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Inexact Newton-type methods for the solution of steady incompressible viscoplastic 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 viscoplastic incompressible fluid flows. The flow through an abrupt contraction and the rotational flow in eccentric annulus with power law and Bingham rheologies are employed as benchmarks. Our results have shown that inexact schemes are more efficient than traditional Newton-type strategies. © 2005 Elsevier B.V. All rights reserved.

Keywords: Inexact Newton; Viscoplastic flow; Stabilized formulations; Finite elements

1. Introduction

This work addresses aspects in the finite element simulation of steady viscoplastic flows with emphasis on nonlinear solution strategies employing inexact Newton-type algorithms.

Several modern material and manufacturing processes involve non-Newtonian fluids, and in particular viscoplastic 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 difficult case of incompressible fluid flows. In these fluids the

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dependence between the viscosity and the shear rate amplifies the nonlinear character of the governing equations. For a comprehensive presentation of numerical methods for non-Newtonian fluid flow computations we refer to [7,16].

The finite element computation of incompressible Newtonian flows involves two sources of potential numerical instabilities associated with the Galerkin formulation of the problem. One source is due to the presence of convective terms in the governing equations. The other source is due to the use of inappropriate combinations of interpolation functions to represent the velocity and pressure fields. These instabilities are frequently prevented by addition of stabilization terms into the Galerkin formulation. In the context of non-Newtonian fluids, the rheological equations are inherently nonlinear, thus increasing the difficulties to find an efficient solution method.

In this work we consider the stabilized finite element formulation proposed by Tezduyar [19] applied to solve steady viscoplastic incompressible flows. This formulation, originally proposed for Newtonian fluids, allows that equal-order-interpolation velocity-pressure elements are employed, circumventing the Babuska-Brezzi stability condition by introducing two stabilization terms. The first term is the streamline upwind Petrov-Galerkin (SUPG) introduced by Brooks and Hughes [6] and the other one is the pressure stabilizing Petrov Galerkin (PSPG) stabilization proposed initially by Hughes et al. [12] for Stokes flows and generalized by Tezduyar et al. [21] to high Reynolds number flows.

It is known that, when discretized, the incompressible Navier–Stokes equations give rise to a system of nonlinear algebraic equations due the presence of convective terms in the momentum equation. Among several strategies to solve nonlinear problems the Newton's methods is attractive because it converges rapidly from any sufficiently good initial guess [8,13]. However, the implementation of Newton's method requires some considerations: Newton's method requires the solution of linear systems at each stage and exact solutions can be too expensive if the number of unknowns is large. In addition, the computational effort spent to find exact solutions for the linearized systems may not be justified when the nonlinear iterates are far from the solution. Therefore, it seems reasonable to use an iterative method [3], such as BiCGSTAB or GMRES, to solve these linear systems only approximately.

The inexact-Newton methods associated with iterative Krylov solvers have been used to reduce computational efforts related to nonlinearities in many problems of computational fluid dynamics, offering a trade-off between the accuracy and the amount of computational effort spent per iteration. According to Kelley [13] its success depends on several factors, such as: quality of initial Newton step, robustness of Jacobian evaluation and proper forcing function choice. Shadid and co-workers presented in [18] 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 [14] discussed the constituents of a broader class of inexact-Newton methods, the Jacobian-free Newton–Krylov methods. In this work we address only the essentials of the inexact-Newton methods and the interested reader should refer to Knoll and Keyes [14], and references therein, for a more detailed presentation.

Many authors have considered finite element formulations in combination with solution algorithms for nonlinear problems arising from non-Newtonian incompressible flow simulations. For instance, in [5] the least-squares method was employed; in [1] a mixed-Galerkin finite element formulation with a Newton– Raphson iteration procedure coupled to an iterative solver was used, while in [17] the authors adopted the Galerkin/least-squares formulation (GLS) associated also with Newton–Raphson algorithm; Meuric et al. in [15] used the SUPG formulation in combination with Newton–Raphson and Picard iterations as a strategy to circumvent 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 have tested the performance of the approximate Jacobian form described by Tezduyar in [20]. This numerically approximated Jacobian is based on Taylor's expansions of the nonlinear terms and presents an alternative and simple way to implement the approximate tangent matrix employed by inexact Newton-type methods. The present 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.

