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Viscoelastic fluid flow simulation using the contravariant deformation formulation

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Abstract

The new formulation for conformation-tensor based viscoelastic fluid models, written in terms of the contravariant deformation tensor as introduced by Hütter et al. (2018), has been approached numerically. It has been implemented in a finite element method framework with the DEVSS-G/SUPG method for stabilisation. A stress-implicit as well as a stress-explicit formulation is presented that allows to integrate the non-linear flow equations, with or without a solvent contribution, forward in time with second-order accuracy. The time-dependent stability in shear flow is maintained using the contravariant deformation, which is tested by solving a perturbed planar Couette flow of an upper-convected Maxwell (UCM) fluid. The stability and accuracy of our implementation has furthermore been tested by solving the flow around a cylinder with confining walls. The new formulation turns out to be more stable as compared to the formulation in terms of the conformation tensor. It enables to simulate the flow of a Giesekus fluid with non-linear parameter $\alpha = 0.01$ and viscosity ratio $\nu = \eta_s/\eta_0 = 0.59$ way beyond the Weissenberg number at which the High Weissenberg Number Problem manifests itself using the standard formulation. The stability appears to be similar to the log-conformation representation. The computed stress profiles up to a Weissenberg number of $Wi = 0.6$ for an Oldroyd-B
fluid with viscosity ratio $\nu = 0.59$, compare well with benchmark results from other studies, including other finite element, finite volume and spectral element methods.

Keywords: conformation-tensor based models, multiplicative decomposition, finite element method, numerical stability, flow around a confined cylinder, planar Couette flow

1. Introduction

Several numerical stabilisation techniques have already been developed for mixed finite element methods using conformation-tensor based differential models for simulating the flow of viscoelastic fluids [1]. For stabilising the velocity-stress interpolation, the DEVSS-G technique [2, 3] with smooth velocity gradient interpolation in the constitutive equation [4, 5] for additional time-dependent stability in shear flow, and variants thereof are often employed. In addition, stabilisation of the convection in the constitutive equation is obtained with SUPG [6]. The decoupling of the momentum balance equation from the constitutive equation using the implicit stress formulation [7] allows for second-order time-integration of these equations avoiding a fully implicit coupled scheme, even for small or zero solvent viscosities. Still, with all these techniques available, until 2004 [8, 9], all methods for numerical simulation of the flow of viscoelastic fluids broke down when the Weissenberg number exceeds a relatively small critical value. This value of $\mathcal{O}(1)$ depends on the problem, the constitutive model, the numerical method and the mesh. The High Weissenberg Number Problem (HWNP) is conjectured to be a numerical instability as a result of the failure of the numerical schemes - that make use of polynomial basis functions for approximating the stress - to balance exponential growth of the stress due to deformation with convection [9].

In Fattal et al. [9], the HWNP is restrained by rewriting the equation for the conformation in terms of the logarithm of the conformation, leading to crucial stabilisation of the numerical schemes. This way, the exponential profiles
become linear in the logarithm of the conformation. In addition, the positive-
definiteness of the conformation is preserved. Hulsen et al. [10] were the first
to implement the log-conformation representation in a finite element method
(FEM) context using the DEVSS/DG formulation. However, the required spec-
tral decomposition in this formulation makes numerical implementation difficult,
especially when it comes to linearisation required for Newton-Raphson iteration

[11] [12] to solve the governing equations in a fully coupled manner. Another
approach that alleviates the HWNP can be found in [13] [14], which use the
 evolution of the unique symmetric positive-definite square root of the confor-
mation. Finally, in [15] a Cholesky decomposition of the conformation tensor
is evolved which keeps positivity of the conformation. All the techniques men-
tioned in this paragraph enable to simulate and/or obtain improved convergence
beyond Weissenberg numbers at which the standard conformation formulation
fails. Note, that similar decompositions of the conformation tensor are used in
[16] [17] for turbulent flow analysis purposes but not for flow computations.

