Numerical Simulation of Visco-Elastic Fluids

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Abstract

In this work we give an overview of differential constitutive equations used in theoretical and numerical description of the visco-elastic fluids. We first give general form of constitutive equation and then we mention some often used differential constitutive equations for visco-elastic fluids. In the second part we present an algorithm based on finite element method for computation of time dependent flows of visco-elastic fluids.

1 Introduction

We consider flow of a visco-elastic, incompressible, homogeneous fluid in a bounded region denoted by Ω. Such a motion is known to be described by the following set of equations, stating the law of mass and momentum conservation

$$\operatorname{div}\vec{v} = 0 \tag{1.1}$$

$$\varrho\Big(\frac{\partial\vec{v}}{\partial t} + (\nabla\vec{v})\vec{v}\Big) = \operatorname{div}\boldsymbol{\sigma} + \varrho\vec{f}. \tag{1.2}$$

Here $\vec{v} = (v_1, v_2, v_3)$ is a velocity vector field, ϱ is a constant density of the fluid, $\vec{f} = (f_1, f_2, f_3)$ is a given field of body forces per mass unit and $\boldsymbol{\sigma}$ is a symmetric stress tensor field. In order to solve these equations, they must be completed by some suitable initial and boundary conditions for the velocity and the stress and by a constitutive equation which gives relation between the stress tensor $\boldsymbol{\sigma}$ and the motion of the fluid represented by th e velocity $\vec{v}$.

1.1 Formulation of the constitutive equation

Let us consider deformation of body Ω. For arbitrary material point from Ω marked X, the position $\vec{x}$ of this point at time t during the process of deformation is described by mapping $\vec{x} = \chi(X, t)$. The positions $\vec{x}$ resp. $\vec{\xi}$ of material point X at times t resp. τ can be connected by relative deformation in the following way (under assumption χ being invertible)

$$\vec{\xi} = \chi(X, \tau) = \chi\big(\chi^{-1}(\vec{x}, t), \tau\big) \equiv \chi_t(\vec{x}, \tau). \tag{1.3}$$

Which says that $\vec{\xi}$ is the position at time τ of material point X which was at time t in the position $\vec{x}$. Then we can define the relative deformation gradient tensor $\boldsymbol{F}_t$ and the relative right Cauchy-Green strain tensor $\boldsymbol{C}_t$ by

$$\boldsymbol{F}_t(\tau) = \nabla_x\chi_t(\vec{x}, \tau) \tag{1.4}$$

$$\boldsymbol{C}_t(\tau) = \boldsymbol{F}_t^T(\tau)\boldsymbol{F}_t(\tau). \tag{1.5}$$

The velocity field and velocity gradient can be expressed in terms of deformation as follows

$$\vec{v}(\vec{x},t) = \frac{\mathrm{d}}{\mathrm{d}\tau}\chi_t(\vec{x},\tau)\big|_{\tau=t} \tag{1.6}$$

$$\nabla\vec{v} = \boldsymbol{L} = \frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{F}_t(\tau)\big|_{\tau=t}. \tag{1.7}$$

Next, we denote by $\boldsymbol{R}_t(\tau)$ and $\boldsymbol{U}_t(\tau)$ the polar decomposition of the deformation gradient in the form

$$\boldsymbol{F}_t(\tau) = \boldsymbol{R}_t(\tau)\boldsymbol{U}_t(\tau) \tag{1.8}$$

where $\boldsymbol{U}_t(\tau)$ is symmetric and positive definite and $\boldsymbol{R}_t(\tau)$ is orthogonal. Then we can define the rate of stretch $\boldsymbol{D} = \frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{U}_t(\tau)\big|_{\tau=t} = \frac{1}{2}(\boldsymbol{L}+\boldsymbol{L}^T)$ and the rate of spin $\boldsymbol{W} = \frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{R}_t(\tau)\big|_{\tau=t} = \frac{1}{2}(\boldsymbol{L}-\boldsymbol{L}^T)$.

1.2 Principles governing formulation of constitutive equations

There are several principles and assumptions which are usually taken into an account when formulating a constitutive equation.

Principle of determinism. The stress can be determined only by history and present state of the material.

Principle of material objectivity. The form of the constitutive equation does not depend on a motion of an observer.