2. 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:

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

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

where ρ and **u** are the density and velocity, **\sigma** is the stress tensor given as

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

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

The essential and natural boundary conditions associated with Eqs. (1) and (2) can be imposed at different portions of the boundary Γ and represented by

$$\mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_g, \tag{4}$$
$$\mathbf{n} \cdot \mathbf{\sigma} = \mathbf{h} \quad \text{on } \Gamma_h, \tag{5}$$

where
$$\Gamma_g$$
 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 experienced by the fluid. Therefore, the deviatoric tensor in Eq. (3) can be expressed by

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

where μ is the proportionality constant known as the dynamic viscosity and ε is the deformation rate tensor or

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2} [\boldsymbol{\nabla} \mathbf{u} + (\boldsymbol{\nabla} \mathbf{u})^{\mathrm{T}}].$$
(7)

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

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

where $\dot{\gamma}$ is the second invariant of the strain rate tensor and $\mu(\dot{\gamma})$ is the apparent viscosity of the fluid [7,16].

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 discussed in [2,7,11,16]; thus for the power law fluids we have

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

where K denotes the consistency index, μ_0 is a nominal viscosity, n is 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

$$\mu(\dot{\gamma}) = \begin{cases} \mu_0 + \frac{\mathbf{\sigma}_Y}{\dot{\gamma}} & \text{if } \dot{\gamma} > \frac{\mathbf{\sigma}_Y}{\mu_r - \mu_0}, \\ \mu_r & \text{if } \dot{\gamma} \leqslant \frac{\mathbf{\sigma}_Y}{\mu_r - \mu_0}, \end{cases}$$
(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 [2,4].

3. Finite element formulation

Let us assume following Tezduyar [19] 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 Eqs. (1) and (2) using SUPG and PSPG stabilizations for incompressible fluid flows [19] 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 $\forall q^h \in V_p^h$:

$$\int_{\Omega} \mathbf{w}^{h} \cdot \rho \left(\mathbf{u}^{h} \cdot \nabla \mathbf{u}^{h} - \mathbf{f} \right) d\Omega + \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{w}^{h}) : \boldsymbol{\sigma}(p^{h}, \mathbf{u}^{h}) d\Omega - \int_{\Gamma} \mathbf{w}^{h} \cdot h \, d\Gamma + \int_{\Omega} q^{h} \nabla \cdot \mathbf{u}^{h} \, d\Omega \\ + \sum_{e=1}^{n_{\text{el}}} \int_{\Omega^{e}} \tau_{\text{SUPG}} \mathbf{u}^{h} \cdot \nabla \mathbf{w}^{h} \cdot \left[\rho(\mathbf{u}^{h} \cdot \nabla \mathbf{u}^{h}) - \nabla \cdot \boldsymbol{\sigma}(p^{h}, \mathbf{u}^{h}) - \rho \mathbf{f} \right] d\Omega \\ + \sum_{e=1}^{n_{\text{el}}} \int_{\Omega^{e}} \frac{1}{\rho} \tau_{\text{PSPG}} \nabla q^{h} \cdot \left[\rho(\mathbf{u}^{h} \cdot \nabla \mathbf{u}^{h}) - \nabla \cdot \boldsymbol{\sigma}(p^{h}, \mathbf{u}^{h}) - \rho \mathbf{f} \right] d\Omega = 0.$$
(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 streamline upwind Petrov/Galerkin (SUPG) term and the second correspond to the pressure stabilization Petrov/Galerkin (PSPG) term. We have calculated the stabilization parameters according to [21], as follows:

$$\tau_{\rm SUPG} = \tau_{\rm PSPG} = \left[\left(\frac{2 \| \mathbf{u}^h \|}{h^\#} \right)^2 + 9 \left(\frac{4\nu}{(h^\#)^2} \right)^2 \right]^{-1/2}.$$
 (12)

Here \mathbf{u}^h is the local velocity vector, v represent the kinematic viscosity and the "element length" $h^{\#}$ is defined to be equal to the diameter of the circle which is area-equivalent to the element.

