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Inexact Newton-Type Methods for the Solution of Steady Incompressible Non-Newtonian Flows with the SUPG/PSPG Finite Element Formulation

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Abstract In this work we evaluate the performance of inexact Newton-type schemes to solve the nonlinear equations arising from the SUPG/PSPG finite element formulation of steady non-Newtonian incompressible fluid flows. The flow in eccentric annuli with Power Law and Bingham fluids is employed as benchmark. Our results have shown that inexact schemes are more efficient than traditional Newton-type strategies.

Key words: Inexact Newton, Non-Newtonian flow, Stabilized formulations, Finite elements.

INTRODUCTION

Several modern material and manufacturing processes involve non-Newtonian fluids. Examples of non-Newtonian behavior can be found in processes for manufacturing coated sheets, optical fibers, foods, drilling muds and plastic polymers. Numerical simulations of non-Newtonian behavior represent a particular and difficulty case in incompressible fluid flows. In these fluids the dependence between the viscosity and the shear rate increases the nonlinear character of the governing equations.

Many works proposed combinations between stabilized finite element formulations and algorithms to solve the nonlinear problems arising from non-Newtonian incompressible flow simulations. In [2], [11] and [13] the authors solve the resulting finite element nonlinear equations with Newton-Raphson algorithm; Meuric *et al*. in [10] used the SUPG formulation with Newton-Raphson and Picard iterations combined as a strategy to circumventing some computational difficulties in annuli flow computations. Some of these strategies employ analytical or directional forms of Jacobians in the Newton method. The analytical derivative of the stabilization terms are often difficult to evaluate. In this work, we consider the stabilized finite element formulation proposed by Tezduyar [15] applied to solve steady non-Newtonian incompressible flows. We also test the performance of the Jacobian form described by Tezduyar in [16]. This numerically approximated Jacobian is based in Taylor's expansions of the nonlinear terms and presents an alternative and simple way to implement the tangent matrix employed by Newton-type methods.

The inexact-Newton method associated with iterative Krylov solvers have been used to reduce computational costs in many problems of computational fluid dynamics, offering a trade-off between accuracy and computational effort spent per iteration. Shadid and co-workers presented in [14] an inexact-Newton method applied to problems involving Newtonian fluids, mass and energy transport, discretized by SUPG/PSPG formulation and equal-order interpolation elements. Recently, Knoll and Keyes [9] discussed the constituents of a broader class of inexact-Newton methods, the Jacobian-Free Newton-Krylov methods. We address here only the essentials of the inexact-Newton methods to solve the nonlinear equations arising from the SUPG/PSPG finite element formulation of steady non-Newtonian incompressible fluid flows and the interested reader should refer to Knoll and Keyes, and the references therein, for a more detailed presentation. The remainder of this paper is organized as follows. Sections 2 and 3 present the governing equations and the SUPG/PSPG finite element formulation. Section 4 introduces the inexact Newton-type schemes under consideration. The test problems are presented in Section 5 and the paper ends with a summary of our main conclusions.

GOVERNING AND CONSTITUTIVE EQUATIONS

Let $\Omega \subset \mathbb{R}^{n_{sd}}$ be the spatial domain, where n_{sd} is the number of space dimensions. Let Γ denote the boundary of Ω. We consider the following velocity-pressure formulation of the Navier-Stokes equations governing steady incompressible flows:

$$\rho(\mathbf{u} \cdot \nabla\mathbf{u} - \mathbf{f}) - \nabla \cdot \boldsymbol{\sigma} = 0 \qquad \text{on } \Omega \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{on } \Omega \tag{2}$$

where ρ and $\mathbf{u}$ are the density and velocity, $\boldsymbol{\sigma}$ is the stress tensor given as

$$\boldsymbol{\sigma}(p,\mathbf{u}) = -p\mathbf{I} + \mathbf{T}, \tag{3}$$

where p is the hydrostatic pressure, **I** is the identity tensor and **T** is the tensor of deviatoric stress.

