Computers & Fluids 79 (2013) 178–189

Contents lists available at SciVerse ScienceDirect

Computers & Fluids

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

Numerical simulation of polymer flows using non-conforming finite elements

Julie Joie [a,b], Didier Graebling [d,c,*]

[a] Institut de Mathématiques de Bordeaux, UMR CNRS 5251 Université Bordeaux 1, 351 cours de la Libération, 33405 Talence, Cedex, France
[b] Centre de Recherche INRIA Bordeaux-Sud-Ouest, Équipe Projet MC2, France
[c] Centre de Recherche INRIA Bordeaux-Sud-Ouest, Équipe Projet Concha, France
[d] IPREM/EPCP, UMR CNRS 5154 Université de Pau et des Pays de l'Adour 2 Avenue Angot, 64053 Pau Cedex 9, France

ARTICLE INFO

Article history:
Received 23 February 2012
Received in revised form 18 January 2013
Accepted 15 March 2013
Available online 8 April 2013

Keywords:
Phan-Thien and Tanner model
Giesekus model
Weissenberg number
Nonconforming finite element method

ABSTRACT

In this paper, we are interested in the simulation of polymer flows for high-Weissenberg numbers. The high-Weissenberg number problem (HWNP) is one of the main difficulties encountered for the numerical simulation of such flows. We develop a numerical approach for two non-linear models: the affine Phan-Thien and Tanner model and the Giesekus model. We consider the 2D case and triangular and quadrilateral meshes. The velocity and the pressure are approximated by non-conforming finite elements while the stress tensor is approximated by P_0 totally discontinuous finite elements. We have considered three popular test-cases: a simple channel, a 4:1 abrupt contraction and a cylinder. Comparisons with analytical solutions and experiences are performed, illustrating the good behavior of our code. Moreover, for the Oldroyd-B model, we have performed comparisons of drag values with data given in the literature. We have been able to obtain simulations for large values of Weissenberg number ($\mathfrak{Wi} > 21$ for the 4:1 contraction), our approach gives a realistic description of polymer flows.

1. Introduction

Despite numerous efforts, computational non-Newtonian fluid mechanics is still a very challenging research area. The high-Weissenberg number problem (HWNP) is one of the main difficulties encountered for the numerical simulation of polymer flows. The source of the problem is the breakdown in convergence of the algorithms at critical values of the Weissenberg number. The frustratingly low value of the Weissenberg number limits the CFD use for the polymer processing industry [19,36].

Besides this major issue, there are two other aspects that have to be carefully treated by the finite element discretization: the choice of approximation spaces satisfying the Babuška–Brezzi compatibility condition and the treatment of the convective terms.

Several well-posed mixed finite element approximation have been developed during the last decades. Most approaches consist in adding ellipticity on the momentum equation in order to stabilize the scheme. King et al. [21] introduce the Elasticity Elliptic Momentum Equation (EEME) method, which is a reformulation of the momentum equation that makes the elliptic character of this equation explicit. Another popular method is the Elastic-Viscous Split Stress (EVSS) finite element method introduced by Rajagopalan et al. [33], which consists in splitting the stress tensor into a viscous part and an elastic part and to perform a change of variables. The Adaptative Viscous Split Stress (AVSS) method of Sun et al. [35], introduced another way to perform this change of variable. Nevertheless, this change of variable is not possible with all the constitutive equation. To overcome this problem, Guénette and Fortin [16] introduced the Discrete Elastic–Viscous Split Stress (DEVSS) finite element method, where the same split is performed, but no change of variable is needed.

Concerning the discretization of the convective term, there exist two main approaches: one based on the Streamline-Upwind method (SU or SUPG) and the other on discontinuous Galerkin methods (dG) following the Lesaint–Raviart scheme. The first class of methods consists in adding streamline upwind artificial diffusivity and was first applied to the computation of viscoelastic flows in 1987 by Marchal and Crochet [26]. The dG method is based on the Lesaint–Raviart method [24] and was first applied to a viscoelastic liquid by Fortin and Fortin [13]. An advantage of this method, is that the velocity-stress tensor spaces compatibility condition required for the three field Stokes problem, can be easily satisfied. Moreover, the dG methods are known to be easy to implement.

For a complete review of these methods one can refers to [1,2,28].