The spatial discretization of Eq. (11) leads to the following system of nonlinear equations:

$$\mathbf{N}(\mathbf{u}) + \mathbf{N}_{\delta}(\mathbf{u}) + \mathbf{K}\mathbf{u} - (\mathbf{G} + \mathbf{G}_{\delta})\mathbf{p} = \mathbf{f}_{\mathbf{u}},$$

$$\mathbf{G}^{\mathrm{T}}\mathbf{u} + \mathbf{N}_{\varphi}(\mathbf{u}) + \mathbf{G}_{\varphi}\mathbf{p} = \mathbf{f}_{p},$$

(13)

where **u** is the vector of unknown nodal values of \mathbf{u}^h and p is the vector of unknown nodal values of p^h . The nonlinear vectors $\mathbf{N}(\mathbf{u})$, $\mathbf{N}_{\delta}(\mathbf{u})$, and $\mathbf{N}_{\varphi}(\mathbf{u})$, the matrices **K**, **G**, \mathbf{G}_{δ} , and \mathbf{G}_{φ} emanate, respectively, from the convective, viscous and pressure terms. The vectors $\mathbf{f}_{\mathbf{u}}$ and \mathbf{f}_{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

3148

the notation we denote by $\mathbf{x} = (\mathbf{u}, \mathbf{p})$ a vector of nodal variables comprising both nodal velocities and pressures. Thus, Eq. (13) can be written as

$$\mathbf{F}(\mathbf{x}) = \mathbf{0},\tag{14}$$

where F(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.

4. Nonlinear solution procedures

Consider the nonlinear problem arising from the discretization of the fluid flow equations described by Eq. (14). We assume that **F** is continuously differentiable in $\mathbb{R}^{n_{sd}}$ and denote its Jacobian matrix by $\mathbf{J} \in \mathbb{R}^{n_{sd}}$. The Newton's method is a classical algorithm for solving Eq. (14) 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 $\mathbf{J}(\mathbf{x}_k)\mathbf{s}_k = -\mathbf{F}(\mathbf{x}_k)$
set $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$ (15)

Newton's method is attractive because it converges rapidly from any sufficiently good initial guess (see [8]). However, one drawback of Newton's method is the need to solve the Newton Eqs. (15) 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 (16)
 $\|\mathbf{F}(\mathbf{x}_k) + \mathbf{J}(\mathbf{x}_k)\mathbf{s}_k\| \leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\|$
set $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$

for some $\eta_k \in [0, 1)$, where $\|\cdot\|$ 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 (15) until a \mathbf{s}_k is determined for which the residual norm satisfies (16). In this context η_k is often called the forcing term, since its role is to force the residual of Eq. (15) to be suitably small. This term can be specified in several ways (see [9]) to enhance efficiency and convergence and will be treated in Section 4.1. Note that, as demonstrated in Kelley [13], convergence is superlinear. In our implementation, following [22] we have used an element-by-element (EBE) BiCGSTAB method to compute \mathbf{s}_k such that Eq. (16) holds.

A particularly simple scheme for solving the nonlinear system of Eqs. (14) is a fixed point iteration procedure known as the successive substitution, also known as the Picard iteration, functional iteration or successive iteration. In the non-Newtonian cases considered here we follow Meuric et al. [15]. Material nonlinearities are treated by using values from the previous iteration level (upstream values) as in case of successive or Picard iterations. The apparent non-Newtonian viscosities are evaluated after each iteration

using the new velocity solution vector. Computational difficulties can be encountered when the apparent viscosities attains infinite values. This happens in the case of the power law approximation that is breaking down at extreme values of shear rate.

4.1. Forcing term

We have implemented the forcing term as a variation of the choice from Eisenstat and Walker [9] that tends to minimize oversolving while giving fast asymptotic convergence to a solution of (14). Oversolving means that the linear equation for the Newton step is solved to a precision far beyond what is needed to correct the nonlinear iteration. Kelley [13] have considered the following measure of the degree to which the nonlinear iteration approximates the solution

$$\eta_k^a = \gamma \|\mathbf{F}(\mathbf{x}_k)\|^2 / \|\mathbf{F}(\mathbf{x}_{k-1})\|^2, \tag{17}$$

where $\gamma \in [0, 1)$ is a parameter. In order to specify the choice at k = 0 and bound the sequence away from 1 we set,

$$\eta_k^b = \begin{cases} \eta_{\max} & k = 0,\\ \min(\eta_{\max}, \eta_k^a) & k > 0, \end{cases}$$
(18)

where the parameter η_{max} is an upper limit of the sequence $\{\eta_k\}$. We have chosen $\gamma = 0.9$ according to Eisenstat and Walker [9], and adopted $\eta_{\text{max}} = 0.1$ arbitrarily in our tests.

