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Nonconforming finite element approximation of the Giesekus model for polymer flows

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ABSTRACT

We present a numerical approximation of the Giesekus equation which is considered as a realistic model for polymer flows. We use nonconforming finite elements on quadrilateral grids which necessitate the addition of two stabilization terms. An appropriate upwind scheme is employed for the convective term. The underlying discrete Stokes problem is then analysed. Finally, numerical tests are presented in order to validate the code, illustrating its good behavior for large Weissenberg numbers. Comparisons with Polyflow® and with the literature are also carried out.

1. Introduction

We are interested in the numerical simulation of polymeric liquids which are, from a rheological point of view, non-Newtonian viscoelastic fluids. Their viscoelastic behavior can be observed in a variety of physical phenomena, such as die swelling or the Weissenberg effect, which are unseen with Newtonian liquids and which cannot be predicted by the Navier–Stokes equations.

Despite numerous efforts, the numerical approximation of polymer flows is still a challenging research area, due to the internal coupling between the viscoelasticity of the liquid and the flow, which is quantified by the Weissenberg number $We = \dot{\lambda}\dot{\gamma}$ with $\dot{\gamma}$ the shear rate and λ the relaxation time.

A major issue to be addressed is the breakdown in convergence of the algorithms at critical values of *We*. The existing commercial codes are generally only able to deal with *We* up to 10, which is insufficient to describe polymer flows in a processing machine.

The rheological behavior of polymers is so complex that many different constitutive equations have been proposed in the literature in order to describe these phenomena, see for instance [13]. We choose here to study the differential model of Giesekus which presents two main advantages. First, it yields a realistic behavior for shear flows, elongational flows and mixed flows. Second, only two material parameters (the viscosity η and the relaxation time λ) are needed to describe the model. However, the Giesekus constitutive law is strongly nonlinear since it involves a quadratic term in the stress tensor.

Our goal is to develop a robust numerical scheme to obtain realistic simulation for high Weissenberg numbers. We consider here the 2D steady case and quadrilateral meshes. We approximate the velocity and the pressure by means of nonconforming finite elements of Rannacher–Turek, which are well-known to be inf-sup stable, and the stress tensor by means of totally discontinuous piecewise functions. The analysis of the underlying discrete Stokes problem has highlighted the necessity of adding two stabilization terms, one in order to recover a Korn type inequality on nonconforming spaces, and the other to attain optimal convergence. Concerning the Giesekus equation, the convective term on the stress tensor is treated using an upwind scheme, similarly to the well-known Lesaint–Raviart scheme.

The paper is organized as follows. In Section 2 we introduce the Giesekus model. In Section 3, we describe the numerical scheme and we perform the numerical analysis of the underlying Stokes problem. In particular the influence of the regularization terms is discussed. The last section is devoted to the numerical results. We first study the convergence rate for the Giesekus model on an academic test-case. Then we consider a benchmark problem, the flow past a cylinder, for which we carry out some comparisons and we illustrate the good behavior of the method for large Weissenberg numbers. The robustness of the scheme is explained by the positive definiteness of the conformation tensor, guaranteed by our choice of discretization.

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2. The Giesekus model

In what follows, we write the vectors in bold letters and the second order tensors in underlined letters.

Giesekus introduced in [6] the following constitutive law, describing the behavior of a polymeric liquid in a polygonal domain $\Omega \subset \mathbb{R}^2$:

$$\lambda\left(\overset{\nabla}{\underline{\tau}} + \frac{\alpha}{\eta}\underline{\tau}\underline{\tau}\right) + \underline{\tau} = 2\eta\underline{D}(\boldsymbol{u}), \tag{1}$$

with $\underline{\tau}$ the viscous stress tensor, $\underline{D}(\boldsymbol{u}) = \frac{1}{2}(\underline{\nabla}\boldsymbol{u} + \underline{\nabla}\boldsymbol{u}^T)$ the strain rate tensor and $\alpha \in]0,1[$ a parameter. We take $\alpha = 0.5$ which is physically acceptable. Here above, $\nabla\boldsymbol{u} = \left(\frac{\partial u_i}{\partial x_j}\right)_{1\leqslant i,j\leqslant 2}$ and $\overset{\nabla}{\underline{\tau}}$ is the upper convective derivative, defined in the steady case by:

$$\overset{\nabla}{\underline{\tau}} = (\boldsymbol{u}\cdot\nabla)\underline{\tau} - \underline{\tau}\nabla\boldsymbol{u}^T - \nabla\boldsymbol{u}\underline{\tau}.$$

