



# Numerical simulation of thermally convective viscoplastic fluids by semismooth second order type methods

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## ABSTRACT

We study the numerical solution of thermally convective viscoplastic fluids with yield stress. Following [12], a Bousinesq approximation of the convection effect is considered. The resulting coupled model is then regularized by means of a local regularization technique. After discretization in space, a second order BDF method is used for the time discretization of the regularized problem, leading, in each time iteration, to a nonsmooth system of equations, which is amenable to be solved by generalized Newton methods. A semismooth Newton algorithm with a modified Jacobian is constructed for the solution of the discrete systems. The paper ends with a detailed computational experiment that exhibits the main properties of the numerical approach.

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## 1. Introduction

The understanding of heat transfer in viscoplastic fluid flow, and its effects on the different material regions, is nowadays a challenging topic in the study of materials with yield stress. Although it is clear that the temperature distribution has an effect on how the rigid zones of the material evolve, a precise determination of such effect, of important practical consequences, has not yet been studied in depth.

A complete model which involves both phenomena demands quite complicated mathematical and computational tools. Recently, a Bousinesq approximation has been studied for the understanding of such coupled phenomena in the Rayleigh–Bénard convection context (cf. [12]). Moreover, in order to track the interface between rigid and fluid regions numerically, the authors in [12] consider an Uzawa type technique, which results in an accurate, but rather slow, solution algorithm.

Typically, for the numerical simulation of viscoplastic materials either a first order method for the original non-differentiable problem (in the convex case) or a second order approach for a globally regularized version of the model are considered. The former provides a good approximation of the solution and its correspondent material properties, but is computationally slow and highly mesh dependent. On the other hand, regularization approaches allow

the use of efficient numerical techniques but important qualitative properties may get lost at the obtained solution if the used regularization is too general [3,8].

A challenge in this respect consists in designing a mixed numerical strategy, which allows to obtain an accurate solution (including material properties) with a fast convergent method. In this respect, the combination of semismooth Newton algorithms with a local regularization of the dual multiplier has been recently successfully considered [5,6].

In this paper, we aim at extending the approach developed in [6] to the case of the coupled heat–fluid flow phenomena, i.e., we consider a second order BDF time discretization of a properly regularized coupled model and solve, in each time step, a nonsmooth system of equations by means of a semismooth Newton algorithm. To do so, we consider a lag operator, as proposed in Baker et al. [1] for the Navier–Stokes equations, and applied it to the coupled model. This strategy, combined with a semismooth Newton method, leads to a fast second order approach for the simulation of the convective viscoplastic flow.

## 2. Problem statement and regularization

We start by considering a square cavity with thermally insulated lateral walls. The upper and lower walls are assumed to be at temperatures 0 and  $\theta_1$ , respectively. We use a Boussinesq approximation and the Rayleigh–Bénard convection model developed in [11,12], i.e., we look for a velocity vector field  $\mathbf{u}$  and a temperature distribution  $\theta$  such that

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$$\frac{1}{Pr}(\partial_t + \mathbf{u} \cdot \nabla)\mathbf{u} - \Delta\mathbf{u} - \nabla \cdot \boldsymbol{\tau} + \nabla p = Ra\theta\hat{z} \quad (2.1a)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2.1b)$$

$$\boldsymbol{\tau} = Bi \frac{\boldsymbol{\mathcal{E}}\mathbf{u}}{\|\boldsymbol{\mathcal{E}}\mathbf{u}\|}, \text{ if } \boldsymbol{\mathcal{E}}\mathbf{u} \neq 0 \quad (2.1c)$$

$$\|\boldsymbol{\tau}\| \leq Bi, \text{ if } \boldsymbol{\mathcal{E}}\mathbf{u} = 0 \quad (2.1d)$$

$$(\partial_t + \mathbf{u} \cdot \nabla)\theta = \Delta\theta \quad (2.1e)$$

where  $\hat{z}$  represents the unit vector in the upward direction and  $\|\cdot\|$  stand for the Frobenius norm. Here  $Bi, Pr$  and  $Ra$  are the Bingham, Prandtl and Rayleigh numbers, respectively. They are given by

$$Bi = \frac{\tau_y}{\rho\beta g\delta_T L}, Pr = \frac{\nu}{\alpha} \text{ and } Ra = \frac{\beta g\delta_T L^3}{\alpha\nu},$$

where  $\nu$  stands for the kinematic viscosity,  $\alpha$  for the thermal diffusivity,  $\beta$  for the coefficient of thermal expansion,  $g$  for the acceleration due to gravity,  $\rho$  for the density of the material,  $\tau_y$  for the yield stress and  $L$  for the vertical separation of the cavity walls. Further,  $\delta_T$  represents the temperature difference between the plates (see Fig. 1).

Let us briefly discuss on the boundary and initial conditions considered. For the temperature evolution equation, we impose that

$$\theta = \begin{cases} \theta_1, & \text{for } 0 \leq x_1 \leq 1 \text{ and } x_2 = 0 \\ 0 & \text{for } 0 \leq x_1 \leq 1 \text{ and } x_2 = L \end{cases} \quad (2.2a)$$

$$\frac{\partial\theta}{\partial n} = 0 \text{ on } \Gamma_N$$

$$\theta(0) = \theta_0,$$

where  $\Gamma_N$  stands for the lateral walls. The condition on  $\Gamma_N$  represents the isolation condition on the lateral walls. For the flow a no-slip boundary condition is imposed on the whole boundary:

$$\mathbf{u} = \mathbf{0} \text{ on } \Gamma$$

$$\mathbf{u}(0) = \mathbf{u}_0. \quad (2.2b)$$

From model (2.1) it can be observed that the constitutive relation (2.1c) is only valid in the sectors where the shear rate tensor is different from zero, while no relation holds in the remaining regions. The model constitutes therefore a *free boundary problem*.