It may happen that η_k^b is small for one or more iterations while \mathbf{x}_k is still far from the solution. A method of safeguarding against this possibility was suggested by Eisenstat and Walker [9] to avoid volatile decreases in η_k . The idea is that if η_{k-1} is sufficiently large we do not let η_k decrease by much more than a factor of η_{k-1} , that is

$$\eta_k^c = \begin{cases} \eta_{\max} & k = 0, \\ \min(\eta_{\max}, \eta_k^a) & k > 0, \ \gamma \eta_{k-1}^2 < 0.1, \\ \min(\eta_{\max}, \max(\eta_k^a, \gamma \eta_{k-1}^2)) & k > 0, \ \gamma \eta_{k-1}^2 > 0.1. \end{cases}$$
(19)

The constant 0.1 is arbitrary. According to Kelley [13] the described safeguarding does improve the performance of the iteration.

There is a chance that the final iterate will reduce $\|\mathbf{F}\|$ far beyond the desired level and that the cost of the solution of the linear equation for the last step will be higher than is really needed. This oversolving in the final step can be controlled by comparing the norm of the current nonlinear residual to the nonlinear norm at which the iteration would terminate

$$\tau_{\rm NL} = \tau_{\rm res} \|\mathbf{F}_0\| \tag{20}$$

and bounding η_k by a constant multiple of $\tau_{NL}/||\mathbf{F}(\mathbf{x}_k)||$. We use the choice proposed by Kelley [13], that is

$$\eta_k = \min\left(\eta_{\max}, \max\left(\eta_k^c, 0.5\tau_{NL} / \|\mathbf{F}(\mathbf{x}_k)\|\right)\right),\tag{21}$$

where $\tau_{\rm NL}$ represent the nonlinear tolerance.

4.2. Jacobian matrix evaluation

To form the Jacobian J required by Newton-type methods we use a numerical approximation described by Tezduyar [20]. Consider the following Taylor expansion for the nonlinear convective term emanating from the Galerkin formulation: R.N. Elias et al. / Comput. Methods Appl. Mech. Engrg. 195 (2006) 3145–3167

3151

$$\mathbf{N}(\mathbf{u} + \Delta \mathbf{u}) = \mathbf{N}(\mathbf{u}) + \frac{\partial \mathbf{N}}{\partial \mathbf{u}} \Delta \mathbf{u} + \cdots,$$
(22)

where Δu is the velocity increment. Discarding the high order terms and omitting the integral symbols we arrive at the following approximation:

$$\mathbf{w} \cdot \rho(\mathbf{u} + \Delta \mathbf{u}) \cdot \nabla(\mathbf{u} + \Delta \mathbf{u}) \cong \mathbf{w} \cdot \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \mathbf{w} \cdot \rho(\mathbf{u} \cdot \nabla)\Delta\mathbf{u} + \mathbf{w} \cdot \rho(\Delta \mathbf{u} \cdot \nabla)\mathbf{u}$$

= $\mathbf{N}(\mathbf{u}) + \mathbf{C}(\mathbf{u}) + \mathbf{C}^{+}(\mathbf{u}).$ (23)

