Numerical analysis of linear viscoelastic flow

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Summary

Two dimensional simulation of the flow of the linear and quasilinear upper-convected Maxwell fluid is performed using the Boundary element method (BEM). In particular, a singular boundary integral approach, which has been established for the viscous incompressible flow problem [1], is modified and extended to capture viscoelastic fluid state. A special attention is given to a proper integration of the conservation and constitutive equations. A velocity-vorticity formulation of the dynamical set of equations is adopted. The flow in a driven cavity and the flow through an abrupt planar contraction with a re-entrant corner is studied [5].

1 Introduction

The Boundary-domain integral method (BDIM) presented in the paper is based on the solution of the Navier-Stokes equations set in velocity-vorticity formulation for different viscoelastic Maxwell fluids. The use of special fundamental solutions accounting for the linear part of the transport phenomena dramatically increases stability and accuracy of the numerical model although no additional stabilisation techniques are used. Particular attention is given to a proper integration of conservation and constitutive equations. The developed numerical scheme is tested on simple test cases to study the stability and accuracy of the solution algorithm.
2 Conservation equations

The analytical description of the motion of a continuous medium is based on conservation of mass, momentum, and energy, and the associated equations of state. The present development will be focused on isothermal laminar flows of incompressible viscoelastic isotropic fluids.

The field functions of interest are the velocity vector field \( \mathbf{v}(r, t) \), and the pressure scalar field \( p(r, t) \) such that the mass and momentum equations are satisfied

\[
\frac{\partial \mathbf{v}}{\partial t} = 0, \quad \rho \frac{D \mathbf{v}}{Dt} = \frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i, \tag{2.1}
\]

written in the Cartesian frame \( x_i \) using Eulerian description, where \( \rho \) is the constant fluid mass density, \( t \) is time, \( g_i \) is gravitational acceleration vector, \( \sigma_{ij} \) denotes the components of the total stress tensor, and the \( D (\cdot) / Dt = \partial (\cdot) / \partial t + v_k \partial (\cdot) / \partial x_k \) represents the Stokes material derivatives.

The field equations (2.1) and (2.2) are to be solved in conjunction with rheological equations of the fluid and boundary and initial conditions of the flow problem. The boundary conditions in general depend on the dependent variables applied, i.e. primitive or velocity-vorticity variables formulation.

3 Constitutive equations

For an incompressible fluid the Cauchy total stress \( \sigma_{ij} \) can be decomposed into a pressure contribution plus an extra deviatoric stress tensor field function \( \tau_{ij} \), and follows:

\[
\sigma_{ij} = -p \delta_{ij} + \tau_{ij}, \tag{3.1}
\]

where \( \delta_{ij} \) is the Kronecker delta. The central problem in the visco-elastic fluid dynamics is the selection of an appropriate rheological model that relates the extra-stress in eq. (3.1) to the flow kinematics. The differential constitutive equations to be considered here are implicit, rate-type rheological models generally associated with the name of Maxwell. For the broad class of materials such as simple fluids with fading memory, the constitutive equation can be expressed through a relation between stress and strain rate tensor and their time derivatives. Components of the stress and strain rate may be covariant (lower-convected) or contravariant (upper-convected).

For an Eulerian reference frame the material time derivative or convected derivative of an arbitrary symmetric, second order tensor \( u_{ij} \), which can be equated to extra-stress tensor \( \tau_{ij} \) or strain rate tensor \( \dot{\varepsilon}_{ij} \), can be formulated in several ways. Let us first define the Stokes material time derivative by expression

\[
\frac{D u_{ij}}{Dt} = \frac{\partial u_{ij}}{\partial t} + \nu_k \frac{\partial u_{ij}}{\partial x_k}, \tag{3.2}
\]
then the upper-convected or codeformational derivative is defined by relation

\[ \nabla u_{ij} = \frac{Du_{ij}}{Dt} - u_{ik}L_{jk} - u_{jk}L_{ik}, \quad (3.3) \]

while the lower-convected derivative is defined as

\[ \hat{u}_{ij} = \frac{Du_{ij}}{Dt} + u_{ik}L_{kj} + u_{jk}L_{ki}, \quad (3.4) \]

where the symbols \( \nabla \) and \( \Delta \) stand for upper or lower convected derivatives, respectively, and the velocity gradient tensor \( L_{ij} \) is defined as

\[ L_{ij} = \frac{\partial v_i}{\partial x_j}. \quad (3.5) \]

