the convergence and the selection of possible type of elements is made by imposing special properties\(^4\), in particular div-stability.

Velocity for the finite volume in figure 2b is calculated as follow,

\[
\begin{align*}
  u &= \left( \frac{u_1^e + u_1^n}{2}, \frac{u_2^e + u_2^n}{2} \right) \\
  (20)
\end{align*}
\]

where: super-indexes \(w\), \(e\), \(s\) and \(n\) make references to the velocity nodes that are at west, east, south and north of the pressure node.

![Fig. 2a. Grids](image1)

![Fig. 2b. 2D finite volume](image2)

Discretization of the domain by this technique can be understood as the superposition of three grids: one for \(u\) component of the velocity in \(x_1\) direction, another for the \(v\) component of the velocity in \(x_2\) direction and a third one for pressure.

Based on the grid defined, the approximation for the differential terms in the equation (18)-(19) can be introduced. Second order derivatives, can be calculated for instance by the following expression:

\[
\begin{align*}
  \frac{\partial^2 u_i}{\partial x_i^2} &= (D_{ii}D_{ii}u_i^{lm}) = \frac{u_i^{l+1,m} - 2u_i^{l,m} + u_i^{l-1,m}}{h^2} \\
  (21)
\end{align*}
\]

where: \(u_i^{l+1,m}, u_i^{l,m}\) and \(u_i^{l-1,m}\) are the velocity of nodes \(l+1,m; l,m\) and \(l-1,m\) respectively, with all nodes located in \(x_1\) direction, and \(h\) denoting the grid spatial size.

The expressions used to calculate the derivatives in problem (18)-(19) have an error of order 2 for velocity and an error of order 1 for pressure.
2.6 Stabilized finite differences

At high Reynolds numbers the convective terms in momentum equation (1) are important and the finite difference approximation is less stable. Spurious oscillations of velocity arise that tends to introduce numerical oscillations in the solution as the Reynolds number increases. An upwind diffusion in the direction of the flow particles has been used in this work. This approximation for the convective terms is:

\[ u_j \frac{\partial u_i}{\partial x_j} \approx u_j \left( D_{0,j} u^{l,m}_i \right) - \frac{h_i u_i \cdot u_j \cdot f \left( P^{l,m}_i \right)}{2 |u|} \left( D_{-j} D_{v,j} u^{l,m}_i \right) \]  (22)

where: \( h_i \) is the size of grid in \( i \) direction, \( f \left( P^{l,m}_i \right) \) is a function of the local Peclet number \( P^{l,m}_i \), and \( |u| \) is the norm of vector \( u_i \). Therefore \( P^{l,m}_i \) and \( f \left( P^{l,m}_i \right) \) are defined as follows.

\[ P^{l,m}_i = \frac{u_j^{l,m} h_i}{\mu^{l,m}_i} \cdot f \left( P^{l,m}_i \right) = \begin{cases} \frac{P^{l,m}_i}{3} & \text{si } 0 \leq P^{l,m}_i \leq 3 \\ P^{l,m}_i & \text{si } 3 \leq |P^{l,m}_i| \end{cases} \]  (23)

These expressions (23) were obtained stabilizing, by an artificial diffusion (24), a one-dimensional convection-diffusion equation.

\[ \frac{h_i \cdot u_j^{l,m} \cdot f \left( P^{l,m}_i \right)}{2} \]  (24)

The term \( f \left( P^{l,m}_i \right) \) increases the accuracy of the SUPG method.

The discrete final expression for the Navier-Stokes equation is obtained after making a discrete approximation in time, by using a Crank-Nicholson approach that it has been linearized by the Picard fixed point method and approximated by a stabilized finite difference scheme.

\[ \rho \left[ \left( \frac{\partial u_j^{l,m}}{\partial t} \right)^{n+1} + \left( u_j^{l,m} \right)^{n+1} \frac{K^{k}}{2} - \left( D_{0,j} u_j^{l,m} \right)^{n+1} \frac{K^{k}}{2} - \frac{h_i u_i \cdot f \left( P^{l,m}_i \right)}{2 \sum (u_i)^2} \left( D_{-j} D_{v,j} u_i^{l,m} \right)^{n+1+K^{k+1}} \right] \]

\[ - \left( u_j^{l,m} \right)^{n+1} \frac{K^{k}}{2} - \left( D_{0,j} u_i^{l,m} \right)^{n+1} \frac{K^{k}}{2} - \left( D_{-j} D_{v,j} u_i^{l,m} \right)^{n+1+K^{k+1}} \]

\[ + \left( D_{-i} P^{r,s} \right)^{n+1+K^{k+1}} = \rho f^{n+K^{k+1}} \]  (25)

where sub-indexes \( r \) and \( s \) are associated to the defined grid for the pressure field. Sub-indexes \( l \) and \( m \) are related to the grid used to calculated the velocities.
2.7 Elimination of pressure

Pressure in equation (25) can be eliminating by using equation (26). A system of equations is obtained in which velocities are the unknowns. This is a convenient choice from the numerical point of view, because the size of the system of linear equations is reduced.