The essential and natural boundary conditions associated with equations (1) and (2) can be imposed at different portions of the boundary Γ, and they are represented by,

$$\mathbf{u} = \mathbf{g} \qquad \text{on } \Gamma_g \tag{4}$$

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \mathbf{h} \qquad \text{on } \Gamma_h \tag{5}$$

where Γ_g and Γ_h are complementary subsets of Γ.

The relationship between the stress tensor and deformation rate for Newtonian fluids is defined by a proportionality constant, that represents the momentum diffusion experimented for the fluid when flowing. Therefore, the deviatoric tensor in (3) can be expressed by,

$$\mathbf{T} = 2\mu\boldsymbol{\varepsilon}(\mathbf{u}) \tag{6}$$

where μ is the proportionality constant known as dynamic viscosity and $\boldsymbol{\varepsilon}$ is deformation rate tensor or

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \tfrac{1}{2}\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right] \tag{7}$$

The fluids that do not obey the relationship expressed in equation (6) are known as non-Newtonian fluids. The main characteristic of these fluids is the dependence of viscosity with others flow parameters, such as, deformation rate and even the deformation history of the fluid. In these cases, equation (6) can be rewritten as,

$$\mathbf{T} = 2\mu(\dot{\gamma})\boldsymbol{\varepsilon}(\mathbf{u}) \tag{8}$$

where $\dot{\gamma}$ is the second invariant of the strain rate tensor and $\mu(\dot{\gamma})$ is the apparent viscosity of the fluid [3], [12].

In this work the non-Newtonian flows considered are viscoplastic fluids described by Power Law and Bingham models. The rheology models and non-Newtonian viscosity relations follow the definitions included in [3], [7], and [12], thus for Power Law fluids we have,

$$\mu(\dot{\gamma}) = \begin{cases} \mu_0 K \dot{\gamma}^{n-1} & \text{if } \dot{\gamma} > \dot{\gamma}_0 \\ \mu_0 K \dot{\gamma}_0^{n-1} & \text{if } \dot{\gamma} \le \dot{\gamma}_0 \end{cases} \tag{9}$$

where K denotes the consistency index, μ_0 is a nominal viscosity, n the Power Law index and $\dot{\gamma}_0$ is the cutoff value for $\dot{\gamma}$. For Bingham fluids we use the bi-viscosity model expressed as,

$$\mu(\dot{\gamma}) = \begin{cases} \mu_0 + \dfrac{\sigma_Y}{\dot{\gamma}} & \text{if } \dot{\gamma} > \dfrac{\sigma_Y}{\mu_r - \mu_0} \\ \mu_r & \text{if } \dot{\gamma} \le \dfrac{\sigma_Y}{\mu_r - \mu_0} \end{cases} \tag{10}$$

where μ_r is the Newtonian viscosity chosen to be at least an order of magnitude larger than μ_0. Typically μ_r is approximately $100\mu_0$ to represent a true Bingham fluid behavior [1].

FINITE ELEMENT FORMULATION

Let us assume following Tezduyar [15] that we have some suitably defined finite-dimensional trial solution and test function spaces for velocity and pressure, $S_{\mathbf{u}}^h$, $V_{\mathbf{u}}^h$, S_p^h and $V_p^h = S_p^h$. The finite element formulation of equations (1) and (2) using SUPG and PSPG stabilizations for incompressible fluid flows [15] can be written as follows: find $\mathbf{u}^h \in S_{\mathbf{u}}^h$ and $p^h \in S_p^h$ such that $\forall \mathbf{w}^h \in V_{\mathbf{u}}^h$ and $\forall q^h \in V_p^h$:

$$\begin{aligned} &\int_\Omega \mathbf{w}^h \cdot \rho\left(\mathbf{u}^h \cdot \nabla \mathbf{u}^h - \mathbf{f}\right) d\Omega + \int_\Omega \boldsymbol{\varepsilon}\left(\mathbf{w}^h\right) : \boldsymbol{\sigma}\left(p^h, \mathbf{u}^h\right) d\Omega - \int_\Gamma \mathbf{w}^h \cdot h \, d\Gamma + \int_\Omega q^h \nabla \cdot \mathbf{u}^h d\Omega \\ &+ \sum_{e=1}^{n_{el}} \int_\Omega \tau_{SUPG} \mathbf{u}^h \cdot \nabla \mathbf{w}^h \cdot \left[\rho\left(\mathbf{u}^h \cdot \nabla \mathbf{u}^h\right) - \nabla \cdot \boldsymbol{\sigma}\left(p^h, \mathbf{u}^h\right) - \rho \mathbf{f}\right] d\Omega \\ &+ \sum_{e=1}^{n_{el}} \int_\Omega \frac{1}{\rho} \tau_{PSPG} \nabla q^h \cdot \left[\rho\left(\mathbf{u}^h \cdot \nabla \mathbf{u}^h\right) - \nabla \cdot \boldsymbol{\sigma}\left(p^h, \mathbf{u}^h\right) - \rho \mathbf{f}\right] d\Omega = 0 \end{aligned} \tag{11}$$

In the above equation the first four integrals on the left hand side represent terms that appear in the Galerkin formulation of the problem (1)-(5), while the remaining integral expressions represent the additional terms which arise in the stabilized finite element formulation of the problem. Note that the stabilization terms are evaluated as the sum of element-wise integral expressions. The first summation corresponds to the SUPG (Streamline Upwind Petrov/Galerkin) term and the second correspond to the PSPG (Pressure Stabilization Petrov/Galerkin) term. The spatial discretization of equation (11) leads to the following system of nonlinear equations,

$$\begin{bmatrix} \mathbf{N}(\mathbf{u})+\mathbf{N}_{\delta}(\mathbf{u})+\mathbf{K} & -(\mathbf{G}+\mathbf{G}_{\delta}) \\ \mathbf{G}^{T}+\mathbf{N}_{\varphi}(\mathbf{u}) & \mathbf{G}_{\varphi} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{\mathbf{u}} \\ \mathbf{f}_{\boldsymbol{p}} \end{bmatrix} \tag{12}$$

where $\mathbf{u}$ is the vector of unknown nodal values of $\mathbf{u}^{h}$ and $\boldsymbol{p}$ is the vector of unknown nodal values of $\boldsymbol{p}^{h}$. The non-linear vectors $\mathbf{N}(\mathbf{u})$, $\mathbf{N}_{\delta}(\mathbf{u})$, and $\mathbf{N}_{\varphi}(\mathbf{u})$ the matrices $\mathbf{K}$, $\mathbf{G}$, $\mathbf{G}_{\delta}$, and $\mathbf{G}_{\varphi}$ emanate, respectively, from the convective, viscous and pressure terms. The vectors $\mathbf{f}_{\mathbf{u}}$ and $\mathbf{f}_{\boldsymbol{p}}$ are due to the boundary conditions (4) and (5). The subscripts δ and φ identify the SUPG and PSPG contributions respectively. In order to simplify the notation we denote by $\mathbf{x}=(\mathbf{u},\boldsymbol{p})$ a vector of nodal variables comprising both nodal velocities and pressures. Thus, equation (12) can be written as,

$$\mathbf{F}(\mathbf{x})=\mathbf{0} \tag{13}$$

where $\mathbf{F}(\mathbf{x})$ represents a nonlinear vector function. For Reynolds numbers much greater than unity and non-Newtonian behavior, the nonlinear character of the equations becomes dominant, making the choice of the solution algorithm, especially with respect to its convergence and efficiency a key issue. The search for a suitable nonlinear solution method is complicated by the existence of several procedures and their variants. In the following section we present the nonlinear solution strategies based on the Newton-type methods evaluated in this work.

NONLINEAR SOLUTION PROCEDURES

Consider the nonlinear problem arising from the discretization of the fluid flow equations described by equation (13). We assume that $\mathbf{F}$ is continuously differentiable in $\mathbb{R}^{n_{sd}}$ and denote its Jacobian matrix by $\mathbf{F}' \in \mathbb{R}^{n_{sd}}$. The Newton's method is a classical algorithm for solving equation (13) and can be enunciated as: given an initial guess $\mathbf{x}_0$, we compute a sequence of steps $\mathbf{s}_k$ and iterates $\mathbf{x}_k$ as follows:

ALGORITHM N

for $k=0$ step 1 until convergence do

solve $\mathbf{F}'(\mathbf{x}_k)\mathbf{s}_k=\mathbf{0}$ (14)

set $\mathbf{x}_{k+1}=\mathbf{x}_k+\mathbf{s}_k$

Newton's method is attractive because it converges rapidly from any sufficiently good initial guess (see Dembo [4]). However, one drawback of Newton's method is the need to solve the Newton equations (14) at each stage. Computing the exact solution using a direct method can be expensive if the number of unknowns is large and may not be justified when $\mathbf{x}_k$ is far from a solution. Thus, one might prefer to compute some approximate solution, leading to the following algorithm:

ALGORITHM IN

for $k=0$ step 1 until convergence do

find some $\eta_k \in [0,1)$ AND $\mathbf{s}_k$ that satisfy

$$\left\|\mathbf{F}(\mathbf{x}_k)+\mathbf{F}'(\mathbf{x}_k)\mathbf{s}_k\right\| \le \eta_k \left\|\mathbf{F}(\mathbf{x}_k)\right\| \tag{15}$$

set $\mathbf{x}_{k+1}=\mathbf{x}_k+\mathbf{s}_k$

For some $\eta_k \in [0,1)$, where $\|\bullet\|$ is a norm of choice. This formulation naturally allows the use of an iterative solver: one first chooses η_k and then applies the iterative solver to (14) until a $\mathbf{s}_k$ is determined for which the residual norm satisfies (15). In this context η_k is often called a forcing term, since its role is to force the residual of (14) to be suitably small. This term can be specified in several ways (see, Eisenstat and Walker [5]) to enhance efficiency and convergence. We adopted $\eta_{max} = 0.1$ arbitrarily in our tests. Following [17], we have used an element-by-element (EBE) BiCGSTAB method to compute $\mathbf{s}_k$ such as equation (15) holds. A particularly simple scheme for solving the nonlinear system of equations (13) is a fixed point iteration procedure known as successive substitution (SS) (also known as Picard iteration, functional iteration or successive iteration). In the non-Newtonian cases approached here we follow Meuric *et al* [10]). Material non-linearities are treated by using values from the previous iteration level (upstream values) such as successive or Picard iterations. The non-Newtonian apparent viscosities are evaluated after each nonlinear iteration using the new velocity solution vector. Computational difficulties can be encountered when the apparent viscosities approach large values. This is the case when the Power Law approximation is breaking down at extreme values of shear rate. Note in the algorithms above that, if we do not build the Jacobian matrix in equations (14) and (15), and the solution of previous iterations were used, we have a successive substitution (SS) method. In this work, we have evaluated the efficiency of Newton and successive substitution methods and their inexact versions. We may also define a mixed strategy combining SS and N (or ISS and IN) iterations, to improve performance, as well shall see. In this strategy the Jacobian evaluation is enabled after *k* successive substitution iterations. Thus, we label the mixed strategy as *k*-SS+N or as *k*-ISS+IN in the case of its inexact counterpart.

To form the Jacobian $\mathbf{F}'$ required by Newton-type methods we use a numerical approximation described by Tezduyar [16]. Consider the following Taylor expansion for the nonlinear convective term emanating from the Galerkin formulation:

$$\mathbf{N}(\mathbf{u} + \Delta\mathbf{u}) = \mathbf{N}(\mathbf{u}) + \frac{\partial \mathbf{N}}{\partial \mathbf{u}} \Delta\mathbf{u} + \ldots \tag{16}$$

where $\Delta\mathbf{u}$ is the velocity increment. Discarding the high order terms and omitting the integral symbols we arrive to the following approximation,

$$\begin{aligned}\rho(\mathbf{u} + \Delta\mathbf{u}) \cdot \nabla(\mathbf{u} + \Delta\mathbf{u}) &\cong \rho(\mathbf{u} \cdot \nabla)\mathbf{u} \\ &+ \rho(\mathbf{u} \cdot \nabla)\Delta\mathbf{u} + \rho(\Delta\mathbf{u} \cdot \nabla)\mathbf{u}\end{aligned} \tag{17}$$

Note that the first term in the right hand side of equation (17) is the corresponding residual vector and the remaining terms represent the numerical approximation of $\partial \mathbf{N} / \partial \mathbf{u}$. If we apply similar derivations to $\mathbf{N}_\delta(\mathbf{u})$ and $\mathbf{N}_\varphi(\mathbf{u})$ we arrive to the SUPG and PSPG contributions to the residual vector and to the approximations of $\partial \mathbf{N}_\delta / \partial \mathbf{u}$ and $\partial \mathbf{N}_\varphi / \partial \mathbf{u}$.