For the linear Maxwell fluid model the extra stress term \( \tau_{ij} \) incorporates both the effects of viscosity and elasticity, as follows

\[ \tau_{ij} + \lambda_1 \frac{\partial \tau_{ij}}{\partial t} = 2\eta_0 \dot{\varepsilon}_{ij}, \quad (3.6) \]

where \( \lambda_1 \) is a material constant for the fluid and is called stress relaxation time, while \( \eta_0 \) stands for the dynamic viscosity. The elasticity is given by the local time derivative of the additional stress tensor, being significant during transient conditions. As the flow develops, the local time derivative loses its influence to finally arrive at steady state where the viscosity is dominant.

The simplest quasilinear Maxwell model may be given in the following form

\[ \tau_{ij} + \lambda_1 \frac{D\tau_{ij}}{Dt} = 2\eta_0 \dot{\varepsilon}_{ij}, \quad (3.7) \]

where the nonlinearity of the model is now due to the local and convective derivative of the stress tensor. The model (3.7) should not be used for practical purposes, but it can be examined due to its simplicity as an appropriate model to study the stability and accuracy of the developed numerical solution algorithm presented herein.

In addition, simple quasilinear or convected viscoelastic constitutive models are Maxwell models, such as upper-convected Maxwell model (UCM) governed by the following constitutive relation

\[ \tau_{ij} + \lambda_1 \nabla \tau_{ij} = 2\eta_0 \dot{\varepsilon}_{ij}, \quad (3.8) \]

or the lower-convected Maxwell model (LCM)

\[ \tau_{ij} + \lambda_1 \hat{\tau}_{ij} = 2\eta_0 \dot{\varepsilon}_{ij}. \quad (3.9) \]

The upper-convected Maxwell model (3.8) is used extensively in testing numerical solution models. Some real fluids behave qualitatively like eq.
(3.8), at least over limited range of kinematics. Let us write the upper-convected model (3.8) in the following explicit manner

\[ \tau_{ij} + \lambda_1 \frac{D\tau_{ij}}{Dt} = 2\eta_0 \dot{\varepsilon}_{ij} + \lambda_1 \left( \tau_{ik} \frac{\partial v_j}{\partial x_k} + \tau_{jk} \frac{\partial v_i}{\partial x_k} \right), \] (3.10)

where the part of Oldroyd’s upper convected derivative has been shifted to the right hand side of the equation. This term may be seen as representing production of stress by interaction with the velocity gradients, in analogy to the equivalent vortex-stretching term. It is quite clear by contracting indices that the trace of \( \tau_{ij} \) is not zero, \( \tau_{kk} \neq 0 \), and evolves with the flow.

4 Summary of governing equations

Combining constitutive eqs. (3.1) and (3.8) and substituting for the total stress \( \sigma_{ij} \) in the momentum conservation eq. (2.2) leads to the following closed set of nonlinear equations [3], [4]

\[ \frac{\partial v_i}{\partial x_j} = 0, \] (4.1)

\[ \rho \frac{Dv_i}{Dt} = \eta_0 \frac{\partial^2 v_i}{\partial x_j \partial x_j} - \frac{\partial P}{\partial x_i} - \lambda_1 \frac{\partial \tau_{ij}^v}{\partial x_j}, \] (4.2)

\[ \tau_{ij} = 2\eta_0 \dot{\varepsilon}_{ij} - \lambda_1 \tau_{ij}^v, \] (4.3)

with \( P = p - \rho g \) representing the modified pressure. The system of eqs. (4.1) - (4.3) is formally identical to the equations govern the motion of newtonian viscous fluid, except the additional upper-convected derivative stress term. The distinguishing feature of this system as compared to a newtonian problem, is the implicit nature of the constitutive equation that forces the extra stresses to remain as dependent variables. The appearance of the additional terms in the momentum equation at the same time increases the nonlinearity of the dynamical system of equations.