Note that the second term in the right hand side of Eq. (23) is the contribution to the nonlinear Galerkin convective matrix $C(\mathbf{u})$ and the remaining matrix completes the numerical approximation of $\partial \mathbf{N}/\partial u$. If we apply similar derivations to $\mathbf{N}_{\delta}(\mathbf{u})$ and $\mathbf{N}_{\omega}(\mathbf{u})$ we obtain

$$\begin{aligned} \tau_{\text{SUPG}}[(\mathbf{u} + \Delta \mathbf{u}) \cdot \nabla] \mathbf{w} \cdot \rho[(\mathbf{u} + \Delta \mathbf{u}) \cdot \nabla](\mathbf{u} + \Delta \mathbf{u}) \\ &\cong \tau_{\text{SUPG}}(\mathbf{u} \cdot \nabla) \mathbf{w} \cdot \rho(\mathbf{u} \cdot \nabla) \mathbf{u} + \tau_{\text{SUPG}}(\mathbf{u} \cdot \nabla) \mathbf{w} \cdot \rho(\mathbf{u} \cdot \nabla) \Delta \mathbf{u} + \tau_{\text{SUPG}}(\mathbf{u} \cdot \nabla) \mathbf{w} \cdot \rho(\Delta \mathbf{u} \cdot \nabla) \mathbf{u} \\ &+ \tau_{\text{SUPG}}(\Delta \mathbf{u} \cdot \nabla) \mathbf{w} \cdot \rho(\mathbf{u} \cdot \nabla) \mathbf{u} \\ &= \mathbf{N}_{\delta}(\mathbf{u}) + \mathbf{C}_{\delta}^{+}(\mathbf{u}) + \mathbf{C}_{\delta}^{++}(\mathbf{u}) \end{aligned}$$
(24)

and

$$\tau_{\text{PSPG}} \nabla q \cdot [(\mathbf{u} + \Delta \mathbf{u}) \cdot \nabla](\mathbf{u} + \Delta \mathbf{u}) \cong \tau_{\text{PSPG}} \nabla q \cdot (\mathbf{u} \cdot \nabla) \mathbf{u} + \tau_{\text{PSPG}} \nabla q \cdot (\mathbf{u} \cdot \nabla) \Delta \mathbf{u} + \tau_{\text{PSPG}} \nabla q \cdot (\Delta \mathbf{u} \cdot \nabla) \mathbf{u}$$
$$= \mathbf{N}_{\varphi}(\mathbf{u}) + \mathbf{C}_{\varphi}(\mathbf{u}) + \mathbf{C}_{\varphi}^{+}(\mathbf{u}),$$
(25)

where again the second terms on the right hand side of Eqs. (24) and (25) are the SUPG and PSPG contributions to the convective matrix and the additional terms also complete the definition of the numerical approximations of $\partial N_{\delta}/\partial u$ and $\partial N_{\phi}/\partial u$. Note that if we do not build the full approximate Jacobian matrix and the solution of previous iterations is used to compute the matrices C, C_{SUPG} and C_{PSPG}, we obtain 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 discussed in the following. 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.

5. Numerical results

In this section we present two examples of practical applications of the nonlinear methods described in the previous sections. The first problem consists of a flow through an abrupt contraction well known in food processing and plastic molding industries. The second is the rotational eccentric annulus flow into borehole wells observed during well drilling operations. Table 1 shows the fluid parameters for the two test problems. In all the numerical experiments no special care was taken with the initial conditions and we have adopted zero value as initialization for pressure and velocity fields. The nonlinear iterations were halted when the maximum and the relative residual Euclidean norms decreased 10 orders of magnitude. In the mixed strategy solutions we switched to the approximate Jacobian updates after five 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 by BiCGSTAB with a fixed tolerance of 10^{-6} . All computations have 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.

3152

Table 1 Fluid properties

Fluid model	Rheology parameters	Flow through an abrupt contraction	Rotational eccentric annulus flow	
Newtonian	Viscosity (kg/m s)	10^{-2}	10^{-2}	
Pseudoplastic ($n = 0.75$)	Nominal viscosity (kg/m s) Cutoff shear rate (Pa) Consistency index (Pa s ⁿ)	$ \begin{array}{l} 10^{-2} \\ 10^{-6} \\ 1.0 \end{array} $	$ \begin{array}{c} 0.15 \\ 10^{-6} \\ 1.0 \end{array} $	
Dilatant ($n = 1.25$)	Nominal viscosity (kg/m s) Cutoff shear rate (Pa) Consistency index (Pa s ⁿ)	$ \begin{array}{l} 10^{-2} \\ 10^{-6} \\ 1.0 \end{array} $	$ \begin{array}{c} 0.15 \\ 10^{-6} \\ 1.0 \end{array} $	
Bingham	Plastic viscosity (kg/m s) Yield stress (Pa)	10^{-2} 10^{-1}	0.15 7.16	

Density = 1.0 kg/m^3 .

