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Pierre Saramito. A damped Newton algorithm for computing viscoplastic fluid flows. 2015. hal-01228347v1

HAL Id: hal-01228347 https://hal.science/hal-01228347v1

Preprint submitted on 12 Nov 2015 (v1), last revised 11 May 2016 (v3)

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A damped Newton algorithm for computing viscoplastic fluid flows

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Abstract – A new damped Newton algorithm for viscoelastic fluid flows is presented in this paper. This algorithm bases on a projection formulation of the viscoplastic problem and an efficient preconditioned iterative solved for the singular Jacobian. A demonstration is provided by the computing a viscoplastic flow in a pipe with a square cross section and performance are compared with the augmented Lagrangian algorithm.

Keywords - viscoplastic fluid; Bingham model; Heschel-Bulkley model; Newton method

Introduction

The numerical resolution of viscoplastic fluid flows is still a challenging task. The augmented Lagrangian method has been introduced in 1969 by Hestenes [18] and Powell [27]. During the 1970s, this approach became popular for solving optimization problems (see e.g. Rockafellar [30]). In 1980, Glowinski [15] and then Fortin and Glowinski [13] proposed to apply it to the solution of the linear Stokes problem and also to others non-linear problems such as Bingham fluid flows. In 1980, Bercovier and Engelman [3] proposed a viscosity function for the regularization of Bingham flow problem. In 1987, another viscosity function was proposed by Papanastasiou [26]. During the 1980s and the 1990s, numerical computations for Bingham flow problems was dominated by the regularization method, perhaps due to its simplicity, while the augmented Lagrangian algorithm leaded not yet convincing results for viscoplastic flow applications. In 1989, Glowinski and le Tallec [16] revisited the augmented Lagrangian method, using new optimization and convex analysis tools, such as subdifferential, but no evidence of the efficiency of this approach to viscoplasticity was showed, while regularization approach becomes more popular in the 1990s with the work of Mitsoulis et al. [19] and Wilson and Taylor [39]. In 2001, Saramito and Roquet [36, 31] showed for the first time the efficiency of the augmented Lagrangian algorithm when combined with auto-adaptive mesh methods for capturing accurately the yield surface. In the 2000s, this approach became mature and a healthy competition developed between the regularization approach and the augmented Lagrangian one. Vola, Boscardin and Latché [38] obtained results for a driven cavity flow with the augmented Lagrangian algorithm while Mitsoulis et al. [20] presented computation for an expansion flow with regularization and Frigaard et al. [21, 14, 29] pointed out some drawbacks of the regularization approach. Finally, at the end of the 2000s decade, the augmented Lagrangian algorithm becomes the most popular way to solve viscoplastic flow problems [22, 11] because of its accuracy, despite the regularization approach runs much more faster. The free software Rheolef library, developped by the author and supporting both the augmented Lagrangian algorithm and an auto-adaptive mesh technique is now widely used for various flow applications (see e.g. [28, 32, 33, 4]).

The main drawback of the augmented Lagrangian algorithm is its computing time for large applications, especially when the Bingham number becomes large. This paper is a contribution to an ongoing effort for the development of faster algorithms for the resolution of the unregularized viscoplastic model. One of the most efficient algorithm to solve nonlinear problems is the Newton method, due to its super-linear convergence properties (see e.g. [24]). This approach has already been investigated for the regularized approach of the viscoplastic problem (see e.g. [5] and most recently [8, 9, 10] for the biviscous regularization). Applying the Newton method to the unregularized viscoplastic problem leads to a singular Jacobian matrix. This difficulty has been recently addressed by using the trusted region algorithm [37], that regularizes the Jacobian matrix but loses the superlinear convergence of the method. In this paper, our contribution is to address directly the singularity of the Jacobian matrix in the Newton method in order to preserve the superlinear convergence. The proposed reformulation of the viscoplastic flow problem is inspired by the work of Alart and Curnier [1] on another non-smooth problem, the frictional contact one, that was successfully addressed by a Newton method.

Section 1 presents the viscoplastic flow problem and its mathematical statement. This problem is reformulated in section 2 in terms of a projection operator and section 3 presents its variational formulation and discretization. Section 4 develops the Newton algorithm and the resolution of the Jacobian matrix while section 5 shows preliminary results for this approach.