For the two-dimensional plane geometry, the eqs. (4.1) - (4.3) provide six relations for the six unknowns, \( v_1, v_2, P, \tau_{11}, \tau_{12}, \) and \( \tau_{22} \). The above field equations are to be solved for appropriate boundary and initial conditions. Assuming that at time level \( t = t_n \) all relevant flow quantities, i.e. \( \tau_{ij}^n = \tau_{ij}^n (r_j, t_n), \tau_{ij}^n = \tau_{ij}^n (r_j, t_n) \) etc., are known, the issue is to determine the field functions at the time level \( t_{n+1} = t_n + \Delta t \).

5 Velocity-vorticity formulation

Introducing the vorticite vector field function \( \omega_i (r_j, t) \) as a curl of the compatibility velocity field \( v_i (r_j, t) \)

\[ \omega_i = \epsilon_{ijk} \frac{\partial v_k}{\partial x_j}, \quad \frac{\partial \omega_j}{\partial x_j} = 0, \] (5.1)
which is a solenoidal vector by the definition, the fluid motion computation procedure is divided into its kinetics and kinematics [1]. The vorticity transport in fluid domain is governed by the nonlinear parabolic diffusion-convection equation obtained as a curl of the momentum eq. (4.1)

$$\frac{D\omega_i}{Dt} = \nu_0 \frac{\partial^2 \omega_i}{\partial x_j \partial x_j} + \frac{\partial \omega_i}{\partial x_j} v_i - \frac{\lambda_1}{\rho} e_{ijk} \frac{\partial^2 \omega_k}{\partial x_j \partial x_k},$$

for $i, j, k, m = 1, 2, 3$, which reduces in two-dimensional plane flow geometry to the scalar vorticity equation

$$\frac{D\omega}{Dt} = \nu_0 \frac{\partial^2 \omega}{\partial x_j \partial x_j} - \frac{\lambda_1}{\rho} e_{ij} \frac{\partial^2 \omega_k}{\partial x_i \partial x_k},$$

for $i, j, k = 1, 2$. The vorticity equation (5.2) expresses the kinetics of the vorticity transfer by diffusion, convection, twisting-stretching, while the elasticity of the fluid acts as a highly nonlinear production term, making the nonlinearity of the equation even more severe, as compared to Newtonian viscous fluid flow.

The kinematics of an incompressible fluid motion is given by the vector potential field function $\psi_i (r_j, t)$ as in the following relation

$$v_i = e_{ijk} \frac{\partial \psi_k}{\partial x_j}, \quad \frac{\partial \psi_j}{\partial x_j} = 0,$$

in which the vector potential $\psi_i$ is considered to be solenoidal. By combining eqs. (5.1) and (5.4) the following kinematic expression is derived in the form of a velocity vector elliptic equation

$$\frac{\partial^2 v_i}{\partial x_j \partial x_j} + e_{ijk} \frac{\partial \omega_k}{\partial x_j} = 0.$$

The eq. (5.5) expresses the kinematics of the incompressible fluid motion, and further the compatibility and restriction conditions to keep velocity and vorticity field functions solenoidal. To improve convergence and stability of the coupled nonlinear velocity - vorticity iterative scheme, the eq. (5.5) is written in its false parabolic form

$$\frac{1}{\alpha} \frac{\partial v_i}{\partial t} = \frac{\partial^2 v_i}{\partial x_j \partial x_j} + e_{ijk} \frac{\partial \omega_k}{\partial x_j},$$

in which the false accumulation term, controlled by the relaxation parameter $\alpha$ value on the left hand side of the equation balances the nonsolenoidality of the velocity and vorticity field.
6 Boundary element model