Hütter et al. [18] recently developed a general approach for including ther-
nal fluctuations in conformation-tensor based (non-)linear viscoelastic models
in accordance with thermodynamic principles. They generalised these models
and reformulated them in terms of a multiplicative decomposition of the con-
formation tensor which they call the **contravariant deformation tensor**, and can
be interpreted as the elastic part of the deformation gradient tensor. One of
the numerical advantages of the reformulation by Hütter et al. [18] is that it
is also relevant for deterministic models, i.e. without fluctuations, and we ant-
ticipate that the HWNP is naturally avoided. The reason for the avoidance is
the resemblance of the evolution equation for the contravariant deformation to
the formulation of the constitutive model in the Brownian configurations fields
method [19], which is not affected by the instability, regarding deformation and
convection [20]. In contrast to approaches [13–15], the contravariant deforma-
tion tensor (CDT) formulation contains deformation rotation, whereas the other
approaches eliminate this rotation of the conformation-related variable to obtain
a symmetric or triangular structure. The inherent rotation is a drawback of the


CDT formulation, making it difficult to obtain a steady state solution directly as, for example, needed in a linear stability analysis. However, the approaches [13–15] contain additional complicated terms in the evolution equation to comply with the restriction to symmetry or triangularity, respectively, making them computationally more expensive and less amenable to the inclusion of thermal fluctuations, in constrast to our CDT formulation.

The goal of this paper is to show that the stability and accuracy of the formulation of differential constitutive models for viscoelastic fluids without fluctuations in terms of the contravariant deformation [18] is similar to the log-conformation formulation. We aim at providing stable numerical methods to solve time-dependent viscoelastic flows, which at a later stage can be extended with fluctuations according to [18].

The paper is organised as follows. The governing equations including the new formulation of viscoelastic models are described in Section 2. The numerical method is explained in Section 3 where two different second-order time-integration schemes for viscoelastic flows are presented: a stress-implicit as well as a stress-explicit formulation. Section 4 presents results for homogeneous flows using the new formulation. Results for the planar Couette problem with an initial perturbation are shown in Section 5. In Section 6 the results for the flow around a cylinder with walls at low and high Weissenberg numbers will be shown, comparing the new formulation with the (log-)conformation representation and with results from the literature. Conclusions are drawn in Section 7.

2. Governing equations

2.1. General aspects

The flow of incompressible viscoelastic fluids for which inertia is neglected is governed by the momentum and mass balance equations,

\[ \nabla p - \nabla \cdot (2\eta_s \mathbf{D}) - \nabla \cdot \mathbf{r} = 0, \]

\[ \nabla \cdot \mathbf{u} = 0, \]

where \( \eta_s \) is the shear viscosity and \( \mathbf{D} \) is the symmetric part of the velocity gradient \( \nabla \mathbf{u} \).

4
with pressure $p$ and velocity vector $u$, $\eta_s$ is the solvent viscosity, $D = (\nabla u + (\nabla u)^\text{T})/2$ is the rate-of-deformation tensor with velocity gradient tensor $(\nabla u)_{i,j} = \partial u_j / \partial x_i$, and $\tau$ is the viscoelastic extra stress tensor. Furthermore, a constitutive equation for $\tau$ is required, relating it to the deformation history of the fluid. Following Hütter et al. [18], in this paper conformation-tensor based viscoelastic models will be used that are formulated in terms of the contravariant deformation tensor $b$, which obeys

$$
\dot{b} = L \cdot b - g(b) = h(L, b),
$$

(3)

with $\dot{}$ the material derivative, $L = (\nabla u)^\text{T}$ is the transposed velocity gradient tensor, and $g(b)$ is a tensor function of $b$ whose form depends on the viscoelastic model. Tensor $b$ is related to the conformation tensor $c$ via

$$
c = b \cdot b^\text{T},
$$

(4)