The complete Giesekus model is obtained by adding the mass and the momentum conservation laws, where the density ρ is supposed to be constant:

$$\nabla\cdot\boldsymbol{u} = 0,$$
$$\rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} - \nabla\cdot\underline{\tau} + \nabla p = \boldsymbol{f},$$

and boundary conditions $\boldsymbol{u} = \boldsymbol{g}$ on $\partial\,\Omega$, $\underline{\tau} = \underline{\tau}^D$ on the inflow boundary $\partial\Omega^- = \{x \in \partial\Omega; \boldsymbol{u}(x)\cdot\boldsymbol{n}(x) < 0\}$. Other boundary conditions for $\boldsymbol{u}$ will be considered in Section 4.2. We take $\boldsymbol{f} \in (L^2(\Omega))^2$, $\boldsymbol{g} \in (H^{1/2}(\partial\Omega))^2$ and $\underline{\tau}^D \in \underline{L}^2_{sym}(\partial\Omega^-)$, with:

$$\underline{L}^2_{sym}(\omega) = \left\{\underline{\tau} = (\tau_{ij})_{1\leqslant i,j\leqslant 2}; \underline{\tau} = \underline{\tau}^T, \tau_{ij} \in L_2(\omega)\right\}.$$

3. Finite element approximation

3.1. Discrete nonlinear formulation

Let $(\mathscr{K}_h)_{h>0}$ be a family of regular meshes of Ω consisting of quadrilaterals: $\overline{\Omega} = \bigcup_{K\in\mathscr{K}_h} K$. We denote by ε_h^{int} the set of internal edges of $\mathscr{K}_h$, by ε_h^{∂} the set of boundary edges and we put $\varepsilon_h = \varepsilon_h^{int} \cup \varepsilon_h^{\partial}$. As usually, let h_K be the diameter of the quadrilateral K and let $h = \max_{K\in\mathscr{K}_h} h_K$.

On every edge e belonging to ε_h^{int}, such that $\{e\} = \partial K_1 \cap \partial K_2$, we define once and for all a unit normal $\boldsymbol{n}_e$. For a given function φ with $\varphi_{|K_i} \in \mathscr{C}(K_i)$ $(1 \leqslant i \leqslant 2)$, we define on e: $\varphi^{in}(\boldsymbol{x}) = \lim_{\varepsilon\searrow 0}\varphi(\boldsymbol{x} - \varepsilon\boldsymbol{n}_e)$, $\varphi^{ex}(\boldsymbol{x}) = \lim_{\varepsilon\searrow 0}\varphi\,(\boldsymbol{x} + \varepsilon\boldsymbol{n}_e)$ as well as the jump $[\varphi] = \varphi^{in} - \varphi^{ex}$ and the average $\{\varphi\} = \frac{1}{2}(\varphi^{in} + \varphi^{ex})$. If $e \in \varepsilon_h^{\partial}$, $\boldsymbol{n}$ is the outward unit normal and $[\varphi]$ is the trace of φ. We agree to denote the $L^2(\omega)$-orthogonal projection of a given function $\varphi \in L^2(\omega)$ on the polynomial space $P_k(k \in \mathbb{N})$ by $\pi_k^{\omega}\varphi$. As usually, we denote by $\varphi^- = \min\{0, \varphi\}$ the negative part of φ and we set $\varphi^+ = \varphi - \varphi^-$. We denote by c any constant independent of h, η and the stabilization parameters. We shall use the notation $\underline{\tau} : \underline{\theta} = \sum_{i,j=1}^{2}\tau_{ij}\theta_{ij}$.