5.1. Flow through an abrupt contraction

An important problem in rheology is the prediction of entry losses when a viscous fluid flows through a contraction at the junction of two tubes of different diameters, and of the exit losses when the fluid leaves the tube and enters a jet. The problem is important in rheometry as well as in technological applications, where contractions are present in most forming devices [7,16].

Fig. 1 shows the geometry of the problem and the boundary conditions and Fig. 2 shows the finite element mesh. We consider an axisymmetric 4:1 contraction, where 4 and 1 are the ratio between the radius of the upstream and downstream tubes, respectively. The boundary ABCD is a fixed and impenetrable wall on which the velocity components of the fluid are assumed zero, while EF is an axis of symmetry. The velocity



Fig. 1. Geometry and boundary conditions for the contraction 4:1 problem.



Fig. 2. Finite element mesh 3600 element mesh and 1911 nodes.

profile adopted as upstream boundary condition may be found in Bose and Carey [5]. The mesh shown in Fig. 2 was built with 3600 triangular elements and 1911 nodes.

Fig. 3a–d (left) present the velocity contour results for the fluid rheologies in Table 1. Fig. 3b–d (right) show the viscosity contour for each fluid rheology. For the pseudoplastic fluid (Fig. 3b) the shear-thinning behavior is observed near to the corner entrance, where the viscosity tends to decrease with the presence of high velocity gradients. The opposite behavior is noted in dilatant fluids. This fluid tends to become less viscous with increase of the shear rate. In the Bingham case, we can note the regions where the fluid displays high viscosity and flows slowly. In Fig. 4a–d we may observe the good agreement between our inexact-Newton results and those obtained by Ansys Flotran [2].

Fig. 5a–d show the relative residual norm convergence towards the nonlinear solution for each fluid type. We note that the solutions for the Newtonian, pseudoplastic and dilatant fluids show a similar trend. The inexact successive substitution (ISS) solutions converge very slowly for these fluids, needing more than



Fig. 3. Flow through an abrupt contraction—velocity and viscosity contours. (a) Newtonian fluid, (left) velocity field, (right) pressure field; (b) pseudoplastic fluid, (left) velocity field, (right) viscosity field; (c) dilatant fluid, (left) velocity field, (right) viscosity field and (d) Bingham fluid, (left) velocity field, (right) viscosity field.



Fig. 4. Velocity profiles validation for the flow through an abrupt contraction. (a) Newtonian fluid, (b) pseudoplastic fluid (n = 0.75), (c) dilatant fluid (n = 1.25) and (d) Bingham fluid.

100 iterations to reach the desired accuracy. The inexact Newton-type solutions (IN and 5-ISS + IN), on the contrary, solved these problems with a good convergence rate, although requiring slightly more nonlinear iterations than their counterparts (N and 5-SS + N). These results indicate that the numerically approximated Jacobians improve the convergence rate of the nonlinear solution. However, as shown in Fig. 5d, for the Bingham fluid the numerically approximated Jacobian has no effect on convergence.

Fig. 6 shows, for each fluid, the total number of nonlinear iterations for each solution method. We can observe that the numerically approximated Jacobians have more influence in the inexact methods. Note also that when we start to evaluate the Jacobians after a few inexact successive substitutions the number of nonlinear iterations decreases to an amount comparable to the IN solution. As can be seen in Fig. 7, the inexact methods are very fast, since they require less effort to compute the solution updates, as shown in Fig. 8, which depicts, for all fluids, the total number of BiCGSTAB iterations for each method.



Fig. 5. Flow through an abrupt contraction influence of numerical Jacobian evaluation in the Newton-type methods. (a) Newtonian fluid, (b) pseudoplastic fluid (n = 0.75), (c) dilatant fluid (n = 1.25) and (d) Bingham fluid.

5.2. Rotational eccentric annulus flow

This problem is based on the fluid dynamics observed in the flow of drilling muds in a borehole 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 [15].



