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NONCONFORMING FINITE ELEMENT APPROXIMATION OF POLYMERS FLOWS FOR LARGE WEISSENBERG NUMBERS

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Abstract. *We present here a numerical scheme for the simulation of polymer flows. We consider here two differential nonlinear models : the Giesekus and the Phan-Thien Tanner models. Their numerical approximation is achieved by means of Crouzeix-Raviart nonconforming finite elements for the velocity and the presure, respectively piecewise constant elements for the stress tensor. We present numerical simulations on a 4:1 contraction illustrating the good behavior of our method for large Weissenberg numbers.*

1 INTRODUCTION

We are interested in the numerical simulation of polymeric liquids which are, from a rheological point of view, viscoelastic non-Newtonian fluids. This is a challenging problem, due to the intrinsic properties of polymers and to the internal coupling between the viscoelasticity of the liquid and the flow, quantified by the Weissenberg number $We = \lambda\dot{\gamma}$ with $\dot{\gamma}$ the shear rate and λ the relaxation time. 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 source of the problem is the breakdown in convergence of the algorithms at critical values of the Weissenberg number.

The rheological behavior of polymers is so complex that many different constitutive equations have been proposed in the literature. We use the nonlinears differentials models of Giesekus and of Phan-Thien Tanner (PTT).

Our goal is to develop a robust numerical scheme to obtain realistic simulation for high Weissenberg numbers. We consider here the 2D case and triangular meshes. We approach the velocity by means of nonconforming finite elements of Crouzeix-Raviart and the stress tensor by means of totally discontinuous piecewise functions. The convective term on the stress tensor is treated using an upwind scheme, similarly to the well-known Lesaint-Raviart scheme.

The outline of this article is the following. In the second section we describe the physical models, then in the third section we present the numerical scheme. Finally, we present numerical tests obtained on 4:1 contraction benchmark illustrating the good behaviour of our method for large Weissenberg numbers, and the positive definiteness of the so-called discrete conformation tensor, which is a crucial point in computational rheology.

2 GOVERNING EQUATIONS

The flow of an incompressible isothermal liquid is described by the mass conservation law :

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

the momentum conservation law :

$$\rho \partial_t \boldsymbol{u} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - div\underline{\tau} + \nabla p = \boldsymbol{0} \tag{2}$$

and a constitutive equation. Here above, $\boldsymbol{u}$ is the velocity, p the pressure, $\underline{\tau}$ the stress tensor and ρ is the density.

We consider here two constitutive equations, the Giesekus equation introduced in [6] and the simplified Phan-ThienTanner equation introduced in [10]. It is useful to introduce the following upper-convected derivative of a given tensor $\underline{A}$:

$$\overset{\triangledown}{\underline{A}} = \partial_t \underline{A} + \boldsymbol{u} \cdot \nabla \underline{A} - \underline{A}(\nabla \boldsymbol{u})^t - \nabla \boldsymbol{u} \underline{A}$$

Then, the Giesekus law is given by:

$$\overset{\triangledown}{\underline{\tau}} + \frac{1}{2G}\,\underline{\tau\tau} + \lambda\,\underline{\tau} = 2\eta\,\underline{D}.$$

Here above, η is the viscosity of the liquid and G is the elastic modulus given by $\frac{\eta}{\lambda}$. $\underline{D}$ is the rate of strain tensor defined by $\underline{D} = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^t)$.

The simplified or affine Phan-Thien and Tanner model can be written as follows:

$$\overset{\triangledown}{\underline{\tau}} + \frac{\epsilon}{G}\,\mathrm{tr}(\underline{\tau})\underline{\tau} + \lambda\,\underline{\tau} = 2\eta\,\underline{D}$$

where ϵ is a non-dimensional adjustable parameter called the extensional parameter.

We consider a bounded polygonal domain Ω of $\mathbb{R}^2$. The corresponding complete models are obtained by adding boundary conditions for $\boldsymbol{u}$ on $\partial\Omega$ and for $\underline{\tau}$ on the inflow boundary $\partial\Omega^- = \{x \in \partial\Omega; \boldsymbol{u}(x)\cdot\boldsymbol{n}(x) < 0\}$, and initial conditions on $\boldsymbol{u}$ and $\underline{\tau}$.