NUMERICAL RESULTS

In this section we present a practical application of the nonlinear methods previously described. The problem is the rotational eccentric annulus flow into borehole wells observed during well drilling operations. In these operations, the mud is pumped through the hollow drill shaft to the drill bit where it enters the wellbore and returns under pressure as a rotational flow to the well surface. The primary functions of the mud are to carry rock cuttings to the surface, to lubricate the drill bit and to control subsurface pressures. The rheology of muds usually exhibits a finite yield stress and shear thinning behavior (Meuric [10]). The drilling mud flow has a tendency to form a helical stream surrounding the drill string due the existence of radial and tangential forces. The radial force is generated by the pressure drop imposed by the mud pump and the tangential force is due to the rotational movement of the drill string. The transport of these rotational forces through the fluid layers is significantly influenced by the fluid viscosity. Extensive numerical investigations of annuli flow were conducted by Escudier *et al* [6]. The effects of eccentricity and inner-cylinder rotation for the flow of several Power Law fluids were studied. We restrict ourselves here to a simple case, the laminar tangential flow in an eccentric annulus for Power Law and Bingham fluids, flowing in a 2D section of a borehole such as given in Figure 1a. The eccentricity is 0.6 and the finite element mesh in Figure 1b comprises 1,600 elements and 800 nodes. The rotational speed imposed at the drill string is 300 RPM for all cases and the borehole wall was considered impenetrable. Table 1 shows the fluid parameters for the test problems. In all the numerical experiments no special care was taken with the initial conditions and we have adopted null value as initialization for pressure and velocity fields. The nonlinear iterations were halted when the maximum and the relative residual Euclidean norms decrease 10 orders of magnitude. In the mixed strategy solutions we switched on the approximate Jacobian updates after 5 successive substitutions or inexact successive substitutions. An engineering criterion was adopted to define the exact nonlinear solution methods. In these, the inner linear equation systems were solved with a fixed tolerance of 10-6. All computations has been performed on the InfoServer Itautec PC Cluster (16 nodes dual Intel Pentium 1 GHz, Intel Fortran compiler and Red Hat Linux) located at the Center for Parallel Computations at COPPE/UFRJ.

Table 1 Fluid Properties

Fluid model	Rheology parameters	Rotational eccentric annulus flow
Pseudoplastic (n = 0.75)	nominal viscosity (kg/m.s)	0.15
	cutoff shear rate (Pa)	10^{-6}
	consistency index ($Pa.s^n$)	1.0
Dilatant (n = 1.25)	nominal viscosity (kg/m.s)	0.15
	cutoff shear rate (Pa)	10^{-6}
	consistency index ($Pa.s^n$)	1.0
Bingham	plastic viscosity (kg/m.s)	0.15
	yield stress (Pa)	7.16

Figs 3a to 3c present velocity (left) and viscosity (right) contours for the fluids considered in this study. Figs 4a to 4c show the relative residual evolution towards the nonlinear solution for each fluid type. For the Power Law fluids we note that the Newton strategies converge faster than the successive substitutions or mixed methods, indicating that the numerically approximated Jacobians improved convergence rate. For the Bingham fluid (see Figure 3c) we observe that convergence is slower than the Power Law fluids. It is also important to note that just the inexact methods were able to reach the desired accuracy. In all other methods the relative residual norm oscillates wildly, indicating serious convergence problems. The inexact Newton method required the smallest number of iterations, which is a clear sign that the numerically approximate Jacobians even here have substantially increased the convergence rate. In Figure 5 we show the total CPU time in seconds for each fluid and nonlinear strategy. We may see in this Figure that the inexact methods are faster. However, it is interesting to note that just for the dilatant fluid the inexact successive substitution method is the fastest. For Bingham and pseudoplastic fluids the inexact Newton method is faster than all other strategies.