1 Problem statement

The Bingham [6, 23] and Herschel-Bulkley [17] models are characterized by the following property: the material starts to flow only if the applied forces exceed a certain limit σ_0 , called the yield limit. The total Cauchy stress tensor is expressed by:

$$\sigma_{tot} = -p.I + \sigma$$

where σ denotes its deviatoric part, and p is the pressure. The conservation of momentum is:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) - \operatorname{div} \sigma + \nabla p = 0$$

where u is the velocity field, and ρ the constant density. The mass conservation leads to:

$$\operatorname{div} \boldsymbol{u} = 0$$

The constitutive equation writes:

$$\sigma = K|2D(\boldsymbol{u})|^{-1+n}2D(\boldsymbol{u}) + \sigma_0 \frac{2D(\boldsymbol{u})}{|2D(\boldsymbol{u})|} \quad \text{if } |D(\boldsymbol{u})| \neq 0$$
$$|\sigma| \leqslant \sigma_0 \quad \text{if } |D(\boldsymbol{u})| = 0$$

or equivalently:

$$2D(\boldsymbol{u}) = \begin{cases} \frac{1}{K^{1/n}} (|\sigma| - \sigma_0)^{1/n} \frac{\sigma}{|\sigma|} & \text{if } |\sigma| > \sigma_0 \\ 0 & \text{otherwise} \end{cases}$$

where $\sigma_0 \ge 0$ is the yield stress, K > 0 is the consistency, n > 0 is the power index, $D(\boldsymbol{u}) = (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)/2$ is the rate-of-deformation tensor, and, for any tensor $\tau = (\tau_{i,j})_{1 \le i,j \le 3}$, the notation $|\tau|$ represents the following matrix norm:

$$|\tau| = \sqrt{\frac{\tau : \tau}{2}} = \frac{1}{\sqrt{2}} \left(\sum_{i,j=1}^{3} \tau_{i,j}^{2} \right)^{\frac{1}{2}}$$

Notice that when $\sigma_0 = 0$ and n = 1, one is led to the classical viscous incompressible fluid. When $\sigma_0 > 0$, rigid zones in the interior of the fluid can be observed. As σ_0 becomes larger, these rigid zones develop and may completely block the flow when σ_0 is sufficiently large. When n = 1 and $\sigma_0 > 0$ the model is called the Bingham one while for a general power law index n > 0 this is the Herschel-Bulkley model.

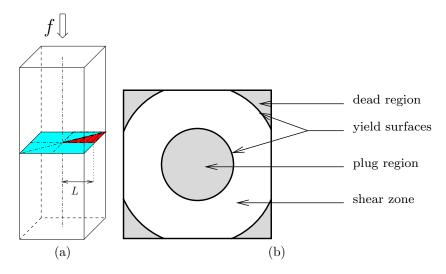


Figure 1: Square tube cross-section: (a) tridimensional view; (b) schematic view of the cross-section.

We consider the fully developed flow in a prismatic tube, as shown on Fig. 1.a (see also [36]). Let (Oz) be the axis of the tube and (Oxy) the plane of the bounded section $\Omega \subset \mathbb{R}^2$. The pressure gradient is written as $\nabla p = (0, 0, -f)$ in Ω , where f > 0 is the constant applied force density. The velocity is written as $\mathbf{u} = (0, 0, u)$, where the third component u along the (Oz) axis depends only upon x and y, and is independent of t and z. The problem can be considered as a two-dimensional one, and the stress tensor σ is equivalent to a two shear stress component vector: $\boldsymbol{\sigma} = (\sigma_{xz}, \sigma_{yz})$. We also use the following notations:

$$\nabla u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$$
$$\operatorname{div} \boldsymbol{\sigma} = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y}$$
$$|\boldsymbol{\sigma}| = \sqrt{\sigma_{xz}^2 + \sigma_{yz}^2}$$

Finally, the problem can be summarized as:

(HB): find σ and u defined in Ω such that:

$$\nabla u = P_0(\boldsymbol{\sigma}) \tag{1a}$$

$$\operatorname{div} \boldsymbol{\sigma} = -f \text{ in } \Omega \tag{1b}$$

$$u = 0 \text{ on } \partial\Omega \tag{1c}$$

where P_0 denotes the following projection operator, defined for all $\boldsymbol{\tau} \in \mathbb{R}^2$ by

$$P_0(\boldsymbol{\tau}) = \begin{cases} \frac{1}{K^{1/n}} (|\boldsymbol{\tau}| - \sigma_0)^{1/n} \frac{\boldsymbol{\tau}}{|\boldsymbol{\tau}|} & \text{when } |\boldsymbol{\tau}| > \sigma_0 \\ 0 & \text{otherwise} \end{cases}$$
 (2)

Here, (1a) expresses the constitutive equation, (1b) the conservation of momentum and (1c) the noslip boundary condition. In the case of a square cross-section, we reduce the domain of computation by using symmetries (see Fig. 1.a).