Finally, the discrete equation used to calculate the velocity field is,

\[
\rho \left[ \left( \frac{\delta u_i}{\delta t} \right)^{n+1}_{k} + \left( u^{n}_{i,m} \right)^{n+1} \right] \cdot \left[ \begin{array}{c}
\left( D_{0,j} u_i^{n}_{j,m} \right)^{n+1}_{k+1} - \frac{h_j \cdot f_{j,m}^{l}}{2} \left( D_{-j} u_i^{n}_{j,m} \right)^{n+1}_{k+1} \\
2 \left( \sum_{k=1}^{n} (u_k) \right)^2 \\
- \left( \mu^{n+1}_{j,m} \right)^{n+1}_{k+1} \left( D_{0,j} u_i^{n}_{j,m} \right)^{n+1}_{k+1} - \left( D_{0,j} \mu^{n+1}_{j,m} \right)^{n+1}_{k+1} \left( D_{0,j} u_i^{n}_{j,m} \right)^{n+1}_{k+1} + \left( D_{0,j} u_i^{n}_{j,m} \right)^{n+1}_{k+1} \\
- \frac{1}{\epsilon} \left( D_{0,j} u_i^{n}_{j,m} \right)^{n+1}_{k+1} \right] = \left( P_{j,m}^{l} \right)^{n+1}_{k+1}
\]

(27)

2.8 Algorithm

A simulation software was built that uses an iterative standard algorithm to solve Navier-Stokes equations for incompressible, non-newtonian flows with time dependent boundary condition. The algorithm is:

Let \( n = 0 \). Read initial velocity condition \( u_i^0 \)

For \( n = 0, 1, 2, \ldots, N-1 \)

Use the boundary conditions for velocity \( u_i^{n+1} \).

Let \( k = 0 \), \( u_i^{n+1} = u_i^n \), \( \mu_h^{n+1} = \mu_h^n \).

Before convergence let:

\( k \leftarrow k+1 \)

Solve problem (26) for \( u_i^{n+1} \).

Calculate the known values for viscosity \( \mu_h^{n+1} \) using (3).

Evaluate convergence

End

Convergence is verified by using an standard procedure. Euclidean discrete norm is used, calculated as the difference between the unknown velocity vectors at the present iteration and those from the last iteration \((k+1)\) and \(k\) of algorithm). The norm is calculated and must be smaller than an \( \epsilon \) value that is calculated in a normalized way with the values of the unknown velocities in the present iteration.
4 RESULTS

The finite-difference penalty method is applied to solve two classical fluid mechanics problems: (1) newtonian flow in a pipe with a sudden contraction and (2) a non newtonian, Casson fluid, developing in a pipe. In both cases, experimental results for velocity measured with laser-Doppler anemometer are available.

Figure 1 shows the geometry, boundary condition and the coordinate system describing problem 1. Numerical simulation was performed to calculate velocity profiles at five axial locations, three before the sudden contraction and two after the contraction. Figure 3 shows the positions where velocity is calculated.

Experimental data are compared to the values calculated with the developed method and with those values calculated with the finite volume method, SIMPLE algorithm.

Figures 4a to 4e shows the velocity distribution at the five locations for a Reynolds number equal to 372.

Results with the proposed methodology, shown with a continuos line, show an overall agreement with experimental values. The accuracy of the proposed method is seem to decrease near the contracted region.

Fig. 3 Axial locations for numerical calculations of velocity.

Fig. 4a. Velocity for position x/D = -0.523

Fig. 4b. Velocity for position x/D = -0.236
The system of discrete equations has been obtained by using a particular iterative projection method, that is known as complete orthogonal method FOM. An small value of tolerance must be used in the FOM scheme, due to the effect of ill conditioning caused by the penalty parameter $\varepsilon$. This value of $\varepsilon$ is very important in order to satisfy continuity requirements in all the domain. When $\varepsilon$ is small FOM method is less effective and convergent solution is difficult to get. A good choice for this value $\varepsilon = 0.01$ was obtained by trial and error for problem 1.

The values used in the calculation were: $1 \times 10^{-5}$ for tolerance in FOM scheme, 1% for Picard iterative cycle, a penalty $\varepsilon$ factor of 0.01 and a grid with 60×79 nodes. The use of an iterative method causes losses of accuracy in the method in those regions where the convective terms are larger. The method is very sensitive to the Krylov space used to built the orthogonal bases in the FOM method and to the tolerance used.
Problem 2:
The second problem studied is the developing flow of a non-newtonian, Casson type fluid, developing in the entrance of a circular pipe.

In this numerical experiment the blood flow is predicted assuming a behavior of a plastic Casson fluid,

\[ \sqrt{\tau} = \sqrt{\tau_0} + \sqrt{\mu_c D} \]  

(28)

where \( \tau_0 \) is the yield stress, \( \mu_c \) is the dynamic Casson viscosity and \( D \) is the deformation rate of the fluid, that is defined in terms of the second invariant of the velocity tensor. When \( \tau \) is lower than \( \tau_0 \) the fluid flow is zero. The numerical simulation was accomplished for the case where: \( \mu_c = 4 \times 10^{-3} \) [Pa·s]; \( \rho = 1050 \) [Kg/m³]; \( Re = 0.107 \) and \( \tau_0 = 0.27 \) [Pa].

A schematic view of the geometry and dimensions is shown in Figure 5.

![Fig.5 Non-newtonian fluid in entrance region of a circular pipe](image)

The numerical experiment in this case aimed to find the local velocity distribution in the entrance region.

The velocity profile for a blood flow, described as a Casson fluid and the same result for a newtonian fluid are show in figure 6. Measured velocity profile at the outlet very well with the numerical simulation for a Casson type of fluid.

![Fig. 6 Velocity distribution at the outlet](image)
5 CONCLUSIONS

A new numerical scheme has been developed and implemented to solve the discretized fluid mechanics governing equations for incompressible, non-newtonian flows in laminar flows. Time integration is performed with a Crank-Nicholson scheme, a fixed Picard point is used to calculate the convective terms, along with a penalty stabilized finite difference method.

The algorithm developed was used to solve two problems: (1) a newtonian flow in a pipe with a sudden contraction and (2) a non-newtonian, Casson-type fluid, in the entrance region of a circular pipe. Comparison with experimental results shows overall agreement in the velocity distributions.

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