The advantage of the boundary element method originate from the application of the Green fundamental solutions as particular weighting function. Since they only describe the linear transport phenomenon, an appropriate selection of a linear differential operator \( \mathcal{L} [\cdot] \) is of key importance in establishing a stable and accurate singular integral representation corresponding to the original differential conservation equation. All differential conservation models can be written as in the following general statement

\[
\mathcal{L} [u] + b = 0, \tag{6.1}
\]

where the linear differential operator \( \mathcal{L} [\cdot] \) can be either elliptic or parabolic and \( u (r_j, t) \) is an arbitrary field function while the nonhomogeneous term \( b (r_j, t) \) is generally used for the nonlinear transport effects.

When solving time dependent flow fields using elliptic fundamental solutions the field function local time derivative \( \partial u / \partial t \), can be approximated in different ways. The finite difference model is usually employed, i.e. such as the following implicit backward first order Euler scheme

\[
\left( \frac{\partial u}{\partial t} \right)^{n+1} \simeq \frac{u^{n+1} - u^n}{\Delta t}, \tag{6.2}
\]

or the three level second order asymmetric difference formulae

\[
\left( \frac{\partial u}{\partial t} \right)^{n+1} \simeq \frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t}. \tag{6.3}
\]

The ability of a viscoelastic fluid flow numerical model depends greatly on the proper integration of constitutive and conservation models [3]. Applying the Euler scheme (6.2) the constitutive eq. (3.10) can be modeled with the following approximative form written for the time level \( n + 1 \)

\[
\tau_{ij} = 2\eta_0 \dot{e}_{ij} - \lambda_1 \left( \frac{\tau_{ij} - \tau_{ij}^n}{\Delta t} + v_k \frac{\partial \tau_{ij}}{\partial x_k} \right) + \lambda_1 \left( \tau_{ik} \frac{\partial v_j}{\partial x_k} + \tau_{jk} \frac{\partial v_i}{\partial x_k} \right), \tag{6.4}
\]

and finally in compact form the "modified" upper-convected derivative \( \tau_{ij}' \) analogous to eq. (3.8)

\[
\tau_{ij} + \lambda_1 \tau_{ij}' = 2\eta_0' \dot{e}_{ij} \tag{6.5}
\]

in which the modified parameters are given as

\[
\eta_0' = \frac{\eta_0}{1 + \lambda_1 / \Delta t}, \quad \text{and} \quad \lambda_1' = \frac{\lambda_1}{1 + \lambda_1 / \Delta t}. \tag{6.6}
\]

with the superscript \( n + 1 \) omitted. Note that at least for the simple linear Maxwell fluid (3.6) the extra stress \( \tau_{ij} \) is given by an explicit relation of viscous contribution and initial stress conditions.
Finally, one can easily summarize the modified governing equations equivalent to eqs. (4.1) - (4.3) written for the velocity-vorticity approach.

\[
\frac{\partial^2 v_i}{\partial x_j \partial x_j} + \epsilon_{ijk} \frac{\partial \omega_k}{\partial x_j} = 0, \quad (6.7)
\]

\[
\frac{D\omega_i}{Dt} = \nu_0 \frac{\partial^2 \omega_i}{\partial x_j \partial x_j} + \frac{\partial \omega_j v_i}{\partial x_j} - \frac{\lambda_1}{\rho} \epsilon_{ijk} \frac{\partial^2 \tau_{km}^v}{\partial x_j \partial x_k}, \quad (6.8)
\]

\[
\tau_{ij} = 2\eta_0 \hat{e}_{ij} - \lambda_1 \tau_{ij}, \quad (6.9)
\]

where the vorticity equation (6.8) simplifies for the plane fluid motion to

\[
\frac{D\omega}{Dt} = \nu_0 \frac{\partial^2 \omega}{\partial x_j \partial x_j} - \frac{\lambda_1}{\rho} \epsilon_{ij} \frac{\partial^2 \tau_{jk}^v}{\partial x_i \partial x_k}. \quad (6.10)
\]