Let L be a characteristic length of the cross-section Ω , i.e. the half-length of an edge of a square section, or the radius of a circular section (also denoted by R for convenience in that case). A characteristic stress is given by $\Sigma = Lf/2$ and a characteristic velocity U is such that $\Sigma = K(U/L)^n$ i.e. $U = (Lf/(2K))^{1/n}L$. The Bingham dimensionless number is defined by the ratio of the yield stress σ_0 by the representative viscous stress Σ :

$$Bi = \frac{2\sigma_0}{Lf}$$

The Bingham number Bi and the power law index n are the only two dimensionless numbers of the problem.

2 Reformulation of the problem

Observe that, for all σ and $\gamma \in \mathbb{R}^2$ and for all $\sigma_0 \ge 0$ and n > 0, the projection operator P_0 introduced in (2) satisfies, for all $r \ge 0$, the following property:

$$\gamma = P_0(\sigma) \Longleftrightarrow \gamma = P_r(\sigma + r\gamma)$$
 (3)

where P_r denotes the following extended projection operator, defined for all $\tau \in \mathbb{R}^2$ by

$$P_r(\boldsymbol{\tau}) = \begin{cases} \varphi_r^{-1}(|\boldsymbol{\tau}|) \frac{\boldsymbol{\tau}}{|\boldsymbol{\tau}|} & \text{when } |\boldsymbol{\tau}| > \sigma_0 \\ 0 & \text{otherwise} \end{cases}$$
(4)

and where φ_r is defined for all $\dot{\gamma} \geqslant 0$ by

$$\varphi_r(\dot{\gamma}) = \sigma_0 + K\dot{\gamma}^n + r\dot{\gamma}$$

Remark that the r parameter, involved in the extended projection operator P_r , interprets as an augmentation parameter, similar to those involved by the augmented Lagrangian formulation.

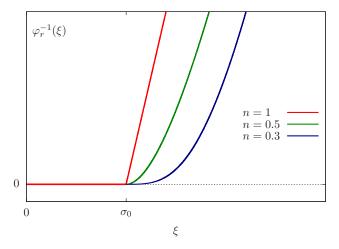


Figure 2: The φ_r^{-1} function for various values of n.

As the function φ_r is strictly increasing in $[0, +\infty[$, it is invertible from $[0, +\infty[$ to $[\sigma_0, +\infty[$ and its inverse denoted by φ_r^{-1} is well defined in $[\sigma_0, +\infty[$ (see Fig. 2).

Let us perform a change of unknown by introducing

$$\boldsymbol{\beta} = \boldsymbol{\sigma} + r \boldsymbol{\nabla} u \Longleftrightarrow \boldsymbol{\sigma} = \boldsymbol{\beta} - r \boldsymbol{\nabla} u$$

Then, problem (1a)-(1c) writes equivalently as

 $(HB)_r$: find u and β such that

$$r\Delta u - \operatorname{div}\boldsymbol{\beta} = f \text{ in } \Omega \tag{5a}$$

$$\nabla u - P_r(\boldsymbol{\beta}) = 0 \text{ in } \Omega \tag{5b}$$

$$u = 0 \text{ on } \partial\Omega \tag{5c}$$

Observe that, from (3), the solution is independent upon $r \in [0, 1[$. An inspection of the regularity of φ_r in zero shows that this function is C^1 only when n < 1 (see also Fig. 2). When n = 1 (Bingham model) we have $\varphi'_r(0) = r + K \neq 0$ and thus $(\varphi_r^{-1})'(\sigma_0^-) = 0$ while $(\varphi_r^{-1})'(\sigma_0^+) = 1/(r + K)$. This loss of regularity in the case n = 1 will impact the convergence properties of the forthcoming Newton method.