In what follows we consider the stationary case and, in order to simplify the presentation, $\boldsymbol{u} = \boldsymbol{0}$ on $\partial\Omega$.

3 NUMERICAL METHOD

3.1 Preliminary notations

Let us first introduce some useful notations. We consider a regular family of triangulation $(\mathcal{T}_h)_{h>0}$ consisting of triangles : $\overline{\Omega} = \bigcup_{T\in\mathcal{T}_h} T$. We agree to denote by ε_h^{int} the set of internal edges of $\mathcal{T}_h$, by ε_h^{∂} the set of edges situated on the boundary $\partial\Omega$ and we put $\varepsilon_h = \varepsilon_h^{int} \cup \varepsilon_h^{\partial}$. As usually, let h_T be the diameter of the triangle T and let $h = \max\limits_{T\in\mathcal{T}_h} h_T$.

On every edge e belonging to ε_h^{int}, such that $\{e\} = \partial T^i \cap \partial T^j$, we define once and for all the unit normal $\boldsymbol{n}$. For a given function φ with $\varphi_{|T_i} \in \mathcal{C}(T_i)$ $(1 \le i \le 2)$, we define on e : $\varphi^{ext}(\boldsymbol{x}) = lim_{\varepsilon\to 0}\varphi(\boldsymbol{x} - \varepsilon\boldsymbol{n})$, $\varphi^{in}(\boldsymbol{x}) = lim_{\varepsilon\to 0}\varphi(\boldsymbol{x} + \varepsilon\boldsymbol{n})$ as well as the jump $[\varphi] = \varphi^{ext} - \varphi^{in}$. If $e \in \varepsilon_h^{\partial}$, $\boldsymbol{n}$ is the outward unit normal and $[\varphi]$ is the trace of φ on e. We agree to denote the $L^2(e)$-orthogonal projection of a given function $\varphi \in L^2(e)$ on P_k $(k \in \mathbb{N})$ by $\pi_k\varphi$ where P_k is the polynomial space of maximum degree k. As usually, we denote by $\varphi^{+(-)}$ the positive, respectively negative, part of φ.

3.2 Discrete formulation

We consider a velocity-pressure-stress tensor formulation of each of the previous models. The velocity and the pressure are approximated by nonconforming finite elements of Crouzeix-Raviart (cf [1]) while the stress tensor is approximated by P_0 discontinuous finite elements. Thus, we introduce the corresponding discrete spaces:

$$\begin{aligned}
\boldsymbol{V}_h &= \left\{\boldsymbol{v} \in \boldsymbol{L}^2(\Omega)\,;(\boldsymbol{v})_{/T} \in \boldsymbol{P}_1,\ \forall T \in \mathcal{T}_h \text{ and } [\pi_0\boldsymbol{v}]_{/e} = 0, \forall e \in \varepsilon_h\right\},\\
Q_h &= \left\{q \in L_0^2(\Omega);\ (q)_{/T} \in P_0,\ \ \forall T \in \mathcal{T}_h\right\},\\
\underline{X}_h &= \left\{\underline{\sigma} \in \underline{X};\ (\underline{\sigma})_{/T} \in \underline{P}_0,\ \ \forall T \in \mathcal{T}_h\right\},
\end{aligned}$$

where $\underline{X}$ is the space of symmetric tensors defined as follows:

$$\underline{X} = \left\{ \underline{\tau} = (\tau_{ij})_{1 \le i,j \le 2} \, ; \tau_{ij} = \tau_{ji}, \; \tau_{ij} \in L_2(\Omega), \; i,j = 1,2 \right\}$$

and

$$L_0^2(\Omega) = \left\{ q \,\in\, L^2(\Omega) : \int_\Omega q dx \,=\, 0 \right\}.$$