Considering the kinetics in the integral representation one has to take into account the parabolic diffusion-convection character of the vorticity transport eq. (6.10). Since only the linear elliptic diffusion-convection differential operator with the first order sink term is employed, i.e.

\[
\mathcal{L} [\cdot] = \nu \frac{\partial^2 (\cdot)}{\partial x_j \partial x_j} - \frac{\partial \bar{v}_j (\cdot)}{\partial x_j} - \beta (\cdot), \quad (6.11)
\]

where the quantities \( \bar{\nu} = \nu_0 \) and \( \bar{v}_j \) are respectively the constant modified viscosity and constant velocity vector, the vorticity eq. (6.10) has to be first rewritten in its elliptic form. Using the time discretization given by eqs. (6.2), and (6.3) the vorticity eq. (6.10) can be formulated as a nonhomogeneous elliptic diffusion-convection equation with a first order reaction term, as follows

\[
\mathcal{L} [\omega] + b = \nu_0 \frac{\partial^2 \omega}{\partial x_j \partial x_j} - \frac{\partial \bar{v}_j \omega}{\partial x_j} - \beta \omega + b = 0, \quad (6.12)
\]

with the following corresponding integral representation

\[
c (\xi) \omega (\xi) + \nu_0 \int_{\Gamma} \omega \frac{\partial u^*}{\partial n} d\Gamma = \nu_0 \int_{\Gamma} \frac{\partial \omega}{\partial n} u^* d\Gamma - \int_{\Gamma} \omega \bar{v}_j n_j u^* d\Gamma + \int_{\Omega} b u^* d\Omega, \quad (6.13)
\]

where \( \beta = 1/\Delta t \) for the Euler time discretization, and the function \( u^* \) is the elliptic diffusion-convection fundamental solution with the first order reaction term. The eq. (6.13) represents the vorticity kinetics in an integral form. The linear vorticity transport representing diffusion and convection for the dominant constant velocity vector \( \bar{v}_j \), is completely represented with the boundary integrals only. The domain integral of the nonhomogeneous nonlinear contribution \( b \), represented as

\[
b = -\frac{\partial \bar{v}_j \omega}{\partial x_j} - \frac{\lambda_1}{\rho} \epsilon_{ij} \frac{\partial^2 \tau_{jk}^v}{\partial x_i \partial x_k} + \frac{1}{\Delta t} \omega^n, \quad (6.14)
\]
includes the convection for the perturbed velocity field \( \tilde{v}_i \), such that \( v_i = \tilde{v}_i + \bar{v}_i \), modified elastic stress part and the initial vorticity conditions combine the following integral representation

\[
\frac{c(\xi)}{\omega(\xi)} + v_0' \int_\Gamma \omega \frac{\partial u^*}{\partial n} d\Gamma = v_0' \int_\Gamma \frac{\partial \omega}{\partial n} u^* d\Gamma - \int_\Gamma \omega \tilde{v}_j u^* d\Gamma
\]

\[
= \int_\Omega \varphi \tilde{v}_j n_j u^* d\Omega + \int_\Omega \omega \tilde{v}_j \frac{\partial u^*}{\partial x_j} d\Omega - \frac{\chi_i}{\rho} e_{ij} \int_\Gamma \frac{\partial \tau^j_{jk}}{\partial x_k} n_i u^* d\Gamma
\]

\[
+ \frac{\chi_i}{\rho} e_{ij} \int_\Omega \frac{\partial \tau^j_{jk}}{\partial x_k} \frac{\partial u^*}{\partial x_i} d\Omega + \frac{1}{\Delta t} \int_\Omega \omega^n u^* d\Omega. \tag{6.15}
\]

The term \( e_{ij} (\partial \tau^j_{jk}/\partial x_k) \) is complex and can be written as in the following symbolic notation expression

\[
e_{ij} \frac{\partial \tau^j_{jk}}{\partial x_k} = e_{ij} \frac{\partial}{\partial x_k} \left( -\frac{1}{\Delta t} \tau^j_{jk} + \nu_m \frac{\partial \tau^j_{jk}}{\partial x_m} - \tau^j_{jm} \frac{\partial v_k}{\partial x_m} - \tau^j_{km} \frac{\partial v_m}{\partial x_m} \right), \tag{6.16}
\]

for \( i, j, k, m = 1, 2 \). The eq. (6.15) represents the integral representation of the vorticity transport in a viscoelastic fluid motion, showing a complete analogy with the integral representation governing the vorticity transport in a Newtonian viscous fluid flow with the exception of the elastic stress terms acting as highly nonlinear vorticity generation terms.