3 Variational formulation and discretization

Consider the following forms:

$$a(u,v) = -r \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad \forall u, v \in H^{1}(\Omega)$$

$$b(v,\tau) = \int_{\Omega} \nabla v \cdot \tau \, dx, \quad \forall \tau \in (L^{2}(\Omega))^{2}, \quad \forall v \in H^{1}(\Omega)$$

$$c(\beta,\tau) = \int_{\Omega} \kappa_{r}(|\beta|) \beta \cdot \tau \, dx, \quad \forall \beta, \tau \in (L^{2}(\Omega))^{2}$$

$$\ell(v) = \int_{\Omega} f v \, dx, \quad \forall v \in L^{2}(\Omega)$$

where κ_r denotes the following function, defined for all $\xi \in \mathbb{R}^+$ by

$$\kappa_r(\xi) = \begin{cases}
\frac{\varphi_r^{-1}(\xi)}{\xi} & \text{when } \xi > \sigma_0 \\
0 & \text{otherwise}
\end{cases}$$

The variational formulation writes:

 $(FV)_r$: find $u \in H_0^1(\Omega)$ and $\beta \in (L^2(\Omega))^2$ such that

$$a(u,v) + b(v,\boldsymbol{\beta}) = \ell(v), \forall v \in H_0^1(\Omega)$$

$$b(u,\boldsymbol{\tau}) - c(\boldsymbol{\beta},\boldsymbol{\tau}) = 0, \forall \boldsymbol{\tau} \in \left(L^2(\Omega)\right)^2$$

This problem is then discretized by using a mixed finite element method (see e.g. [36]). The velocity u is approximated by continuous piecewise polynomials of order $k \ge 1$ while the shear stress vector $\boldsymbol{\beta}$ is approximated by discontinuous k-1 polynomials. In the present paper, all computations are performed with k=1, i.e. piecewise affine and continuous velocities and piecewise constant stresses. As the corresponding approximated problem is similar to the continuous one, it is not developed here. For the purpose of simplicity, we also continue to work with the continuous problem in the next section, dedicated to the Newton method.

4 Newton method

The problem can be expressed in a compact form:

find
$$u \in H_0^1(\Omega)$$
 and $\boldsymbol{\beta} \in (L^2(\Omega))^2$ such that

$$F(u, \boldsymbol{\beta}) = 0$$

where F is defined in variational form for all $v \in H^1(\Omega)$ and $\tau \in (L^2(\Omega))^2$ by

$$\langle F(u, \boldsymbol{\beta}), (v, \boldsymbol{\tau}) \rangle = a(u, v) + b(\boldsymbol{\beta}, v) + b(\boldsymbol{\tau}, u) - c(\boldsymbol{\beta}, \boldsymbol{\tau})$$

and where $\langle .,. \rangle$ denotes the duality product induced by the L^2 pivot space i.e. $\langle \varphi, \phi \rangle = \int_{\Omega} \varphi \phi \, dx$ for all φ, ϕ defined in Ω .

The Newton method defines the sequence $(u_k, \beta_k)_{k \ge 0}$ by recurrence as:

- k = 0: let $(u_0, \boldsymbol{\beta}_0) \in H_0^1(\Omega) \times (L^2(\Omega))^2$ being given.
- $k \ge 0$: let $(u_{k-1}, \beta_{k-1}) \in H_0^1(\Omega) \times (L^2(\Omega))^2$ being known. Find $(\delta u, \delta \beta) \in H_0^1(\Omega) \times (L^2(\Omega))^2$ such that

$$F'(u_{k-1}, \boldsymbol{\beta}_{k-1}) \cdot (\delta u, \delta \boldsymbol{\beta}) = -F(u_{k-1}, \boldsymbol{\beta}_{k-1})$$

and then defines

$$u_k = u_{k-1} + \delta u$$
 and $\boldsymbol{\beta}_k = \boldsymbol{\beta}_{k-1} + \delta \boldsymbol{\beta}$

At each step $k \ge 0$, this algorithm solves a linear subproblem involving the Jacobian F'. The Newton method has only local convergence properties, i.e. the initial value should be close enough to the solution. In order to circumvent this limitation, a globalized Newton variant is used here. It is based on a damping strategy, as described and implemented in the Rheolef free software FEM library [35].