Fig. 5 (continued)

In this problem 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. [10]. The effects of eccentricity and inner-cylinder rotation on 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 Newtonian, power law and Bingham fluids, in a 2D section of a borehole given in Fig. 9. The eccentricity is 0.6 and the finite



Flow Through an Abrupt Contraction

Fig. 6. Nonlinear algorithms performance-number of nonlinear iterations by method.



Flow Through an Abrupt Contraction

Fig. 7. Nonlinear algorithms performance—CPU time (s) by method.



Flow Through an Abrupt Contraction

Fig. 8. Nonlinear algorithms performance-number of BiCGSTAB iterations by method.



Fig. 9. 2D cross section scheme of a borehole well showing the drill string at center and rotation direction.

element mesh in Fig. 10 comprises 1600 elements and 800 nodes. The rotational speed imposed at the drill string is 300 RPM for all cases, while the borehole wall is considered impenetrable.



Fig. 10. Finite element mesh: 1600 elements and 800 nodes.

Fig. 11a–d (left) present the velocity contour for the several fluids considered in this study. Fig. 11b–d (right) show the viscosity contour for each fluid. In Fig. 12a–d we plot the velocity profiles along the dashed line in the annulus for all fluids. We may observe that our inexact Newton solutions are in good agreement with solutions obtained by using Ansys Flotran [2].

Fig. 13a–d show the relative residual evolution towards the nonlinear solution for each fluid type. For the Newtonian and power law fluids we note that the Newton strategies converge faster than the successive substitutions or mixed methods, indicating that in these experiments the numerically approximated Jacobians also improved convergence rate. In particular, for the Newtonian case convergence is very fast. We observe that the convergence rate of the inexact Newton method and the inexact mixed method is superlinear only for the Newtonian fluid.

For the Bingham fluid (see Fig. 13d) we observe that convergence is slower than for the power law fluids. It is also important to note that only 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 approximated Jacobians have even in this case substantially increased the convergence rate.

In Figs. 14–16 we show respectively the total number of nonlinear iterations, the total CPU time in seconds, and the total number of inner (BiCGSTAB) iterations for each fluid and nonlinear strategy. We may see in these figures that although the inexact methods require more nonlinear iterations, they need less inner (BiCGSTAB) iterations. Consequently, as shown in Fig. 14, the inexact methods are faster. However, it is interesting to note that only in the case of 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. In the case of a Newtonian fluid, we observed that the inexact mixed method (5-ISS + IN) is the fastest.

6. 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.



Fig. 11. Rotational eccentric annulus flow—velocity and viscosity contours. (a) Newtonian fluid, (left) velocity field, (right) pressure field; (b) pseudoplastic fluid, (left) velocity field, (right) viscosity field; (c) dilatant fluid, (left) velocity field, (right) viscosity field and (d) Bingham fluid, (left) velocity field, (right) viscosity field.



Fig. 12. Velocity profile validation for the rotational eccentric annulus flow. (a) Newtonian fluid, (b) pseudoplastic fluid (n = 0.75), (c) dilatant fluid (n = 1.25) and (d) Bingham fluid.

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



Fig. 12 (continued)

substitution scheme and a mixed strategy to improve performance of Newton's method. Extensive tests in two 2D benchmark problems considering Newtonian, power law and Bingham fluids have shown that the inexact Newton method or the inexact mixed method, both with numerically approximated Jacobians are



Fig. 13. Rotational eccentric annulus flow—influence of numerical Jacobian evaluation in the Newton-type methods. (a) Newtonian fluid, (b) pseudoplastic fluid (n = 0.75), (c) dilatant fluid (n = 1.25) and (d) Bingham fluid.

faster than the classical methods also using the same approximate form for the tangent operator. 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.

Rotational Eccentric Annulus Flow

Fig. 14. Nonlinear algorithms performance-CPU time (s) by method.

Rotational Eccentric Annulus Flow

Fig. 15. Nonlinear algorithms performance-number of nonlinear iterations by method.

Rotational Eccentric Annulus Flow

Fig. 16. Nonlinear algorithms performance-Number of BiCGSTAB iterations by method.