The velocity eq. (5.6) is recognised as a nonhomogeneous parabolic diffusion equation thus employing the linear parabolic diffusion differential operator as follows

\[
\mathcal{L}[\cdot] = a \frac{\partial^2 (\cdot)}{\partial x_j \partial x_j} - \frac{\partial (\cdot)}{\partial t}, \tag{6.17}
\]

and consequently the following can be written

\[
\mathcal{L}[v_i] + b_i = \alpha \frac{\partial^2 v_i}{\partial x_j \partial x_j} - \frac{\partial v_i}{\partial t} + b_i = 0, \tag{6.18}
\]

with the following corresponding integral representation written in a time increment form for a false transient time step \( \Delta t = t_F - t_{F-1} \)

\[
c(\xi) v_i(\xi, t_F) + \alpha \int_{t_{F-1}}^{t_F} v_i \frac{\partial u^*}{\partial n} dt d\Gamma = \alpha \int_{t_{F-1}}^{t_F} \frac{\partial v_i}{\partial n} u^* dt d\Gamma
\]

\[
+ \int_\Omega \int_{t_{F-1}}^{t_F} b u^* dt d\Omega + \int_\Omega v_{i,F-1} u^*_{F-1} d\Omega, \tag{6.19}
\]

where \( u^* \) is the parabolic diffusion fundamental solution. The eq. (6.19) represents the kinematics or the compatibility conditions in an integral form.
The linear part or the potential part of the flow motion is completely represented with the boundary integrals only, while domain integral of the nonhomogeneous nonlinear contribution $b_i$ shown as

$$b_i = \alpha e_{ijk} \frac{\partial \omega_k}{\partial x_j}$$

(6.20)

includes the contribution of the rotational motion part.

### 7 Test example

The extended numerical algorithm, which included visco-elastic state of the fluid, was tested for standard test case of driven cavity. Computational mesh, used for computations, consisted of 30x30 nonuniform subdomains with ratio of 4 between the longest and the smallest boundary element, and symmetric with respect to the center of the cavity and the time step value of $\Delta t = 0.1$ was considered. Figure 7.1 presents velocity $v_x$ profiles along the vertical through the geometric centre of the cavity for the time steps $t = 0.1$ and $t = 1.0$ for the newtonian fluid ($\lambda_1 = 0$). On the figure 7.2 the corresponding $v_x$ profiles are given for the linear viscoelastic fluid ($\lambda_1 = 0.1$). The elasticity effect is well evident. In both cases of flow simulations the profiles converge to the steady state results of Ghia [6] for the $Re = 100$ value.

![Figure 7.1: Velocity $v_x$ profiles along the vertical through the geometric centre of the cavity for the time steps $t = 0.1$ and $t = 1.0$ for the newtonian fluid ($\lambda_1 = 0$)](image-url)
Figure 7.2: Velocity $v_x$ profiles along the vertical through the geometric centre of the cavity for the time steps $t = 0.1$ and $t = 1.0$ for the viscoelastic fluid ($\lambda_1 = 0.1$)

8 Conclusions

Boundary-domain integral approach to the solution of visco-elastic fluid motion problems is presented. Different Maxwell fluid models are accounted for to show the applicability of the proposed BEM model. All attractive features of the BEM model, based on the application of different fundamental solutions and macro element technique, already established in a viscous fluid dynamics case, are presented [2]. The numerical scheme is verified on the test case of driven cavity and computational results show that the scheme is stable and accurate.

References