We approach the velocity by nonconforming finite elements of Rannacher–Turek (see [14]) whose degrees of freedom are the mean values across the edges, and the pressure and the stress tensor by totally discontinuous piecewise functions. Let $\widehat{K} = [-1, 1] \times [-1, 1]$, $\Psi_K : \widehat{K} \to K$ the bilinear one-to-one transformation and $\widehat{Q}_1^{rot} = \text{vect}\{1, \hat{x}, \hat{y}, \hat{x}^2 - \hat{y}^2\}$. Then we define the space $Q_K = \{v; v\circ\Psi_K \in \widehat{Q}_1^{rot}\}$ and we introduce the discrete spaces:

$$\boldsymbol{V}_h = \{\boldsymbol{v}_h \in (L^2(\Omega))^2; \boldsymbol{v}_{h|K} \in (Q_K)^2\ \forall K \in \mathscr{K}_h,$$
$$\frac{1}{|e|}\int_e [\boldsymbol{v}_h]ds = 0\ \forall e \in \varepsilon_h^{int}\},$$
$$\boldsymbol{V}_h^{\boldsymbol{g}} = \{\boldsymbol{v}_h \in \boldsymbol{V}_h; \int_e \boldsymbol{v}_h ds = \int_e \boldsymbol{g} ds\ \forall e \in \varepsilon_h^{\partial}\},$$
$$Q_h = \{q_h \in L_0^2(\Omega); q_{h|K} \in P_0\ \forall K \in \mathscr{K}_h\},$$
$$\underline{X}_h = \left\{\underline{\theta}_h \in \underline{L}^2_{sym}(\Omega); (\underline{\theta}_h)_{|K} \in \underline{P}_0\ \forall K \in \mathscr{K}_h\right\}.$$

We consider the following discrete formulation:

$$\begin{cases} (\boldsymbol{u}_h, p_h, \underline{\tau}_h) \in \boldsymbol{V}_h^{\boldsymbol{g}} \times Q_h \times \underline{X}_h \\ a^{\gamma,\delta}(\boldsymbol{u}_h, \boldsymbol{v}_h) + b(p_h, \boldsymbol{v}_h) \\ \qquad + c_0(\boldsymbol{v}_h, \underline{\tau}_h) = f(\boldsymbol{v}_h) & \forall \boldsymbol{v}_h \in \boldsymbol{V}_h^{\boldsymbol{0}} \\ b(q_h, \boldsymbol{u}_h) = 0 & \forall q_h \in Q_h \\ c(\boldsymbol{u}_h, \underline{\tau}_h; \underline{\theta}_h) + d(\underline{\tau}_h, \underline{\theta}_h) = l(\underline{\theta}_h) & \forall \underline{\theta}_h \in \underline{X}_h. \end{cases} \tag{2}$$

The previous forms are defined by:

$$a^{\gamma,\delta}(\cdot,\cdot) = a_0(\cdot,\cdot) + \gamma J(\cdot,\cdot) + \delta R(\cdot,\cdot),$$
$$b(q_h, \boldsymbol{v}_h) = -\sum_{K\,\in\,\mathscr{K}_h}\int_K q_h\nabla\cdot\boldsymbol{v}_h\,dx,$$
$$c(\cdot,\cdot;\cdot) = -2\eta\ c_0(\cdot,\cdot) + c_1(\cdot,\cdot;\cdot) - c_2(\cdot,\cdot;\cdot),$$
$$d(\cdot,\cdot) = d_0(\cdot,\cdot) + d_1(\cdot,\cdot),$$
$$f(\boldsymbol{v}_h) = \sum_{K\in\mathscr{K}_h}\int_K \boldsymbol{f}\cdot\boldsymbol{v}_h\,dx,$$
$$l(\underline{\theta}_h) = -\sum_{e\in\varepsilon_h^{\partial}\cap\partial\Omega^-}\int_e(\boldsymbol{u}_h\cdot\boldsymbol{n})^-\underline{\tau}^D : \underline{\theta}_h\,ds,$$