As F is Gâteau differentiable, the Jacobian F' is defined, for all $\delta u \in H^1(\Omega)$ and $\delta \beta \in (L^2(\Omega))^2$ and $v \in H^1(\Omega)$ and $\tau \in (L^2(\Omega))^2$ by

$$\langle F'(u, \boldsymbol{\beta}).(\delta u, \delta \boldsymbol{\beta}), (v, \boldsymbol{\tau}) \rangle = a(\delta u, v) + b(\delta \boldsymbol{\beta}, v) + b(\boldsymbol{\tau}, \delta u) - c_1(\boldsymbol{\beta}; \delta \boldsymbol{\beta}, \boldsymbol{\tau})$$

where c_1 denotes the following form:

$$c_1(\boldsymbol{\beta}; \, \delta \boldsymbol{\beta}, \boldsymbol{\tau}) = \int_{\Omega} \left(P'_r(\boldsymbol{\beta}) \delta \boldsymbol{\beta} \right) . \boldsymbol{\tau} \, \mathrm{d}x$$

and, for all $\beta \in \mathbb{R}^2$, we denote by $P'_r(\beta)$ the following 2×2 matrix:

$$P'_r(\boldsymbol{\beta}) = \begin{cases} \frac{\varphi_r^{-1}(|\boldsymbol{\beta}| - \sigma_0)}{|\boldsymbol{\beta}|} \boldsymbol{I} + \frac{|\boldsymbol{\beta}| \left(\varphi_r^{-1}\right)' (|\boldsymbol{\beta}| - \sigma_0) - \varphi_r^{-1}(|\boldsymbol{\beta}| - \sigma_0)}{|\boldsymbol{\beta}|^3} \boldsymbol{\beta} \otimes \boldsymbol{\beta} & \text{when } |\boldsymbol{\beta}| > \sigma_0 \\ 0 & \text{otherwise} \end{cases}$$

Here, $(\varphi_r^{-1})'$ denotes the derivative of the inverse of the function φ_r , defined for all $\xi \geqslant \sigma_0$ by

$$\left(\varphi_r^{-1}\right)'(\xi) = \frac{1}{\varphi_r'\left(\varphi_r^{-1}(\xi)\right)} = \frac{1}{r + nK\left(\varphi_r^{-1}(\xi)\right)^{-1+n}}$$

Let A, B and C_1 the operators associated to the bilinear forms a(.,.), b(.,.) and $c_1(\boldsymbol{\beta}_{k-1};.,.)$ respectively. The linear problem satisfied by $(\delta u, \delta \boldsymbol{\beta})$ writes also:

$$\begin{pmatrix} A & B^* \\ B & -C_1 \end{pmatrix} \begin{pmatrix} \delta u \\ \delta \boldsymbol{\beta} \end{pmatrix} = \begin{pmatrix} -F_u \left(u_{k-1}, \boldsymbol{\beta}_{k-1} \right) \\ -F_{\boldsymbol{\beta}} \left(u_{k-1}, \boldsymbol{\beta}_{k-1} \right) \end{pmatrix}$$

Notice that A is linear symmetric definite negative while C_1 is nonlinear symmetric semi-definite positive. Recall that we expect the existence of subdomains of Ω with nonzero measure where $\nabla u = 0$ and $|\beta| < \sigma_0$. In these subdomains, the matrix $P'_r(\beta)$ is zero. Thus, the Jacobian F' is not expected to be invertible in general. Moreover, as A is negative, F' is indefinite (i.e. it has both positive and negative eigenvalues). As F' is singular, there exists an infinity of solutions: it is sufficient to choose one of them for the damped Newton method to converge. To this purpose, we use Saad and Schultz' GMRES algorithm [34] for solving this indefinite and possibly singular linear system. It can be considered as a generalization of Paige and Saunders' MINRES algorithm [25] which applies more specifically to symmetric and definite systems, possibly singular. This algorithm is implemented in the Rheolef free software FEM library [35] together with the damped Newton method. The convergence rate of the GMRES algorithm can be dramatically increased by supplying a preconditioner, i.e. another matrix, easier to invert, and close to the Jacobian matrix. In this paper, we consider a preconditioner which is based on the Jacobian of the regularized problem. A similar idea was suggested by Aposporidis [2] in the context of a fixed point algorithm and a different reformulation of the viscoplastic flow problem.

