Journal of Non-Newtonian Fluid Mechanics 000 (2016) 1–16

Contents lists available at ScienceDirect

Journal of Non-Newtonian Fluid Mechanics

journal homepage: www.elsevier.com/locate/jnnfm

An accelerated dual proximal gradient method for applications in viscoplasticity

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ARTICLE INFO

Article history:
Received 10 March 2016
Revised 15 September 2016
Accepted 16 September 2016
Available online xxx

MSC:
49M29
74C10
76M10

Keywords:
Fast proximal gradient methods
Augmented Lagrangian methods
Viscoplastic fluids
Adaptive finite elements

ABSTRACT

We present a very simple and fast algorithm for the numerical solution of viscoplastic flow problems without prior regularisation. Compared to the widespread alternating direction method of multipliers (ADMM / ALG2), the new method features three key advantages: firstly, it accelerates the worst-case convergence rate from $O(1/\sqrt{k})$ to $O(1/k)$, where k is the iteration counter. Secondly, even for nonlinear constitutive models like those of Casson or Herschel–Bulkley, no nonlinear systems of equations have to be solved in the subproblems of the algorithm. Thirdly, there is no need to augment the Lagrangian, which eliminates the difficulty of choosing a penalty parameter heuristically.

In this paper, we transform the usual velocity-based formulation of viscoplastic flow problems to a dual formulation in terms of the stress. For the numerical solution of this dual problem we apply FISTA, an accelerated first-order optimisation algorithm from the class of so-called proximal gradient methods. Finally, we conduct a series of numerical experiments, focussing on stationary flow in two-dimensional square cavities.

Our results confirm that Algorithm FISTA*, the new dual-based FISTA, outperforms state-of-the-art algorithms such as ADMM / ALG2 by several orders of magnitude. We demonstrate how this speedup can be exploited to identify the free boundary between yielded and unyielded regions with previously unknown accuracy. Since the accelerated algorithm relies solely on Stokes-type subproblems and nonlinear function evaluations, existing code based on augmented Lagrangians would require only few minor adaptations to obtain an implementation of FISTA*.

1. Introduction

Viscoplasticity is a wide-spread phenomenon in both natural and man-made applications. The rich rheology of viscoplastic fluids is encountered in geophysics, considering the examples of lava flows or lahars [1,2]. Certain types of mineral oils, mud or slurry suspensions also exhibit viscoplastic features. In the consumer goods industry, toothpaste, hair gel, tomato sauce or dough serve as classical examples of such fluids [3].

The characteristic feature of a viscoplastic fluid is its ability to resist stress in the material up to a critical threshold, the so-called yield stress τ_0. This behaviour is generally due to friction-type interactions between the molecules or particles of the fluid. Consequently, viscoplastic fluids behave like a rigid material at small stress. They only start shearing like a viscous liquid if the stress exceeds the threshold posed by the yield stress.

1.1. Mathematical models for viscoplastic fluid flows

We consider the problem of steady, creeping viscoplastic flow in a cavity, represented by the bounded domain $\Omega \subset \mathrm{R}^d$ with (Lipschitz) boundary $\partial\Omega = \Gamma$. In practice, $d \in \{2, 3\}$. Our objective is to solve for functions $\boldsymbol{u}$: $\Omega \to \mathrm{R}^d$, p: $\Omega \to \mathrm{R}$ and $\boldsymbol{\tau} : \Omega \to \mathrm{R}^{d\times d}_{\mathrm{sym}}$, representing the flow velocity, pressure and deviatoric part of the stress, respectively. Furthermore, with the symmetric gradient operator $\mathcal{D} := (\nabla + \nabla^\top)/2$, we denote the strain-rate tensor by $\dot{\gamma} : \Omega \to \mathrm{R}^{d\times d}_{\mathrm{sym}}$, which is linked to the flow velocity through the relation $\dot{\gamma} = \mathcal{D}\boldsymbol{u}$.