Recently, it has been shown that the breakdown in convergence of the algorithms is related with the lack of positivity of the

* Corresponding author at: IPREM/EPCP, UMR CNRS 5154 Universitéde Pau et des Pays de l'Adour 2 Avenue Angot, 64053 Pau Cedex 9, France.
E-mail addresses: julie.joie@inria.fr (J. Joie), didier.graebling@univ-pau.fr (D. Graebling).

0045-7930/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compfluid.2013.03.012

so-called conformation tensor at the discrete level [37,23]. The conformation tensor can be interpreted as a tensorial measure of the molecular orientation and stretching of the chain. This tensor denotes the average of the dyadic product of the end-to-end vector of a polymer chain. Grmela introduced a class of rheological models based on the conformation tensor [17]. In these models, the conformation tensor is assumed to be symmetric and positive definite. In the last few years, numerical schemes preserving the positive definiteness of the discrete conformation tensor have been proposed in the literature based on the approach of Fattal and Kupferman [12]. They consider a log-conformation formulation of the constitutive equation written in terms of $\boldsymbol{\psi} = ln\boldsymbol{C}$ and then put $\boldsymbol{C}_h = e^{\psi_h}$. This method has been widely used [18,9,22]. An alternate log-conformation formulation has been introduced by Coronado et al. [6]. Those methods lead to stongly nonlinear reformulations of the considered problems and therefore, their computation is very costly. Lee and Xu employed the framework of Riccati equations to preserve the discrete positivity [23].

Among the rheological models developed for describe the polymer liquid flows, the Giesekus model is one of the most realistic [14,15]. This model presents two main advantages. First, it yields a realistic behavior for all flows except for the biaxial extension[1] [20]. Second, only two material parameters, the relaxation time λ and the viscosity η, are needed to describe the model. These parameters can be easily determined using dynamic rheology experiments. However, the Giesekus constitutive law is strongly nonlinear since it involves a quadratic term in the stress tensor. Here, we also consider the simplified or affine Phan-Thien–Tanner model [30,31].

In this paper, we consider a low order non-conforming finite element method to approach the velocity and the pressure and dG finite elements to approach the stress tensor. The presented methodology is implemented in the academic C++ library Concha.[2] To validate the code, convergence tests and comparisons with analytical solutions are performed. We have also computed the cylinder drag values for an Oldroyd-B liquid in order to compare our numerical scheme with other proposed in the literature. For the 4:1 abrupt contraction geometry, we present velocities and stress comparisons between experimental data [32] and our code. Finally, this geometry allows to show simulations for high Weissenberg numbers.

The paper is structured as follows: in Section 2, we present the rheological models used. Section 3 is devoted to the description of the numerical schemes. In the last section, we present the numerical results.

2. Governing equations

In the case of incompressible isothermal flows, the motion of a liquid is described by:

- The mass conservation law,

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

where $\boldsymbol{u}$ is the velocity of the liquid.

- The momentum conservation law,

$$\rho\left(\frac{\partial}{\partial t}\boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) - \nabla\cdot\tau + \nabla p = \boldsymbol{0}, \tag{2}$$

where $\boldsymbol{\tau}$, p and ρ are respectively the extra-stress tensor, the pressure and the density of the fluid.

- And a constitutive equation.

The rheological behaviour of a polymer liquid can be described by two types of differential constitutive equations:

- The quasi-linear differential models:

$$\boldsymbol{\tau} + \lambda\overset{\square}{\boldsymbol{\tau}}_a = 2\eta\boldsymbol{D}, \tag{3}$$

with $\overset{\square}{\boldsymbol{\tau}}_a$ the Gordon–Schowalter convected derivative of the extra-stress tensor.

- The nonlinear differential models:

$$f(\boldsymbol{\tau}) + \lambda\overset{\triangledown}{\boldsymbol{\tau}} = 2\eta\boldsymbol{D}, \tag{4}$$

with $f(\boldsymbol{\tau})$ a nonlinear function of the extra-stress tensor.

$\boldsymbol{D}$ is the Oldroyd strain-rate tensor given by:

$$\boldsymbol{D} = \frac{1}{2}\{\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^t\}. \tag{5}$$

η and λ are respectively the zero-shear viscosity and the relaxation time of the polymer liquid.