The Jacobian of the regularized problem is invertible, thus easier to invert than the unregularized one. Also, when the regularization parameter tends to zero, the Jacobian of the regularized problem becomes close to those of the unregularized one, thus increasing the convergence rate of the GMRES algorithm for solving the unregularized problem. For all $\varepsilon > 0$, let us introduce the regularized function $\varphi_{r,\varepsilon}$ is defined for all $\dot{\gamma} \in \mathbb{R}^+$ by

$$\varphi_{r,\varepsilon}(\dot{\gamma}) = r\dot{\gamma} + K\dot{\gamma}^n + \frac{\sigma_0 \dot{\gamma}}{(\dot{\gamma}^2 + \varepsilon^2)^{\frac{1}{2}}}$$

and the regularized projection operator, defined for all $au \in \mathbb{R}^2$ by

$$P_{r,\varepsilon}(\boldsymbol{\tau}) = \begin{cases} \varphi_{r,\varepsilon}^{-1}(|\boldsymbol{\tau}|) \frac{\boldsymbol{\tau}}{|\boldsymbol{\tau}|} & \text{when } |\boldsymbol{\tau}| > \sigma_0 \\ 0 & \text{otherwise} \end{cases}$$

As $\varphi_{r,\varepsilon}$ is strictly increasing from $]0,+\infty[$ to $]0,+\infty[$, its inverse $\varphi_{r,\varepsilon}^{-1}$ is well defined. The regularized problem writes:

 $(HB)_{r,\varepsilon}$: find u and β , defined in Ω , such that

$$r\Delta u - \operatorname{div} \boldsymbol{\beta} = f \text{ in } \Omega \tag{6a}$$

$$\nabla u - P_{r,\varepsilon}(\beta) = 0 \text{ in } \Omega$$
 (6b)

$$u = 0 \text{ on } \partial\Omega$$
 (6c)

The Jacobian F_{ε} has an expression which is similar to those of the unregularized one, just replacing φ_r by $\varphi_{r,\varepsilon}$. The Jacobian F'_{ε} is expected to be close to the unregularized one F' and it is also non-singular, so easier to invert than F'. Thus, it is a good candidate to be a preconditioner, as shown in the next section. For practical computations, the evaluations of φ_r^{-1} and $\varphi_{r,\varepsilon}^{-1}$ are also performed by a Newton method with a stopping criterion at the machine precision (about 10^{-15} in double precision). This criterion is reached in very few iterations, as φ_r is regular.

5 Numerical results and performances

Fig. 3 shows the convergence of the Newton method for various values of the power law index n and an uniform mesh with h = 1/160. The residue at iteration k is computed as the L^2 norm of

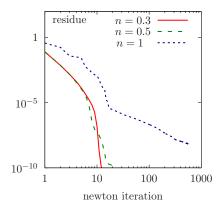


Figure 3: Damped Newton method for the Herschel-Bulkley problem: residue vs Newton iterations for various n, with Bi = 0.1, r = 0.5, $\varepsilon = 10^{-5}$ and h = 1/160.

 $F(u_k, \boldsymbol{\beta}_k)$. The stopping criteria on the residue is 10^{-12} and the preconditioner uses $\varepsilon = 10^{-5}$. Observe that, for both n = 0.3 and n = 0.5, the convergence is very fast, less than 20 iterations: this is the expected behavior of the Newton method when F is sufficiently regular. Changing the value of the parameter r has few influence on performances and all computations presented in this paper are performed with r = 0.5. When n = 1 (Bingham model), the convergence is much more slower: it is asymptotically linear in log-log scale, which means that the residue decreases as $1/k^{\alpha}$. This slow down of the convergence rate is probably due to the lower regularity of F when n = 1 (see also Fig. 2).

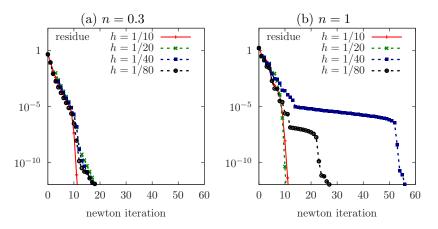


Figure 4: Damped Newton method for the Herschel-Bulkley problem: residue vs Newton iterations for various mesh refinement h with Bi = 0.5, r = 0.5 and $\varepsilon = 10^{-5}$. (a) n = 0.3; (b) n = 1.

Observe on Fig. 4.a that when n = 0.3, the convergence is asymptotically *mesh-invariant* (for the mesh-invariance property of nonlinear algorithms, see [35, chap. 8]). Conversely, when n = 1 (Fig. 4.b), the convergence rate depends mesh refinement and there are long plateau where the residue decreases slowly.