Further we assume that our material is a simple fluid, i.e. the stress at a material point is determined by the deformation gradient at this point. Under these principles the stress tensor $\boldsymbol{\sigma}$ for simple, isotropic, incompressible fluid can be expressed in the following general form

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\tau} = -p\boldsymbol{I} + \mathop{\mathcal{F}}_{s=0}^{\infty}\big(\boldsymbol{C}_t(t-s)\big) \tag{1.9}$$

where p is the pressure, $\boldsymbol{\tau}$ is the extra stress, $\boldsymbol{C}_t$ is relative Cauchy-Green tensor and $\mathcal{F}$ is the response functional which must obey the principle of material objectivity.

1.3 Differential models

Since we want to use the constitutive equation in a numerical simulation it is more suitable to have the constitutive equation in differential form. In general there are two ways how to formulate a differential constitutive equation. We can express the response functional $\mathcal{F}$ by some differential approximation and restrict us to "a few terms". The other way is to formulate constitutive relation from some mechanical model or molecular theory (e.g. spring-dashpot, bead-spring or dumbbell models) and generalize it.

1.4 Oldroyd type models

It was observed by Oldroyd that the convected time derivative $\frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}t} = \frac{\partial\boldsymbol{T}}{\partial t} + (\nabla\boldsymbol{T})\vec{v}$ of a tensor is not objective. The objective form of the time derivative of a tensor can be written in the form

$$\frac{\mathcal{D}_a\boldsymbol{T}}{\mathcal{D}t} = \frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}t} + \boldsymbol{TW} + (\boldsymbol{TW})^T - a\big(\boldsymbol{TD} + (\boldsymbol{TD})^T\big) \tag{1.10}$$

where $-1 \le a \le 1$ is a parameter. The special cases with $a=-1, a=1$ and $a=0$ are called lower, upper and co-rotational convected time derivative. In the constitutive equations used in space-fixed reference frame this objective time derivative must be used.

A general form of the constitutive equation suggested by Oldroyd is

$$\lambda_1 \frac{\mathcal{D}_a \boldsymbol{\tau}}{\mathcal{D}t} + \boldsymbol{\tau} + \boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) = 2\mu\left[\lambda_2 \frac{\mathcal{D}_a \boldsymbol{D}}{\mathcal{D}t} + \boldsymbol{D}\right], \tag{1.11}$$

where $\lambda_1 \geq 0$ and $\lambda_2 \geq 0$ are relaxation and retardation time and $\mu \geq 0$ is the viscosity coefficient. There are several variants of this general model.

- Models with $\boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) \neq 0$

Oldroyd 8-constant model	$\boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) = \nu_1 \operatorname{Tr}(\boldsymbol{\tau}\boldsymbol{D})\boldsymbol{I} + \mu_0 \operatorname{Tr}(\boldsymbol{\tau})\boldsymbol{D} + 2\mu\nu_2 \operatorname{Tr}(\boldsymbol{D}^2)\boldsymbol{I}$
Larson model	$\boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) = 2\operatorname{Tr}(\boldsymbol{\tau}\boldsymbol{D}) f(\operatorname{Tr}\boldsymbol{\tau})(\boldsymbol{\tau} + \boldsymbol{I})$
Phan-Thien-Tanner model	$\boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) = \nu\boldsymbol{\tau} \operatorname{Tr}\boldsymbol{\tau}$ or $\boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) = \nu\boldsymbol{\tau} \exp(\operatorname{Tr}\boldsymbol{\tau})$

- Models with $\boldsymbol{\gamma}(\boldsymbol{\tau}, \nabla\vec{v}) = 0$
  - Jeffreys type models $\lambda_2 \neq 0$

Oldroyd A fluid	$\lambda_1 > \lambda_2 > 0, \quad a = -1$
Oldroyd B fluid	$\lambda_1 > \lambda_2 > 0, \quad a = 1$

  - Maxwell type models $\lambda_2 = 0$

Johnson-Segalman	$-1 < a < 1$
Lower convected Maxwell model	$a = -1$
Upper convected Maxwell model	$a = 1$

These models can be generalized as for example the extra-stress $\boldsymbol{\tau}$ can be expressed as a sum of partial stresses $\boldsymbol{\tau} = \sum \boldsymbol{\tau}^i$ and for each partial stress $\boldsymbol{\tau}^i$ there is prescribed a constitutive equation with different relaxation times λ_1^i. Other generalization are the White-Metzner fluids where the parameters $\lambda_1, \lambda_2, \mu$ are considered as a functions of $\frac{1}{2}\operatorname{Tr}\boldsymbol{D}^2$. However, these parameters has to satisfy certain identities, as we try to show in Appendix.