Note that $b$ is generally an unsymmetric tensor. Moreover, it can be seen that $b$ is not unique since an arbitrary rotation of $b$ according to $b' = b \cdot R$, with $R$ a rotation tensor, does not change the conformation. Hence, no steady state for $b$ is to be expected in steady-state flows. As will be shown later, the tensor $b$ is unsteady in shear flow, even if $c$ is steady. A general form of the evolution equation for $c$ is

$$
\dot{c} = L \cdot c + c \cdot L^\text{T} - f(c),
$$

(5)

with $f(c)$ an isotropic, model specific tensor function of $c$. Substituting Eqs. (3)-(4) into Eq. (5) by applying the product rule for differentiation, it can be shown that

$$
g(b) = \frac{1}{2} f(c) \cdot b^\text{T}.
$$

It has been argued by Hütter et al. [18] that for numerical reasons it is preferable to write viscoelastic models extended with fluctuations in terms of $b$ rather than in $c$. One argument is that, as a consequence of Eq. (4), $c$ is always (semi-)positive definite. Moreover, the formulation in terms of $b$ is expected to be numerically more stable than the formulation in terms of $c$, even without
fluctuations. That is, the evolution equation of \( b \) shows close similarities with the stochastic evolution equation in the method of Brownian configuration fields \([19]\), which is immune to the numerical instability that causes the high Weisenberg number problem (HWNP) \([20]\). The stability comes from the intrinsic balance between deformation and convection in the evolution equation for \( b \).

2.2. Constitutive models

In this paper, two viscoelastic fluid models will be considered: the upper-convected Maxwell (UCM)/Oldroyd-B model and the Giesekus model. As opposed to the UCM model, the Oldroyd-B model has a solvent contribution and therefore \( \eta_s \neq 0 \) for the Oldroyd-B model while \( \eta_s = 0 \) for the UCM model. For the considered models, \( g(b) \) and \( \tau \) are given by \([18]\):

- **UCM/Oldroyd-B model:**
  \[
g(b) = \frac{1}{2\lambda} (b - b^{-T}),
  \]
  with \( \lambda \) the relaxation time. The extra stress expression for this model is
  \[
  \tau = G(c - I),
  \]
  with \( G \) the shear modulus.

- **Giesekus model:**
  \[
g(b) = \frac{1}{2\lambda} \left( c - I + \alpha(c - I)^2 \right) \cdot b^{-T},
  \]
  where the dimensionless parameter \( \alpha \) determines the magnitude of the anisotropic drag. The extra stress expression for this model is the same as for the UCM/Oldroyd-B model:
  \[
  \tau = G(c - I).
  \]

The Giesekus model (Eq. (9)) reduces to the UCM/Oldroyd-B model (Eq. (7)) for \( \alpha = 0 \).
2.3. Polar decomposition of the contravariant deformation

The contravariant deformation can be written as follows (see Eq. (4)):

\[ b = V \cdot R, \]  

\[ (11) \]

where \( V = \sqrt{c} \) is a symmetric, positive definite tensor and \( R \) is a rotation tensor. It should be noted that large differences in the rotations in regions of the flow where shear deformation is dominant result in large gradients in \( b \). This can be shown by substituting the decomposition of Eq. (11) into Eq. (3) applying the product rule, then using Eq. (6) by rewriting Eq. (5) and again applying the product rule, and finally left-multiplying with \( V^{-1} \), right-multiplying with \( R^T \) and rearranging terms. This gives

\[ \dot{R} \cdot R^T = \frac{1}{2}(V^{-1} \cdot L \cdot V - V \cdot L^T \cdot V^{-1}) + \frac{1}{2}(\dot{V} \cdot V^{-1} - V^{-1} \cdot \dot{V}), \]  

\[ (12) \]

which is a skew-symmetric tensor. If the material derivative of \( V \) vanishes \( (\dot{V} = 0) \), for example in the case of stationary homogeneous flow, Eq. (12) reduces to

\[ \dot{R} \cdot R^T = \frac{1}{2}(V^{-1} \cdot L \cdot V - V \cdot L^T \cdot V^{-1}). \]  

\[ (13) \]

Setting the right-hand side of Eq. (13) to zero and then left- and right-multiplying it by \( V \), it can be seen that the rotation rate of \( b \) equals zero if both \( \dot{V} = 0 \) and \( L \cdot c \) is a symmetric tensor. For steady shear flow, \( \dot{R} \neq 0 \) since \( L \cdot c \) is asymmetric for this flow and \( b \) is thus sinusoidal with a frequency determined by the skew-symmetric part of \( V^{-1} \cdot L \cdot V \), see Eq. (13). In steady extensional flow, however, \( L \cdot c \) is diagonal and therefore \( \dot{R} = 0 \).