In order to obtain a numerical solution for (2.1) the flow vector field together with the regions where the material moves with plastic deformation ( $\boldsymbol{\mathcal{E}}\mathbf{u} \neq 0$ ) and the regions where the material behaves like a rigid solid ( $\boldsymbol{\mathcal{E}}\mathbf{u} = 0$ ) have to be determined. This task can be accomplished either by using direct projection techniques or regularization approaches (see [7] and the references therein).

As mentioned in the introduction, our approach consist in using a local regularization considering both primal and dual information. More precisely, if we consider (2.1c) and (2.1d), the following equation can be verified to hold:

$$\max(0, \|\boldsymbol{\mathcal{E}}\mathbf{u}\|)\boldsymbol{\tau} = Bi\boldsymbol{\mathcal{E}}\mathbf{u}. \quad (2.3)$$

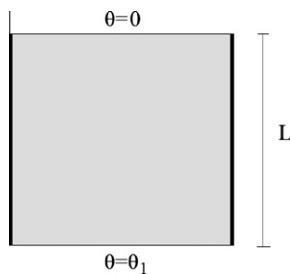


Fig. 1. Geometry of the problem.

Since the main difficulty of the latter corresponds to the case where  $\boldsymbol{\mathcal{E}}\mathbf{u} = 0$ , we consider the following regularized version of (2.3):

$$\max\left(\frac{Bi}{\gamma}, \|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\|\right)\boldsymbol{\tau}_\gamma = Bi\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma, \quad (2.4)$$

where  $\gamma \gg 1$  corresponds to the regularization parameter.

The proposed methodology leads therefore to the following regularized dual multiplier (non-Newtonian component of the stress tensor):

$$\boldsymbol{\tau}_\gamma = \begin{cases} Bi \frac{\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma}{\|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\|} & \text{if } \|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\| \geq \frac{Bi}{\gamma} \\ \gamma\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma & \text{if } \|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\| < \frac{Bi}{\gamma} \end{cases} \quad (2.5)$$

Note that (2.5) can also be obtained, in the case of steady state Bingham flow, from the dual problem by using a Tikhonov regularization technique (see [6]). Moreover, the resulting regularized problem is also related to the bi-viscosity approximation proposed by Beverly and Tanner [2].

Altogether, we obtain the following regularized coupled system of partial differential equations:

$$\frac{1}{Pr}(\partial_t + \mathbf{u}_\gamma \cdot \nabla)\mathbf{u}_\gamma - \Delta\mathbf{u}_\gamma - \nabla \cdot \boldsymbol{\tau}_\gamma + \nabla p_\gamma = Ra\theta_\gamma\hat{z} \quad (2.6a)$$

$$\nabla \cdot \mathbf{u}_\gamma = 0$$

$$\boldsymbol{\tau}_\gamma = \begin{cases} Bi \frac{\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma}{\|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\|} & \text{if } \|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\| \geq \frac{Bi}{\gamma} \\ \gamma\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma & \text{if } \|\boldsymbol{\mathcal{E}}\mathbf{u}_\gamma\| < \frac{Bi}{\gamma} \end{cases} \quad (2.6b)$$

$$(\partial_t + \mathbf{u}_\gamma \cdot \nabla)\theta_\gamma = \Delta\theta_\gamma, \quad (2.6c)$$

with the boundary and initial conditions (2.2a) and (2.2b) for the temperature and flow equations, respectively.

As was proved in [5,6], the proposed type of regularization turns out to be consistent, i.e., the regularized solutions converge to the original one as the parameter  $\gamma$  tends to infinity.

### 3. Numerical treatment

Hereafter, the superscript  $h$  will be used for the discretized functions, and the notation  $\text{diag}(\vec{a})$  stands for a diagonal matrix with the components of the vector  $\vec{a}$  in the diagonal.

#### 3.1. Space discretization

Consider a suitable discretization in space (either by finite elements or finite differences). We therefore obtain the following semi-discretized approximation for the flow Eqs. (2.6a) and (2.4):

$$\frac{1}{Pr}\mathbf{M}^h\partial_t\mathbf{u}^h(t) + \mathbf{A}^h\mathbf{u}^h(t) + \frac{1}{Pr}(\mathbf{u}^h(t) \cdot \nabla^h)\mathbf{u}^h(t) + \nabla^h \cdot \boldsymbol{\tau}^h(t) + \nabla^h p^h(t) - RaM^h\theta^h(t)\hat{z} = 0 \quad (3.1a)$$

$$-(\nabla^h)^\top \mathbf{u}^h(t) = 0 \quad (3.1b)$$

$$\text{diag}(m^h)\boldsymbol{\tau}^h(t) = \mathcal{E}^h\mathbf{u}^h(t). \quad (3.1c)$$

where  $m^h := \max\left(\frac{Bi}{\gamma}\vec{e}, N(\mathcal{E}^h\mathbf{u}^h(t))\right)$ ,  $\vec{e}$  denotes the vector of all ones, and  $\mathbf{u}^h(t)$ ,  $\boldsymbol{\tau}^h(t)$  and  $p^h(t)$  are the time-dependent discrete approximations for the velocity, the regularized stress tensor and the pressure, respectively. Further,  $\mathbf{u}_0^h(t)$  stands for the discrete approximation of the initial condition and  $\mathbf{M}^h$  corresponds to the vectorial mass matrix in the case of finite elements or to the identity matrix in the case of finite differences.  $\mathbf{A}^h$  is the discrete approximation of the vectorial Laplacian, and  $\nabla^h$  and  $\nabla^h$  are matrices representing the discrete versions of the vectorial divergence and the scalar gradient,

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