1.5 Oldroyd B model with equations of motion

Now we add to the system (1.1)-(1.2) the constitutive equation for Oldroyd B model in the following equivalent form

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\mu_v \boldsymbol{D} + \boldsymbol{\tau}, \tag{1.12}$$

$$\lambda \frac{\mathcal{D}_a \boldsymbol{\tau}}{\mathcal{D}t} + \boldsymbol{\tau} = 2\mu_e \boldsymbol{D}, \tag{1.13}$$

where $\lambda = \lambda_1$, $\mu_v = \mu\frac{\lambda_2}{\lambda_1}$ and $\mu_e = \mu - \mu_v$. Next, let us transform these equations into a non-dimensional form

$$\operatorname{div}\vec{v} = 0, \tag{1.14}$$

$$\operatorname{Re}\big(\frac{\partial\vec{v}}{\partial t} + (\nabla\vec{v})\vec{v}\big) = -\nabla p + (1-\alpha)\Delta\vec{v} + \operatorname{div}\boldsymbol{\tau} + \vec{f}, \tag{1.15}$$

$$\operatorname{We}\big(\frac{\partial\boldsymbol{\tau}}{\partial t} + (\nabla\boldsymbol{\tau})\vec{v} + \beta_a(\boldsymbol{\tau}, \nabla\vec{v})\big) + \boldsymbol{\tau} = 2\alpha\boldsymbol{D}, \tag{1.16}$$

where the function β_a and the non-dimensional coefficients are

$$\beta_a(\boldsymbol{\tau}, \nabla\vec{v}) = \boldsymbol{\tau W} + (\boldsymbol{\tau W})^T - a\big(\boldsymbol{\tau D} + (\boldsymbol{\tau D})^T\big), \quad -1 \le a \le 1, \tag{1.17}$$

$$\alpha = \frac{\mu_e}{\mu_e + \mu_v}, \tag{1.18}$$

$$\mathrm{Re} = \frac{LV\varrho}{\mu_e + \mu_v} \quad \text{(Reynolds number)}, \tag{1.19}$$

$$\mathrm{We} = \frac{V\lambda}{L} = \frac{\lambda}{T} \quad \text{(Weissenberg number)}, \tag{1.20}$$

and L is a characteristic length, V is a characteristic velocity, $T = \frac{L}{V}$ is a characteristic time of the problem.

2 Numerical scheme

In recent years there have been several publications on numerical treatment of the problem with viscoelastic fluids. In [1] there is investigated a finite element approximation for visco-elastic fluid flow obeying the Oldroyd B constitutive equation. The unknown pressure, velocity and stress $(p, \vec{V}, \boldsymbol{\tau})$ are approximated by P_1 continuous, P_2 continuous and P_1 discontinuous finite elements and the upwinding by discontinuous finite elements is used for the convection of the stress. Under assumption that the continuous problem admits sufficiently smooth and small solution there is shown using the fixed point techniques the existence of the approximate solution and the error bounds. In [6] the similar results are obtained with P_1 continuous approximation of the stress and upwinding by SUPG method. In [5] the same method is applied to decoupled algorithm and there is shown that the fixed point algorithm is contracting in some neighbourhood of the solution of the continuous problem.

Our approach is based on the papers [7] and [8] where the fractional θ-step time discretization with decoupled system is investigated for slow flows. (i.e. convective term in (1.15) is neglected.) We combine this idea with FE solver of the Navier-Stokes equation developed in [9] (see also [10]).