CONCLUSIONS

We have tested the performance of inexact Newton-type algorithms to solve nonlinear systems of equations arising from the SUPG/PSPG finite element formulation of steady incompressible viscoplastic flows. We employed a numerically approximated Jacobian based on Taylor's expansion of the nonlinear convective terms emanating from the Galerkin and stabilization terms. We also introduced an inexact successive substitution scheme and a mixed strategy, to improve performance of Newton's method. Extensive tests in a 2D benchmark problem considering Power Law and Bingham fluids have shown that the inexact Newton method or the inexact mixed method, both with numerically approximated Jacobians are robust and fast. However, in all Bingham fluid test cases the numerically approximated Jacobian has little effect. Further experiments are needed to investigate other important issues, such the effects of globalization procedures, more robust preconditioners and other Jacobian forms. Of particular interest here is the development of numerically approximated Jacobian terms for the viscous terms, to accelerate convergence especially for Bingham fluids.

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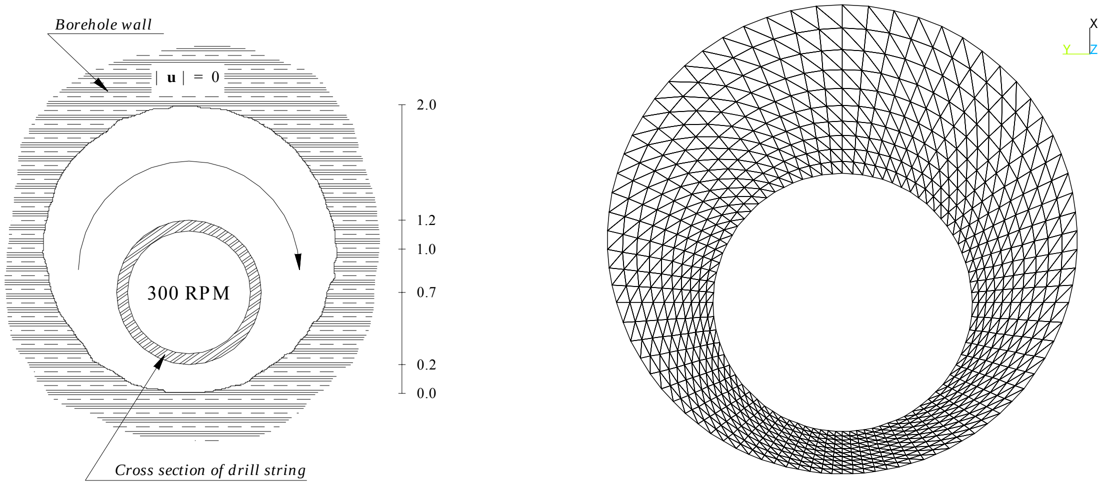
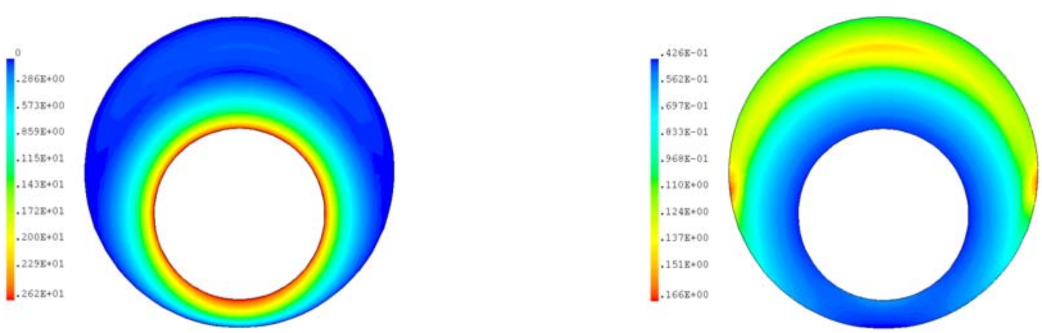
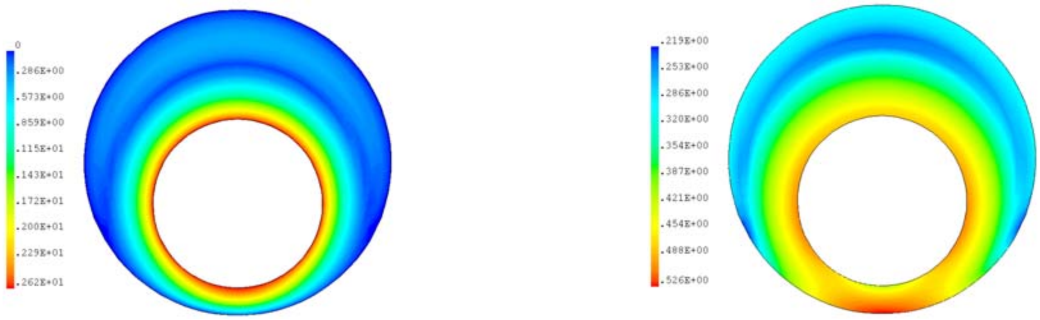