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References

- A.N. Alexandrou, T.M. McGilvreay, G. Burgos, Steady Herschel–Bulkley fluid flow in three-dimensional expansions, J. Non-Newtonian Fluid Mech. 100 (2001) 77–96.
- [2] Ansys Inc. Theory Reference; 2003. Available from: http://www.ansys.com>.
- [3] R. Barret, M. Berry, T.F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine, H. van der Vorst, Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, SIAM, Philadelphia, 1994.
- [4] C.R. Beverly, R.I. Tanner, Numerical analysis of three-dimensional Bingham plastic flow, J. Non-Newtonian Fluid Mech. 42 (1992) 85–115.
- [5] A. Bose, G.F. Carey, Least-squares p r finite element methods for incompressible non-Newtonian flows, Comput. Methods Appl. Mech. Engrg. 180 (1999) 431–458.
- [6] A.N. Brooks, T.J.R. Hughes, Streamline upwind/Petrov–Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier–Stokes equation, Comput. Methods Appl. Mech. Engrg. 32 (1982) 199–259.
- [7] M.J. Crochet, A.R. Davies, K. Walters, Numerical Simulation of Non-Newtonian Flow, Elsevier Science Publishers B.V., 1984.
- [8] R.S. Dembo, S.C. Eisenstat, T. Steihaug, Inexact Newton methods, SIAM J. Numer. Anal. 19 (1982) 400–408.
- [9] S.C. Eisenstat, H.F. Walker, Choosing the forcing terms in inexact Newton method, SIAM.J. Sci. Comput. 17 (1) (1996) 16–32.
- [10] M.P. Escudier, P.J. Oliveira, F.T. Pinho, Fully developed laminar flow of purely viscous non-Newtonian liquids through annuli, including the effects of eccentricity and inner-cylinder rotation, Int. J. Heat and Fluid Flow 23 (1) (2002) 52–73.

- [11] D.K. Gartling, Finite element methods for non-Newtonian flows, Report SAND92-0886, CFD Department, Sandia National Laboratories, Albuquerque, NM, 1992.
- [12] T.J.R. Hughes, L.P. Franca, M. Balestra, A new finite element formulation for computational fluid dynamics: V. circumventing the Babuška–Brezzi condition: a stable Petrov–Galerkin formulation of the stokes problem accommodating equal-order interpolations, Comput. Methods Appl. Mech. Engrg. 59 (1986) 85–99.
- [13] C.T. Kelley, Iterative Methods for Linear and Nonlinear Equations, Frontiers in Applied Mathematics, SIAM, Philadelphia, 1995.
- [14] D.A. Knoll, D.E. Keyes, Jacobian-free Newton–Krylov methods: a survey of approaches and applications, J. Comput. Phys. 193 (2004) 357–397.
- [15] O.F.J. Meuric, R.J. Wakeman, T.W. Chiu, K.A. Fisher, Numerical flow simulation of viscoplastic fluids in annuli, Can. J. Chem. Eng. 76 (1998) 27–40.
- [16] R.G. Owens, T.N. Phillips, Computational Rheology, Imperial College Press, 2002.
- [17] D. Perić, S. Slijepčević, Computational modelling of viscoplastic fluids based on a stabilised finite element method, Engrg. Comput. 18 (3/4) (2001) 577–591.
- [18] J.N. Shadid, R.S. Tuminaro, H.F. Walker, An inexact Newton method for fully-coupled solution of the Navier–Stokes equations with heat and mass transport, J. Comput. Phys. 137 (1997) 155–185.
- [19] T.E. Tezduyar, Stabilized finite element formulations for incompressible flow computations, Adv. Appl. Mech. 28 (1991) 1-44.
- [20] T.E. Tezduyar, Finite Elements in Fluids: Lecture Notes of the Short Course on Finite Elements in Fluids. Computational Mechanics Division, vol. 99–77, Japan Society of Mechanical Engineers, Tokyo, Japan, 1999.
- [21] T.E. Tezduyar, S. Mittal, S.E. Ray, R. Shih, Incompressible flow computations with stabilized bilinear and linear equal-orderinterpolation velocity-pressure elements, Comput. Methods Appl. Mech. Engrg. 95 (1992) 221–242.
- [22] C.C. Tsai, T.J. Liu, Comparison of three solvers for viscoelastic fluid flow problems, J. Non-Newtonian Fluid Mech. 60 (1995) 155–177.