Fig. 5.a shows the convergence properties of the Jacobian solver with the GMRES algorithm for various meshes and the preconditioner based on the regularized problem with $\varepsilon = 10^{-5}$. For the smallest meshes, the Jacobian system is solved with few iterations while the convergence rate becomes slower with mesh refinement and the largest meshes are still the most difficult to solve. Fig. 5.b shows that the preconditioner efficiency increases when ε decreases, as the regularized

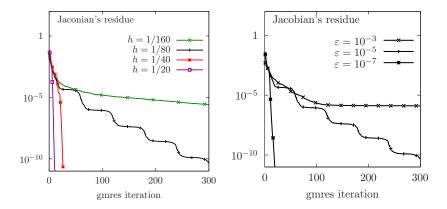


Figure 5: Preconditioning the Jacobian by using the regularized problem: Bi = 0.1, n = 0.5 and r = 0.5. (a) $\varepsilon = 10^{-5}$ and varying h; (b) h = 1/80 and varying ε .

Jacobian approaches better the exact one. Using too small ε , lower than 10^{-7} , could interfere with the finite machine precision, about 10^{-15} for double precision. Increasing the machine precision, e.g. quadruple precision could be usefull here, in order to continue to decrease ε and increase the solver efficiency.

An inexact variant of the Newton [12] method is possible and very efficient here. The idea is to stop the inner GMRES iteration when the residue of the Jacobian system reaches a ratio, e.g. 10%, of the residue of the current Newton iteration. For simplicity, let us denote $\chi = (u, \beta)$ and consider the Jacobian system:

$$F'(\chi).\delta\chi = -F(\chi)$$

In that case, the iterative GMRES solver stops when the residue is less than $0.1 \times ||F(\chi)||$. This modification maintains the superlinear convergence property of the Newton method and each linear solver call requires only very few iterations, thanks to the efficient preconditioner.

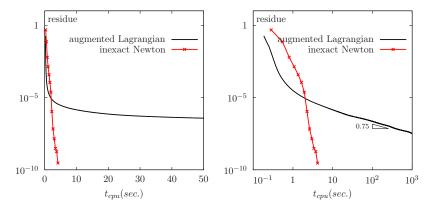


Figure 6: Comparison between the inexact damped Newton method and the augmented Lagrangian algorithm (AL) for the Herschel-Bulkley problem: residu vs CPU time, in seconds when Bi = 0.1, n = 0.5, h = 1/80 (r = 0.5, $\varepsilon = 10^{-7}$ for Newton and r = 7 for AL) (a) in semi-log scale; (b) in log-log scale.

Fig. 6 plots a comparison of the present inexact preconditioned damped Newton algorithm with the classical Uzawa/augmented Lagrangian method, as proposed in [36]. The augmentation parameter r for the augmented Lagrangian algorithm (AL) has been specially optimized (r = 7) for the present mesh (a pipe sector with h = 1/80 and 5781 elements) in order to present the best

possible convergence rate. Both algorithms are implemented in the Rheolef free software FEM library [35]. The Poisson matrix with no-slip boundary condition used by the AL is factored in sparse format one time for all, thanks to the SUITESPARSE library [7]. At each iteration of the AL, a linear system is solved, based on this factorization. For the present inexact Newton algorithm, the Jacobian matrix of the regularized problem, used as preconditioner, is also factored by the same way. This factorization has too be performed at each iteration of the Newton method, so each iteration of the Newton method is expected to be slower than its AL counterpart. For this reason, Fig. 6 compares these two methods in term of the CPU time. Observe the dramatic efficiency of the Newton algorithm, which converge in less than 5 seconds to a residue less than 10^{-10} while the AL becomes slower and slower in semi-log scale and adopts an asymptotic behavior, as shown in semi-log scale, where the residue behaves as $1/t^{\alpha}$, with $\alpha \approx 0.75$. After about 15 minutes, the residue is of about 10^{-7} and, by extrapolation, reaching 10^{-10} would requires one day of computation.

Conclusion

For the first time, a Newton method is proposed for the unregularized viscoplastic fluid flow problem. It leads to a superlinear convergence for Herschel-Bulkley fluids when 0 < n < 1. At each iteration, the singular Jacobian system is solved by an iterative method and an efficient preconditioner based on the regularized problem and an inexact approach permits to increase the performances of the algorithm. A demonstration is provided by the computing a viscoplastic flow in a pipe with a square cross section and performances are compared with the augmented Lagrangian algorithm. Future work will extends this approach to larger flow problems such as flows around obstacles and tridimensional geometries.

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