The most common mathematical descriptions of viscoplastic behaviour are given by the Bingham [4], the Casson [5] and the shear-thinning Herschel–Bulkley model [6]. With viscosity or consistency parameters μ, $\kappa > 0$ and an exponent $1 < r < 2$, they can

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[1] Supported by a UC Doctoral Scholarship and the OptALI Exchange Programme

http://dx.doi.org/10.1016/j.jnnfm.2016.09.004

be formulated as

$$|\boldsymbol{\tau}| \le \tau_0 \qquad \text{if } \dot{\gamma} = 0 \tag{1.1a}$$

$$\boldsymbol{\tau} = \begin{cases} 2\mu\dot{\gamma} + \tau_0 \frac{\dot{\gamma}}{|\dot{\gamma}|} & \text{(Bingham)} \\ \left(\sqrt{2\mu|\dot{\gamma}|} + \sqrt{\tau_0}\right)^2 \frac{\dot{\gamma}}{|\dot{\gamma}|} & \text{(Casson)} \\ 2^{r-1}\kappa|\dot{\gamma}|^{r-2}\dot{\gamma} + \tau_0\frac{\dot{\gamma}}{|\dot{\gamma}|} & \text{(Herschel-Bulkley)} \end{cases} \qquad \text{if } \dot{\gamma} \neq 0. \tag{1.1b}$$

Here, $|\cdot|$ denotes the Frobenius norm on $\mathbb{R}^{d\times d}_{\text{sym}}$.

In what follows, we consider a non-dimensionalised formulation that has been re-scaled with respect to a characteristic length L and velocity U, which reduces the dimensional constitutive relations (1.1) to

$$|\boldsymbol{\tau}| \le \text{Bi} \qquad \text{if } \dot{\gamma} = 0 \tag{1.2a}$$

$$\boldsymbol{\tau} = \begin{cases} 2\dot{\gamma} + \text{Bi} \frac{\dot{\gamma}}{|\dot{\gamma}|} & \text{(Bingham)} \\ \left(\sqrt{2|\dot{\gamma}|} + \sqrt{\text{Bi}}\right)^2 \frac{\dot{\gamma}}{|\dot{\gamma}|} & \text{(Casson)} \\ 2^{r-1}|\dot{\gamma}|^{r-2}\dot{\gamma} + \text{Bi}\frac{\dot{\gamma}}{|\dot{\gamma}|} & \text{(Herschel-Bulkley)} \end{cases} \qquad \text{if } \dot{\gamma} \neq 0. \tag{1.2b}$$

The Bingham number $\text{Bi} := \frac{\tau_0 L}{\mu U}$ (Bingham, Casson) or $\text{Bi} := \frac{\tau_0 L^{r-1}}{\kappa U^{r-1}}$ (Herschel–Bulkley) quantifies the deviation of the viscoplastic flow from (generalised) Newtonian behaviour.

Any of these constitutive relations, along with equations for conservation of momentum and mass, yield a system for the unknown flow variables. Denoting by $\boldsymbol{f}\colon \Omega \to \mathbb{R}^d$ a non-dimensionalised density of body forces, we have

$$-\text{Div}\,\boldsymbol{\tau} + \nabla p = \boldsymbol{f} \quad \text{in } \Omega \tag{1.3}$$

$$\text{div}\,\boldsymbol{u} = 0 \quad \text{in } \Omega. \tag{1.4}$$

To close the system, we incorporate the boundary condition

$$\boldsymbol{u} = \boldsymbol{u}_\text{D} \quad \text{on } \Gamma, \tag{1.5}$$

where $\boldsymbol{u}_\text{D}\colon \Gamma_\text{D} \to \mathbb{R}^d$ is given. We use the notation div (resp. Div) for the (rowwise) divergence operator.