We introduce the following discrete formulation of the Giesekus problem:

$$\left\{ \begin{array}{lll} (\boldsymbol{u}_h, p_h, \underline{\tau}_h) \in \boldsymbol{V}_h \times Q_h \times \underline{X}_h & & \\ a\,(\boldsymbol{u}_h, \boldsymbol{u}_h; \boldsymbol{v}_h) + b\,(p_h, \boldsymbol{v}_h) + c_0(\boldsymbol{v}_h, \underline{\tau}_h) & = l\,(\boldsymbol{v}_h) & \forall \boldsymbol{v}_h \in \boldsymbol{V}_h \\ b\,(q_h, \boldsymbol{u}_h) & = 0 & \forall q_h \in Q_h \\ c\,(\boldsymbol{u}_h, \underline{\tau}_h; \underline{\theta}_h) + d\,(\underline{\tau}_h, \underline{\tau}_h; \underline{\theta}_h) & = 0 & \forall \underline{\theta}_h \in \underline{X}_h \end{array} \right. \tag{3}$$

A similar formulation can be obtained for the PTT model by changing correspondingly $d(\cdot,\cdot;\cdot)$. The form $a(\cdot,\cdot;\cdot)$ can be decomposed into two parts:

$$a(\boldsymbol{u}_h, \boldsymbol{u}_h; \boldsymbol{v}_h) = a_0(\boldsymbol{u}_h, \boldsymbol{u}_h; \boldsymbol{v}_h) + \gamma\, a_1(\boldsymbol{u}_h, \boldsymbol{v}_h)\,.$$

The term $a_0(\cdot,\cdot;\cdot)$ represents the approximation of the following convective term:

$$a_0\,(\boldsymbol{u}_h, \boldsymbol{u}_h; \boldsymbol{v}_h) = \sum_{T \,\in\, \mathcal{T}_h} \int_T \rho \boldsymbol{u}_h \boldsymbol{\nabla} \boldsymbol{u}_h \cdot \boldsymbol{v}_h \, dx,$$

plus eventually an upwinding stabilization whereas the bilinear forrm $a_1(\cdot,\cdot)$ is defined by:

$$a_1(\boldsymbol{u}_h, \boldsymbol{v}_h) = \eta \sum_{e \,\in\, \varepsilon_h^{\text{int}}} \frac{1}{|e|} \int_e [\boldsymbol{u}_h \cdot \boldsymbol{n}]\, [\boldsymbol{v}_h \cdot \boldsymbol{n}] \; ds$$

and γ is a stabilization parameter. This term stabilizes the formulation thanks to a discrete Korn type inequality for discontinuous spaces [3].

The form $b(\cdot,\cdot)$ is the classical one involving the divergence of the velocity:

$$b(q_h, \boldsymbol{v}_h) = -\sum_{T \,\in\, \mathcal{T}_h} \int_T q_h \nabla \cdot \boldsymbol{v}_h \, dx.$$

The nonlinear forms $c(\cdot,\cdot;\cdot)$ and $d(\cdot,\cdot;\cdot)$ are defined by:

$$c(\cdot,\cdot;\cdot) = -2\eta\, c_0(\cdot,\cdot) + c_1(\cdot,\cdot;\cdot) + c_2(\cdot,\cdot;\cdot)\,, \qquad d(\cdot,\cdot;\cdot) = d_0(\cdot,\cdot) + \, d_1(\cdot,\cdot;\cdot)\,.$$

Here above, $c_0(\cdot,\cdot)$ is the linear form:

$$c_0(\underline{\tau}_h, \boldsymbol{v}_h) = \sum_{T \,\in\, \mathcal{T}_h} \int_T \underline{\tau}_h : \underline{D}(\boldsymbol{v}_h) \; dx,$$

$c_2(\cdot,\cdot;\cdot)$ represents the objective derivative:

$$c_2(\boldsymbol{u}_h,\underline{\tau}_h;\underline{\sigma}_h) = -\lambda \sum_{T\,\in\,\mathcal{T}_h} \int_T \underline{\tau}_h\,(\underline{\nabla}\boldsymbol{u}_h)^t : \underline{\sigma}_h\,dx - \lambda \sum_{T\,\in\,\mathcal{T}_h} \int_T \underline{\nabla}\boldsymbol{u}_h\,\underline{\tau}_h : \underline{\sigma}_h\,dx.$$