The Gordon–Schowalter convected derivative of the tensor $\boldsymbol{A}$ is defined by the following relationship:

$$\overset{\square}{\boldsymbol{A}}_a = \frac{\partial}{\partial t}\boldsymbol{A} + \boldsymbol{u}\cdot\nabla\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{\Omega} - \boldsymbol{\Omega}\cdot\boldsymbol{A} - a\{\boldsymbol{A}\cdot\boldsymbol{D} + \boldsymbol{D}\cdot\boldsymbol{A}\}, \tag{6}$$

where a is a parameter $\in[-1,1]$. $\boldsymbol{\Omega}$ is the vorticity tensor defined by:

$$\boldsymbol{\Omega} = \frac{1}{2}\{(\nabla\boldsymbol{u})^t - \nabla\boldsymbol{u}\}. \tag{7}$$

According to the chosen values for a, we obtain:

$$\begin{cases} \text{the upper-convected derivative for } a = 1 : \overset{\triangledown}{\boldsymbol{\tau}} = \frac{\partial}{\partial t}\boldsymbol{\tau} + \boldsymbol{u}\cdot\nabla\boldsymbol{\tau} - \{\boldsymbol{\tau}\cdot\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^t\cdot\boldsymbol{\tau}\}, \\ \text{the Jaumann or co-rotational derivative for } a = 0 : \overset{\circ}{\boldsymbol{\tau}} = \frac{\partial}{\partial t}\boldsymbol{\tau} + \boldsymbol{u}\cdot\nabla\boldsymbol{\tau} + \boldsymbol{\tau}\cdot\boldsymbol{\Omega} + \boldsymbol{\Omega}\cdot\boldsymbol{\tau}, \\ \text{lower-convected derivative for } a = -1 : \overset{\triangle}{\boldsymbol{\tau}} = \frac{\partial}{\partial t}\boldsymbol{\tau} + \boldsymbol{u}\cdot\nabla\boldsymbol{\tau} + \boldsymbol{\tau}\cdot(\nabla\boldsymbol{u})^t + \nabla\boldsymbol{u}\cdot\boldsymbol{\tau} \end{cases} \tag{8}$$

If we replace the time derivative by an objective time derivative, a linear model such as the Maxwell model could be transformed into a quasi-linear model. The Oldroyd-B model can be regarded as an extension of the Upper Convected Maxwell (UCM) model. The deviatoric term of the stress is split into a polymeric part and a solvent or Netwonian part: $\boldsymbol{\tau} = \boldsymbol{\tau}_p + \boldsymbol{\tau}_s$. The constitutive equation of this model is given by:

$$\boldsymbol{\tau}_s = 2\eta_s\boldsymbol{D},$$

$$\boldsymbol{\tau}_p + \lambda\overset{\triangledown}{\boldsymbol{\tau}}_p = 2\eta_p\boldsymbol{D}.$$

The viscosity of this liquid is defined by: $\eta = \eta_s + \eta_p$.

In this work, we consider two non-linear viscoelastic liquids: the simplified version of the Phan-Thien–Tanner model [30,31] and the Giesekus model [14,15].

According to the choice of the function $f(\boldsymbol{\tau})$ in (4), we obtain:

- The simplified or affine Phan-Thien–Tanner model (PTT):

$$f(\boldsymbol{\tau}) = \left(1 + \frac{\epsilon\lambda}{\eta}\mathrm{tr}\{\boldsymbol{\tau}\}\right)\boldsymbol{\tau} \Rightarrow \boldsymbol{\tau} + \frac{\epsilon\lambda}{\eta}\mathrm{tr}\{\boldsymbol{\tau}\}\boldsymbol{\tau} + \lambda\overset{\triangledown}{\boldsymbol{\tau}} = 2\eta\boldsymbol{D}, \tag{9}$$

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

- The Giesekus model:

$$f(\boldsymbol{\tau}) = \boldsymbol{\tau} + \frac{\alpha}{G}\boldsymbol{\tau}\cdot\boldsymbol{\tau} \Rightarrow \boldsymbol{\tau} + \frac{\alpha}{G}\boldsymbol{\tau}\cdot\boldsymbol{\tau} + \lambda\overset{\triangledown}{\boldsymbol{\tau}} = 2\eta\boldsymbol{D}, \tag{10}$$

where α is a constant $\in$ [0,1] and $G = \eta/\lambda$ is called the elastic modulus.

[1] For this flow, the expected behaviour is possible but is not in good agreement with the experimental data.

[2] http://sites.google.com/site/conchapau/.