1.2. Variational formulation

In the following, we use boldface letters for spaces to denote d-fold Cartesian products, e.g. for a space A we write $\boldsymbol{A} := A^d$. To obtain a mathematically rigorous formulation of the viscoplastic flow problem (1.2)–(1.5) in Sobolev spaces, we consider

$$\begin{aligned} U &:= \boldsymbol{W}^{1,r}(\Omega) \\ U_{0*} &:= \{\boldsymbol{u} \in \boldsymbol{W}^{1,r}(\Omega) | \text{div}\boldsymbol{u} = 0\} \\ U_{*0} &:= \{\boldsymbol{u} \in \boldsymbol{W}^{1,r}(\Omega) | \boldsymbol{u}|_\Gamma = 0\} \\ U_{00} &:= \{\boldsymbol{u} \in \boldsymbol{W}^{1,r}(\Omega) | \text{div}\boldsymbol{u} = 0 \text{ and } \boldsymbol{u}|_\Gamma = 0\}, \end{aligned}$$

with $r = 2$ in the Bingham and Casson settings. We use the dual of the latter space to fix the inhomogeneity $\boldsymbol{f} \in U_{00}^*$ and we pick boundary values $\boldsymbol{u}_\text{D} \in U_\text{D}$, where

$$U_\text{D} := \{\boldsymbol{u}_\text{D} \in \boldsymbol{W}^{1-1/r,r}(\Gamma) | \int_\Gamma \boldsymbol{u}_\text{D}\cdot\boldsymbol{n}\,\text{d}s = 0\}.$$

Furthermore, we define the convex set of admissible solutions

$$U_{0\text{D}} := \{\boldsymbol{u} \in \boldsymbol{W}^{1,r}(\Omega) | \text{div}\boldsymbol{u} = 0 \text{ and } \boldsymbol{u}|_\Gamma = \boldsymbol{u}_\text{D}\}.$$

For the strain-rate and stress tensors, we will also need spaces of symmetric matrices whose entries satisfy an integrability condition of order r or r^*, respectively, where $1/r + 1/r^* = 1$:

$$Q := L^r(\Omega)^{d\times d}_{\text{sym}} \quad S := L^{r^*}(\Omega)^{d\times d}_{\text{sym}}.$$

By generalising the ideas of Duvaut and Lions [7,8] and Huilgol and You [9], we conclude that the system (1.2)–(1.5) is a strong formulation of the following variational inequality problem of the second kind: find $\boldsymbol{u} \in U_{0\text{D}}$ such that for all test velocity fields $\boldsymbol{v} \in U_{0\text{D}}$

$$a(\mathcal{D}\boldsymbol{u}, \mathcal{D}\boldsymbol{v} - \mathcal{D}\boldsymbol{u}) + j(\mathcal{D}\boldsymbol{v}) - j(\mathcal{D}\boldsymbol{u}) \ge \langle \boldsymbol{f}, \boldsymbol{v} - \boldsymbol{u}\rangle_{U_{00}^*, U_{00}}. \tag{1.6}$$

This variational inequality is composed of the elliptic form $a\colon Q \times Q \to \mathbb{R}$,

$$a(\dot{\boldsymbol{\gamma}}, \dot{\boldsymbol{\delta}}) := 2\int_\Omega \dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\delta}}\,\text{d}x \quad \text{(Bingham)}$$

$$a(\dot{\boldsymbol{\gamma}}, \dot{\boldsymbol{\delta}}) := 2\int_\Omega \dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\delta}}\,\text{d}x + 2\sqrt{2\text{Bi}}\int_\Omega \frac{\dot{\boldsymbol{\gamma}}}{\sqrt{|\dot{\boldsymbol{\gamma}}|}} : \dot{\boldsymbol{\delta}}\,\text{d}x \quad \text{(Casson)}$$

$$a(\dot{\boldsymbol{\gamma}}, \dot{\boldsymbol{\delta}}) := 2^{r-1}\int_\Omega |\dot{\boldsymbol{\gamma}}|^{r-2}\dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\delta}}\,\text{d}x \quad \text{(Herschel–Bulkley)}$$