where

$$c_0(\underline{\tau}_h, \boldsymbol{v}_h) = \sum_{K\in\mathscr{K}_h}\int_K \underline{\tau}_h : \underline{D}(\boldsymbol{v}_h)\,dx,$$
$$c_2(\boldsymbol{u}_h, \underline{\tau}_h; \underline{\theta}_h) = \lambda\sum_{K\in\mathscr{K}_h}\int_K(\underline{\tau}_h\underline{\nabla}\boldsymbol{u}_h^T + \underline{\nabla}\boldsymbol{u}_h\underline{\tau}_h) : \underline{\theta}_h\,dx,$$
$$d_0(\underline{\theta}_h, \underline{\tau}_h) = \sum_{K\in\mathscr{K}_h}\int_K \underline{\theta}_h : \underline{\tau}_h\,dx,$$
$$d_1(\underline{\tau}_h, \underline{\theta}_h) = \frac{\lambda}{2\eta}\sum_{K\in\mathscr{K}_h}\int_K(\underline{\tau}_h\underline{\tau}_h) : \underline{\theta}_h\,dx.$$

The form $c_1(\cdot,\cdot;\cdot)$ approximates the convective term $\boldsymbol{u}\cdot\nabla\underline{\tau}$. We extend the approach of Lesaint–Raviart [10] for constant vectors $\boldsymbol{u}$ to the present nonconforming approximation of the velocity. Thus we approach $\int_\Omega \boldsymbol{u}\cdot\nabla\underline{\tau} : \underline{\theta}\,dx$ by $-\sum_{e\in\varepsilon_h}\int_e\{\boldsymbol{u}_h\cdot\boldsymbol{n}_e\}^-[\underline{\tau}_h] : \underline{\theta}_h^{in}\,ds$. Finally, an integration by parts together with the fact that $\pi_0^K\nabla\cdot\boldsymbol{u}_h = 0$ for any $K \in \mathscr{K}_h$ allow us to write the previous term as follows:

$$c_1(\boldsymbol{u}_h, \underline{\tau}_h; \underline{\theta}_h) = \lambda\sum_{e\in\varepsilon_h}\int_e F_e(\underline{\tau}_h, \boldsymbol{u}_h, \boldsymbol{n}_e) : [\underline{\theta}_h]ds,$$

where $F_e(\underline{\tau}_h, \boldsymbol{u}_h, \boldsymbol{n}_e) = \{\boldsymbol{u}_h\cdot\boldsymbol{n}_e\}^+\underline{\tau}_h^{\text{in}} + \{\boldsymbol{u}_h\cdot\boldsymbol{n}_e\}^-\underline{\tau}_h^{\text{ex}}$ is the numerical flux. We take:

$$a_0(\boldsymbol{u}_h, \boldsymbol{v}_h) = \sum_{K\in\mathscr{K}_h}\int_K\frac{\rho}{2}(\boldsymbol{u}_h\cdot\underline{\nabla}\boldsymbol{u}_h\cdot\boldsymbol{v}_h - \boldsymbol{u}_h\cdot\underline{\nabla}\boldsymbol{v}_h\cdot\boldsymbol{u}_h)dx.$$

The additional forms $J(\cdot,\cdot)$ and $R(\cdot,\cdot)$ ensure the discrete coercivity and are defined by:

$$J(\boldsymbol{u}_h, \boldsymbol{v}_h) = \eta\sum_{e\in\varepsilon_h^{\text{int}}}\frac{1}{|e|}\int_e[\pi_1^e(\boldsymbol{u}_h\cdot\boldsymbol{n}_e)][\pi_1^e(\boldsymbol{v}_h\cdot\boldsymbol{n}_e)]ds,$$
$$R(\boldsymbol{u}_h, \boldsymbol{v}_h) = \eta\sum_{K\in\mathscr{K}_h}\int_K(\underline{D}(\boldsymbol{u}_h) - \pi_0^K\underline{D}(\boldsymbol{u}_h)) : \underline{D}(\boldsymbol{v}_h)dx.$$

The stabilization parameters γ, δ are independent of h.

Another possibility for the approximation of viscoelastic flows is to introduce the strain rate tensor $\underline{d} = \underline{D}(\boldsymbol{u})$ as a fourth unknown and to split the stress tensor $\underline{\tau}$ (see [7] for the DEVSS method). Then the elimination of $\underline{d}$ at the discrete level yields a three-fields formulation with an additional term similar to our regularization term $R(\cdot,\cdot)$.

The nonlinear problem (2) is solved by Newton's method.