Additionally, the expression for the rotation rate \( \dot{R} \cdot R^T \) in Eq. (13) can be used to determine the frequency of the rotation of \( b \) for the UCM model in steady shear analytically. For this purpose, an eigen-decomposition of \( V \) is inserted in Eq. (13), see Appendix A. The exact solution for \( c \) in steady state is used for expressing the eigenvalues and normalised eigenvectors entirely in terms of the Weissenberg number \( Wi = \lambda \dot{\gamma} \), where \( \dot{\gamma} \) is the shear rate. The result is

\[ \omega = \frac{1}{2 \sqrt{\text{Wi}^2 + 1}}, \]  

\[ (14) \]
where \( \omega \) is the angular frequency. Note that \( \omega/\dot{\gamma} \to 1/2 \) for \( Wi \to 0 \) \( (\dot{\gamma} \neq 0) \), which is the maximum value of \( \omega/\dot{\gamma} \), and \( \omega/\dot{\gamma} \to 1/(2Wi) \) for \( Wi \to \infty \).

3. Numerical discretisation methods

The governing equations of Sec. 2 are discretised in space using the finite element method and the method of lines for the time discretisation applying backward differencing formulas (BDF). For numerical stabilisation of the momentum balance (Eq. (1)) and constitutive equation (Eq. (3)), the DEVSS-G/SUPG method is employed. DEVSS-G \([2,3]\) stabilisation of the momentum balance is required due to an issue regarding the compatibility between the velocity and stress approximation spaces. It involves adding to Eq. (1) a viscous term containing the velocity gradient \( \nabla u \) with the projected velocity gradient \( G^T \) subtracted from it. As a result there is an extra dependent field variable \( G \), for which an additional projection equation is needed, besides the velocity \( u \), pressure \( p \) and contravariant deformation \( b \). Note that the viscoelastic extra stress \( \tau \) depends on \( b \) via Eq. (4) and Eqs. (8) and (10). The DEVSS-G stabilisation is a result of the difference in approximation spaces for \( L = (\nabla u)^T \) and \( G \). Besides, \( G \) is used as the velocity gradient in the constitutive equation \([3\text{–}5]\), which further improves the numerical stability for time-dependent shear flows \([2\text{–}2]\), as will be shown later.

In order to stabilise the convection term in the constitutive equation (Eq. (3)), the SUPG method \([6]\) is applied. This method uses a modified test function \( \tilde{d} = d + \kappa u \cdot \nabla d \), with test function \( d \) for the standard Galerkin method and \( \kappa \) the SUPG-parameter, which puts more weight to the upwind direction of the streamline.

3.1. Weak formulation

For discretisation of the flow problem using FEM with DEVSS-G/SUPG for stabilisation, the domain \( \Omega \) is divided into elements and the field variables \( u \), \( p \), \( G \) and \( b \) are approximated using linear combinations of nodal values of the
solution and polynomial functions on each element:

\[
\begin{align*}
\mathbf{u} &= \sum_i u_i \phi_i(\mathbf{x}), \\
p &= \sum_i p_i \psi_i(\mathbf{x}), \\
\mathbf{G} &= \sum_i G_i \zeta_i(\mathbf{x}), \\
b &= \sum_i b_i \theta_i(\mathbf{x}),
\end{align*}
\]