the nonsmooth functional $j\colon Q \to \mathbb{R}$,

$$j(\dot{\boldsymbol{\gamma}}) := \text{Bi}\int_\Omega |\dot{\boldsymbol{\gamma}}|\,\text{d}x$$

and, on the right-hand side, a duality pairing between U_{00} and its dual, which can be represented as

$$\langle \boldsymbol{f}, \boldsymbol{v} - \boldsymbol{u}\rangle_{U_{00}^*, U_{00}} = \int_\Omega \boldsymbol{f}\cdot(\boldsymbol{v} - \boldsymbol{u})\,\text{d}x$$

provided that $\boldsymbol{f} \in \boldsymbol{L}^{r^*}(\Omega)$. The colon represents the Frobenius inner product of two $d \times d$ matrices, the dot the scalar product of two vectors in $\mathbb{R}^d$.

It is an important observation that for each of the three viscoplastic models, the term $a(\mathcal{D}\boldsymbol{u}, \mathcal{D}\boldsymbol{v} - \mathcal{D}\boldsymbol{u})$ possesses special structure: with the functional $b\colon Q \to \mathbb{R}$ defined by

$$b(\dot{\boldsymbol{\gamma}}) := \int_\Omega |\dot{\boldsymbol{\gamma}}|^2\,\text{d}x \quad \text{(Bingham)}$$

$$b(\dot{\boldsymbol{\gamma}}) := \int_\Omega |\dot{\boldsymbol{\gamma}}|^2\,\text{d}x + \frac{4\sqrt{2\text{Bi}}}{3}\int_\Omega |\dot{\boldsymbol{\gamma}}|^{3/2}\,\text{d}x \quad \text{(Casson)}$$

$$b(\dot{\boldsymbol{\gamma}}) := \frac{2^{r-1}}{r}\int_\Omega |\dot{\boldsymbol{\gamma}}|^r\,\text{d}x \quad \text{(Herschel–Bulkley)}$$

we may write

$$a(\mathcal{D}\boldsymbol{u}, \mathcal{D}\boldsymbol{v} - \mathcal{D}\boldsymbol{u}) = \langle \nabla_{\boldsymbol{u}} b(\mathcal{D}\boldsymbol{u}), \mathcal{D}(\boldsymbol{v} - \boldsymbol{u})\rangle_{Q^*, Q}$$

as a directional derivative of $b \circ \mathcal{D}$ at $\boldsymbol{u}$ in direction $\boldsymbol{v} - \boldsymbol{u}$. Consequently, we may identify the variational inequality (1.6) as a first-order optimality condition of the convex, and hence equivalent minimisation problem

$$\min_{\boldsymbol{u}\in U} b(\mathcal{D}\boldsymbol{u}) + j(\mathcal{D}\boldsymbol{u}) - \langle \boldsymbol{f}, \boldsymbol{u}\rangle_{\boldsymbol{L}^{r^*}(\Omega), \boldsymbol{L}^r(\Omega)} + \iota_{U_{0\text{D}}}(\boldsymbol{u}), \tag{VP}$$

where the indicator functional

$$\iota_{U_{0\text{D}}}(\boldsymbol{u}) = \begin{cases} 0 & \text{if } \boldsymbol{u} \in U_{0\text{D}} \\ +\infty & \text{if } \boldsymbol{u} \notin U_{0\text{D}} \end{cases}$$

enforces the incompressibility constraint (1.4) and the Dirichlet boundary condition (1.5).

For full details of the derivation of Problem (VP), and results regarding existence and uniqueness of solutions, we refer to [10, Chapter 4].

While the Bingham and Casson flow problems are posed in Hilbert spaces, the Herschel–Bulkley model demands for a mathematical treatment in more general Banach spaces. Despite extra theoretical challenges, a very practical consequence of this fact is

Please cite this article as: T. Treskatis et al., An accelerated dual proximal gradient method for applications in viscoplasticity, Journal of Non-Newtonian Fluid Mechanics (2016), http://dx.doi.org/10.1016/j.jnnfm.2016.09.004