For the approximation of the convective term $\boldsymbol{u}\cdot\nabla\underline{\tau}$, we follow the approach of Lesaint-Raviart (cf [9]) and we adapt it for a nonconforming velocity field. Thus we approach $\displaystyle\int_\Omega \boldsymbol{u}\cdot\nabla\underline{\tau} : \underline{\sigma}dx$ by :

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

where $F_e(\underline{\tau}_h,\boldsymbol{u}_h,\boldsymbol{n}) = (\pi_0^e\boldsymbol{v}_h\cdot\boldsymbol{n})^+\underline{\tau}_h^{\mathrm{in}} + (\pi_0^e\boldsymbol{v}_h\cdot\boldsymbol{n})^-\underline{\tau}_h^{\mathrm{ext}}$.

The form $d_0(\cdot,\cdot)$ is defined as:

$$d_0(\underline{\sigma}_h,\underline{\tau}_h) = \sum_{T\,\in\,\mathcal{T}_h} \int_T \underline{\sigma}_h : \underline{\tau}_h\,dx$$

and $d_1(\cdot,\cdot;\cdot)$ takes into account the quadratic term:

$$d_1(\underline{\tau}_h,\underline{\tau}_h;\underline{\sigma}_h) = \frac{1}{2G} \sum_{T\,\in\,\mathcal{T}_h} \int_T \underline{\tau}_h\underline{\tau}_h : \underline{\sigma}_h\,dx.$$

Finally, the righthand-side term is defined as:

$$l(\boldsymbol{v}_h) = \sum_{T\,\in\,\mathcal{T}_h} \int_T \boldsymbol{f}\cdot\boldsymbol{v}_h\,dx$$

where $\boldsymbol{f}\in L^2(\Omega)$ is the data of the problem.

This nonlinear problem is solved by means of Newton's method. This necessitates the computation of the following jacobian matrix:

$$\begin{pmatrix} A_{0,\boldsymbol{u}}+\gamma A_1 & B & C_0 \\ B^t & 0 & 0 \\ -2\eta\,C_0^t + C_{1,\boldsymbol{u}} + C_{2,\boldsymbol{u}} & 0 & D_0 + C_{1,\underline{\tau}} + C_{2,\underline{\tau}} + D_{1,\underline{\tau}} \end{pmatrix}.$$

The corresponding forms are defined as follows, where $\boldsymbol{u}^i$ and $\underline{\tau}^i$ are the previous

Newton iterates:

$$
\begin{aligned}
a_{0,\boldsymbol{u}}(\boldsymbol{u}_h, \boldsymbol{v}_h) &= \sum_{T \in \mathcal{T}_h} \int_T ((\boldsymbol{u}^i \cdot \nabla)\boldsymbol{u}_h \boldsymbol{v}_h + (\boldsymbol{u}_h \cdot \nabla)\boldsymbol{u}^i \boldsymbol{v}_h)\, dx, \\
c_{1,\boldsymbol{u}}(\boldsymbol{u}_h, \underline{\sigma}_h) &= \sum_{T \in \mathcal{T}_h} \int_{\partial T^-} \boldsymbol{u}_h \cdot \boldsymbol{n}\, \underline{\tau}^{\text{ext}} : \left(\underline{\sigma}_h^{\text{int}} - \underline{\sigma}_h^{\text{ext}}\right) ds, \\
c_{1,\underline{\tau}}(\underline{\tau}_h, \underline{\sigma}_h) &= \sum_{T \in \mathcal{T}_h} \int_{\partial T^-} \boldsymbol{u}^i \cdot \boldsymbol{n}\, \underline{\tau}_h^{\text{ext}} : \left(\underline{\sigma}_h^{\text{int}} - \underline{\sigma}_h^{\text{ext}}\right) ds, \\
c_{2,\boldsymbol{u}}(\boldsymbol{u}_h, \underline{\sigma}_h) &= -\lambda \sum_{T \in \mathcal{T}_h} \int_T \underline{\tau}^i \left(\underline{\nabla} \boldsymbol{u}_h\right)^t : \underline{\sigma}_h\, dx - \lambda \sum_{T \in \mathcal{T}_h} \int_T \underline{\nabla} \boldsymbol{u}_h\, \underline{\tau}^i : \underline{\sigma}_h\, dx, \\
c_{2,\underline{\tau}}\ (\underline{\tau}_h, \underline{\sigma}_h) &= -\lambda \sum_{T \in \mathcal{T}_h} \int_T \underline{\tau}_h \left(\underline{\nabla} \boldsymbol{u}^i\right)^t : \underline{\sigma}_h\, dx - \lambda \sum_{T \in \mathcal{T}_h} \int_T \underline{\nabla} \boldsymbol{u}^i\, \underline{\tau}_h : \underline{\sigma}_h\, dx, \\
d_{1,\underline{\tau}}(\underline{\tau}_h, \underline{\sigma}_h) &= \sum_{T \in \mathcal{T}_h} \frac{1}{2G} \int_T \left(\underline{\tau}_h\, \underline{\tau}^i + \underline{\tau}^i\, \underline{\tau}_h\right) : \underline{\sigma}_h\, dx.
\end{aligned}
$$

A complete analysis of the underlying Newtonian case (for $\lambda = 0$) has been performed, and the optimal convergence rate has been obtained (cf [2]). As regards the Giesekus constitutive law, the discrete positivity of the conformation tensor has been shown for (3) for a given velocity and under certain hypotheses. The study of the existence of solutions for the full model is ongoing work, based on the discrete positivity and on energy estimates.

Finally, an analogous method has been proposed on quadrilaterals, using Rannacher-Turek finite elements and an additional regularisation term. All previous results can then be extended on quadrilaterals (cf [7]).

4 NUMERICAL TESTS

For all considered tests, we chose $\eta = 1000$ Pa.s and $\rho = 1000$ kg/m3. For each value of λ, we compute the largest Weissenberg number for a corresponding Newtonian fluid as follows:

$$We = \lambda \frac{3\bar{\boldsymbol{u}}}{a}$$

where $\bar{\boldsymbol{u}}$ is the inflow velocity in the thin channel and a its thickness. The considered geometry here is a 4:1 planar contraction presented in Fig. 1. The abrupt contraction in the geometry allows to highlight the particular behaviour of polymer flows. On the inflow Γ_1, we impose a constant velocity $(v, 0)$ with $v = 0.1$ m/s whereas on the outflow Γ_3 we impose a homogeneous Nemann condition. On Γ_3, we impose $\boldsymbol{v} = \boldsymbol{0}$ and we take Γ_4 as a symmetry axis.

Other benchmark test-cases have also been studied as for instance a 4:1:4 contraction and flows past a cylinder.

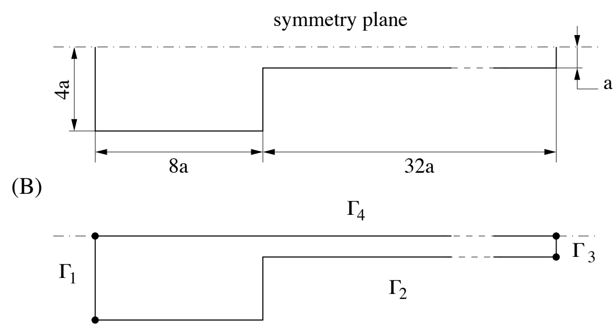

Figure 1: 4:1 planar contraction

4.1 Validation of the code

The CFD codes for polymer liquids are generally only able to deal with We up to 10. The most popular code for the simulation of polymer flows is Polyflow developped by the Cesame team (*http://www.ansys.com/products/polyflow*). We have implemented our method in the C++ library Concha developped by the INRIA team Concha (*http://uppa-inria.univ-pau.fr/concha*). This method has been yet numerically validated for the Newtonian case.
In Fig. 2, we compare the results obtained with these two codes for a Giesekus liquid and