2.1 Time discretization

For the discretization in time we use the fractional θ-step method in combination with the operator splitting method. Suppose we have the following problem

$$m\frac{\mathrm{d}U(t)}{\mathrm{d}t} + A\big(U(t)\big) = 0 \tag{2.21}$$

$$U(0) = U_0, \tag{2.22}$$

where m is a constant vector in $\mathbf{R}^s$ and $U : [0,T] \to \mathbf{R}^s$. The non-linear operator $A : \mathbf{R}^s \to \mathbf{R}^s$ is split into two parts $A = A_1 + A_2$. Then for $\theta \in (0, \frac{1}{2})$ we solve

$$m\frac{U^\theta - U^0}{\theta\Delta t} + A_1\big(U^\theta\big) = -A_2\big(U^0\big) \tag{2.23}$$

$$m\frac{U^{1-\theta} - U^\theta}{(1-2\theta)\Delta t} + A_2\big(U^{1-\theta}\big) = -A_1\big(U^\theta\big) \tag{2.24}$$

$$m\frac{U^1 - U^{1-\theta}}{\theta\Delta t} + A_1\big(U^1\big) = -A_2\big(U^{1-\theta}\big) \tag{2.25}$$

where $U^0 = U(t)$, $U^\theta = U(t+\theta\Delta t)$, $U^{1-\theta} = U(t + (1-\theta)\Delta t)$ and $U^1 = U(t+\Delta t)$.

In our problem, we have $U = (p, \vec{v}, \boldsymbol{\tau})^T$ and we can use the following decomposition

$$A_1(U) = \begin{pmatrix} \operatorname{div} \vec{v} \\ \mathrm{Re}(\nabla\vec{v})\vec{v} + \nabla p - (1-\alpha)\Delta\vec{v} - \operatorname{div}\boldsymbol{\tau} - \vec{f} \\ (1-\omega)\boldsymbol{\tau} - 2\alpha\boldsymbol{D} \end{pmatrix} \tag{2.26}$$

$$A_2(U) = \begin{pmatrix} 0 \\ 0 \\ \mathrm{We}\big((\nabla\boldsymbol{\tau})\vec{v} + \beta_a(\boldsymbol{\tau}, \nabla\vec{v})\big) + \omega\boldsymbol{\tau} \end{pmatrix}. \tag{2.27}$$

The coefficients m are $(0, \mathrm{Re}, \mathrm{We})^T$ and $\omega \in (0,1)$ is the splitting parameter. This decomposition of A results in two different problems which are solved apart. In the 1^{st} and 3^{rd} time sub-step we obtain Navier-Stokes problem for the unknowns $(p, \vec{v})$ and in the 2^{nd} sub-step we have to solve the transport problem for the unknown $\boldsymbol{\tau}$.

2.2 Spatial discretization

Let $\mathbf{T}_h$ be a regular decomposition of the domain Ω into quadrilaterals. We define finite dimensional spaces

$$L_h = \{q_h \in L^2(\Omega); q_h/T = \text{const.}, \forall T \in \mathbf{T}_h\} \quad \text{for the approximation of } p, \tag{2.28}$$

$$S_h = \{v_h \in L^2(\Omega); v_h/T \in \tilde{Q}_1(T), F_\Gamma(v_h/T) = F_\Gamma(v_h/\tilde{T}), \forall T \in \mathbf{T}_h, \tilde{T} \cap T = \Gamma\}, \tag{2.29}$$

$$H_h = S_h \times S_h \quad \text{for the approximation of } \vec{v}, \tag{2.30}$$

$$M_h = \{\boldsymbol{\eta} \in L^2(\Omega)^4; \eta_{ij} = \eta_{ji}, \eta_{ij}/T \in P_1(T), \forall T \in \mathbf{T}_h\} \quad \text{for the approximation of } \boldsymbol{\tau}, \tag{2.31}$$

where $F_\Gamma(v) = |\Gamma|^{-1} \int_\Gamma v(\vec{x}) \mathrm{d}\gamma$ or $F_\Gamma(v) = v(m_\Gamma)$ are the nodal functionals. (m_Γ is midpoint of the edge Γ) $\tilde{Q}_1(T)$ is a finite element space generated by $\{x^2 - y^2, x, y, 1\}$. (Called "rotated bilinear" finite elements.)