(a) (b)

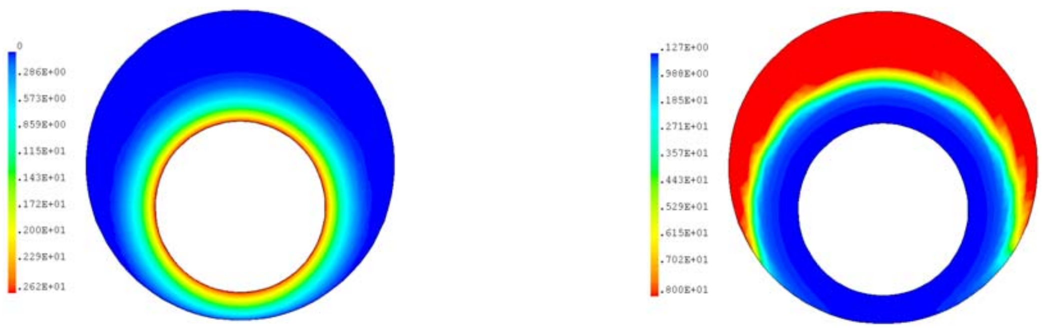
Fig. 1 (a) 2D cross section scheme of a borehole well showing the drill string at center and rotation direction. (b) Finite element mesh: 1,600 elements and 800 nodes.