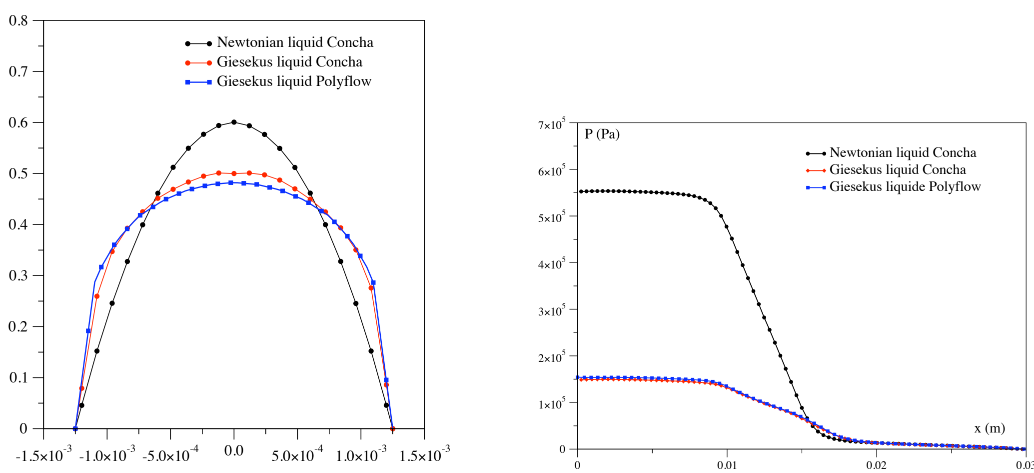

Figure 2: Comparisons with Polyflow

for a Weissenberg number equal to 7.68. This is the highest value for which Polyflow still converges. We have used a mesh consisting of 25 794 triangles with Concha, respectively 14 866 with Polylow. We observe a good agreement between the two approaches. Moreover, the modification of the velocity profiles and the shut down of the pressure are typical behaviours of non-Newtonian fluids.

We are now interested in the behaviour of our numerical scheme for different Weissenberg numbers. We present in Fig.3, respectively in Fig.4, the streamlines for a Giesekus liquid, repctively for a PTT liquid with $\epsilon = 0.05$, for We varying between 0, which corresponds to the Newtonian case, and 21. We note that for the two models, the recirculation vortices clearly grow with We. This phenomena is also in agreement with the theory and can be explained by the emergence of normal stresses in the secondary shear flow.

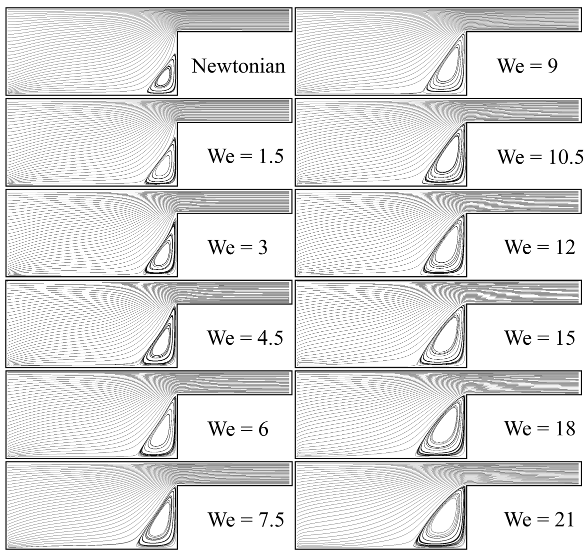

Figure 3: Streamlines for a Giesekus liquid

4.2 Positive definiteness of the conformation tensor for the Giesekus model

The loss of convergence of the numerical schemes at high Weissenberg numbers has often been associated with the loss of the positive definiteness of the conformation tensor at the discrete level. Note that the continuous conformation tensor is known to be positive definite. Numerical schemes preserving this property allow for energy estimates to be established, which generally ensure the stability. Recently, two different approaches in order to preserve the discrete positivity have been proposed. Fattal and Kupferman (cf [5]) employ the logarithm of the conformation tensor and re-write the constitutive equation, while Lee and Xu (cf [8]) use the similarity between the constitutive equation and a differential Riccati equation.