2.2.1 The Navier-Stokes problem.

In the first sub-step of our time stepping scheme we have to solve the following problem for the unknowns $\vec{v}^{\,\theta}$ and p^θ, i.e.

$$\begin{aligned} \operatorname{div} \vec{v}^{\,\theta} &= 0 \\ \mathrm{Re}\Big(\frac{\vec{v}^{\,\theta}}{\theta\Delta t} + (\nabla\vec{v}^{\,\theta})\vec{v}^{\,\theta}\Big) + \nabla p^\theta + c\Delta\vec{v}^{\,\theta} &= \vec{g}, \end{aligned} \tag{NS}$$

where the constant c and the right hand side $\vec{g}$ are given by

$$\begin{aligned} c &= \frac{\alpha\theta\Delta t}{\mathrm{We} + (1-\omega)\theta\Delta t} - (1-\alpha) \\ \vec{g} &= \vec{f}^{\,\theta} + \frac{\mathrm{Re}}{\theta\Delta t}\vec{v}^{\,0} + \frac{\theta\Delta t}{\mathrm{We} + (1-\omega)\theta\Delta t} \operatorname{div}\boldsymbol{\eta} \\ \boldsymbol{\eta} &= \frac{\mathrm{We}}{\theta\Delta t}\boldsymbol{\tau}^0 - \mathrm{We}\big((\nabla\boldsymbol{\tau}^0)\vec{v}^{\,0} - \beta_a(\boldsymbol{\tau}^0, \nabla\vec{v}^{\,0})\big) - (1-\omega)\boldsymbol{\tau}^0. \end{aligned}$$

The stress tensor $\boldsymbol{\tau}^\theta$ can be computed explicitly with known $\vec{v}^{\,\theta}$ from

$$\mathrm{We}\frac{\boldsymbol{\tau}^\theta}{\theta\Delta t} + (1-\omega)\boldsymbol{\tau}^\theta = 2\alpha\boldsymbol{D}(\vec{v}^{\,\theta}) + \boldsymbol{\eta} \tag{2.32}$$

This problem is discretized by standard finite element method with streamline diffusion or SUPG method for convective term, linearized by fixed point defect correction iteration and linear sub-problems are solved by multigrid method with SOR, ILU or block-wise Gauss-Seidel smoothing. The situation for the third step is the same if we replace the superscripts θ and 0 by the superscripts 1 and $1-\theta$.

2.2.2 The transport problem

In the second step of our method we first compute explicitly the velocity $\vec{v}^{1-\theta}$ from

$$\mathrm{Re}\frac{\vec{v}^{1-\theta}}{(1-2\theta)\Delta t} = \mathrm{Re}\frac{\vec{v}^{\,\theta}}{(1-2\theta)\Delta t} - \mathrm{Re}(\nabla\vec{v}^{\,\theta})\vec{v}^{\,\theta} - \nabla p^{\theta} + (1-\alpha)\Delta\vec{v}^{\,\theta} + \operatorname{div}\boldsymbol{\tau}^{\theta} + \vec{f}^{\,\theta}$$

and finally with known $\boldsymbol{\eta}$

$$\boldsymbol{\eta} = \mathrm{We}\frac{\boldsymbol{\tau}^{\theta}}{(1-2\theta)\Delta t} - (1-\omega)\boldsymbol{\tau}^{\theta} + 2\alpha\boldsymbol{D}(\vec{v}^{\,\theta})$$

we solve system for $\boldsymbol{\tau}^{1-\theta}$

$$\text{(T)} \qquad \mathrm{We}\Big(\frac{(1+\omega)\boldsymbol{\tau}^{1-\theta}}{(1-2\theta)\Delta t} + (\nabla\boldsymbol{\tau}^{1-\theta})\vec{v}^{1-\theta} + \beta_a(\boldsymbol{\tau}^{1-\theta}, \nabla\vec{v}^{1-\theta})\Big) = \boldsymbol{\eta}.$$

Here in order to ensure solvability of this problem we get restriction on the length of the time step Δt

$$\text{(2.33)} \qquad \Delta t \le \frac{1}{2|a|(1-2\theta)\|\boldsymbol{D}\|_{\infty}}.$$

This equation is discretized by the FE method with SD or SUPG method for the convection of $\boldsymbol{\tau}$. To solve the resulting algebraic system we follow the work [7] and use the conjugate gradient method with some preconditioning.

3 Conclusion

We are working on implementation of this algorithm and we plan to compute different testing problems which we would like to compare with some experimental measurements in polymer processing or blood rheology experiments.

In the future we would like to develop this algorithm for the use with White-Metzner models, i.e. $\lambda, \mu_e, \mu_v \approx |\boldsymbol{D}|^2$. This algorithm also should be enriched by some adaptive capabilities, probably h-adaptivity, and by some parallel version of the solver in order to be able to compute efficiently real 3-dimensional problems.

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