(a) Pseudoplastic fluid, (left) Velocity field, (right) Viscosity field

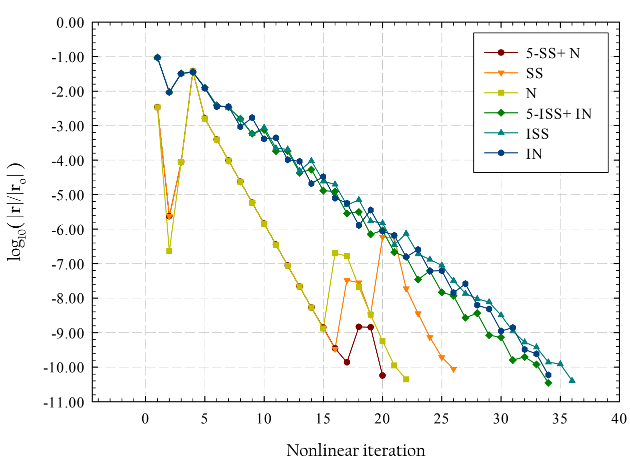


(b) Dilatant fluid, (left) Velocity field, (right) Viscosity field

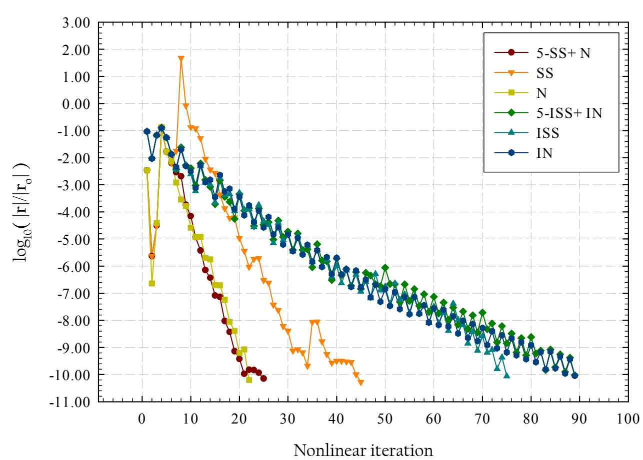


(c) Bingham fluid, (left) Velocity field, (right) Viscosity field

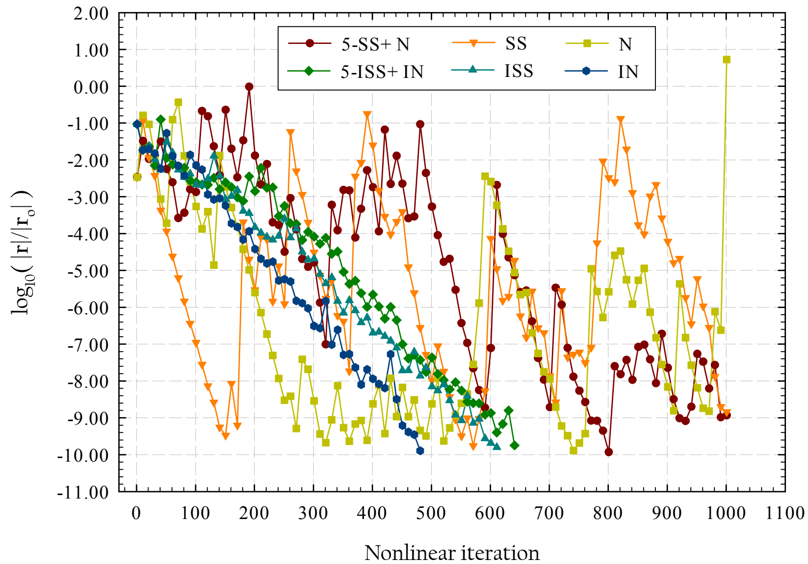
Fig. 2 Rotational eccentric annulus flow – Velocity and Viscosity contours.



(a) Pseudoplastic fluid (n = 0.75)



(b) Dilatant fluid (*n* = 1.25)



(c) Bingham fluid

Fig. 3 Rotational eccentric annulus flow - Influence of numerical Jacobian evaluation in the Newton-type methods

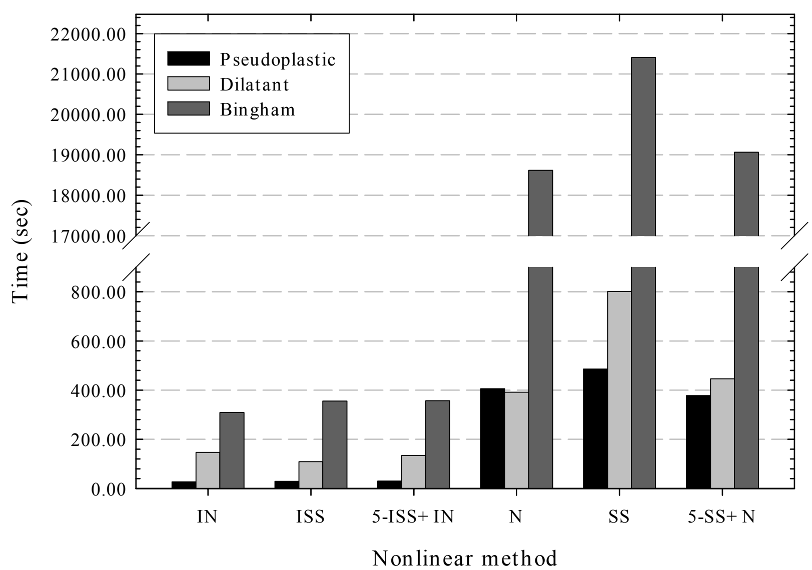


Fig.4 Nonlinear algorithms performance – CPU time (seconds) by method.