In [4], this approach was adapted to the Giesekus equation and to the finite element method presented above. Thanks to the well-known properties of algebraic Ricatti equation, they show that under certains hypotheses, Newton's method for (3) yields positive definite iterates, which moreover converge towards the maximal positive definite solution.

To illustrate this result, we present in Fig.5 and Fig.6 the positive eigenvalues of the discrete conformation tensor, given by $\underline{C}_h = \dfrac{\lambda}{\eta}\underline{\tau}_h + \underline{I}$, for rather high Weissenberg numbers,

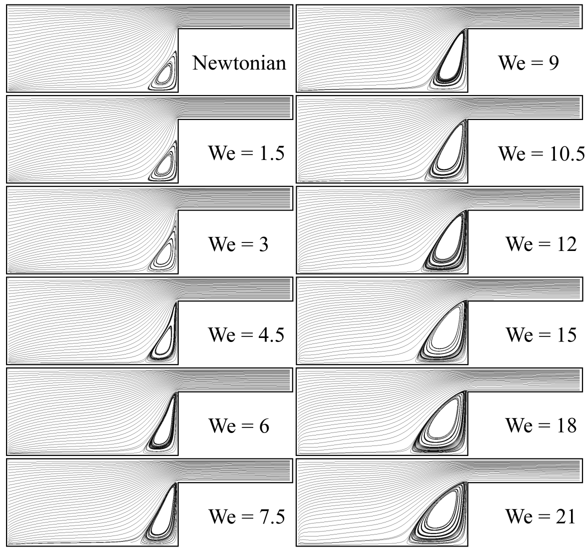

Figure 4: Streamlines for a PTT liquid

up to 33.5. For higher values of We, the Newton method doesn't converge, which can be explained by the loss of positive definiteness of C_h.

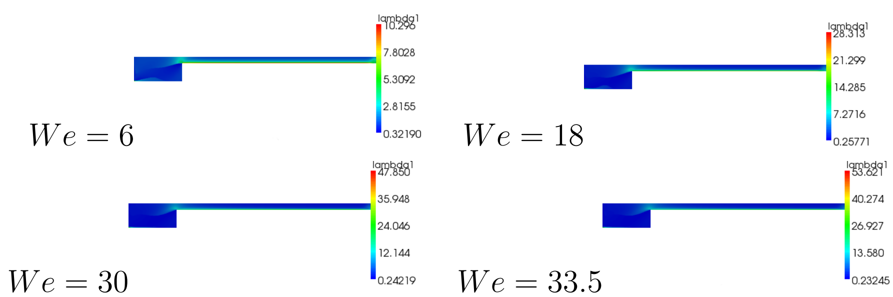

Figure 5: First eigenvalue of the conformation tensor

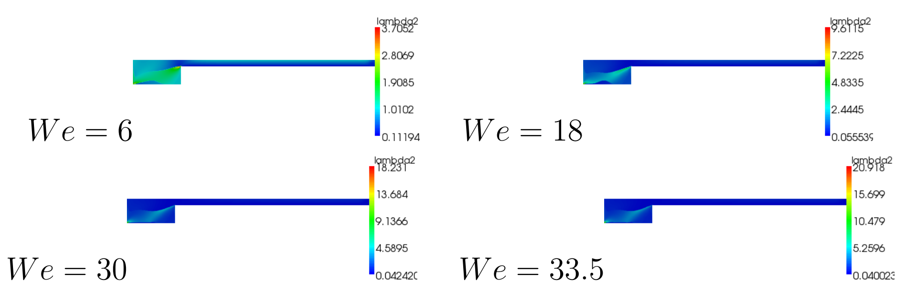

Figure 6: Second eigenvalue of the conformation tensor

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