(15) (16) (17) (18)

where \(\phi_i(\mathbf{x}), \psi_i(\mathbf{x}), \zeta_i(\mathbf{x})\) and \(\theta_i(\mathbf{x})\) are global interpolation functions. Let the finite element approximation spaces for \(\mathbf{u}, p, \mathbf{G}\) and \(b\) be denoted by \(\mathcal{U}_h\), \(\mathcal{P}_h\), \(\mathcal{G}_h\) and \(\mathcal{B}_h\), respectively. After multiplying the momentum balance, mass balance, projection and constitutive equation by test functions \(\mathbf{v}, q\), \(\mathbf{H}\) and \(\hat{d}\) respectively, then integrating them over the domain and applying integration by parts and Gauss’ theorem to the momentum balance, the discretised weak formulation of these equations becomes: find \(\mathbf{u} \in \mathcal{U}_h\), \(p \in \mathcal{P}_h\), \(\mathbf{G} \in \mathcal{G}_h\) and \(b \in \mathcal{B}_h\) such that for all test functions \(\mathbf{v} \in \mathcal{U}_h\), \(q \in \mathcal{P}_h\), \(\mathbf{H} \in \mathcal{G}_h\) and \(d \in \mathcal{B}_h\):

\[
\begin{align*}
((\nabla \mathbf{v})^T, 2\eta_h \mathbf{D} + \beta(\nabla \mathbf{u} - \mathbf{G}^T) + \tau(\mathbf{b})) - (\nabla \cdot \mathbf{v}, p) &= 0, \\
(q, \nabla \cdot \mathbf{u}) &= 0, \\
(\mathbf{H}, (-\nabla \mathbf{u} + \mathbf{G}^T)) &= 0, \\
(\hat{d} + \kappa \mathbf{u} \cdot \nabla \hat{d}, \frac{\partial \mathbf{b}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{b} - \mathbf{G} \cdot \mathbf{b} + g(\mathbf{b})) &= 0,
\end{align*}
\]

(19) (20) (21) (22)

where in Eq. (22) the material derivative is split into a local time-derivative term and a convective term, since an Eulerian grid is employed. Furthermore, \((.,.)\) indicates the \(L^2\)-inner product on the domain \(\Omega\), which is divided into elements of type quadratic triangle. The SUPG-parameter is \(\kappa = h/2U\), with \(h\) a characteristic element size in the direction of velocity obtained by mapping of the reference element \(\hat{\Omega}\) and \(U = \|\mathbf{u}\|\) the velocity magnitude, both determined in each integration point separately. The DEVSS parameter is taken as \(\beta = \lambda G\). Note, that the Dirichlet boundary conditions are enforced strongly by requiring that \(\mathbf{v} = 0\) on the Dirichlet boundary and that the Neumann boundary term vanishes because of the type of boundary conditions we will use. The interpolation of the velocity is quadratic, while the pressure, projected velocity gradient
and contravariant deformation are interpolated linearly. All the unknowns are continuous across element boundaries.

3.2. Time integration

For the time discretisation of the equations, the considered time interval is divided into a number of time steps. The time step $\Delta t$ is taken constant, the current time being equal to $t_n = n\Delta t$, where $n$ is the number of steps already performed. In the following, the evaluation of field variables at a discrete time will be denoted by a subscript; $\mathbf{\tau}_n = \mathbf{\tau}(t = t_n)$ for example for the viscoelastic extra stress. Two formulations for the time discretisation of the equations will be used: the explicit and implicit stress formulations for viscoelastic fluid flow.

3.2.1. Explicit stress formulation

In the explicit stress formulation \cite{24, 28}, the updated viscoelastic extra stress $\mathbf{\tau}_{n+1}$ is first calculated explicitly from the constitutive equation (Eq. (22)) via Eq. (4) and Eqs. (8) and (10) and then substituted into the momentum balance (Eq. (19)). A semi-extrapolated second-order (BDF2) time-integration scheme with velocity prediction is applied to Eq. (22) for solving $\mathbf{b}_{n+1}$:

\begin{equation}
(d + \kappa \hat{\mathbf{u}}_{n+1} \cdot \nabla d, \frac{3}{2} \frac{\mathbf{b}_{n+1}}{\Delta t} + \hat{\mathbf{u}}_{n+1} \cdot \nabla \mathbf{b}_{n+1}) = (d + \kappa \hat{\mathbf{u}}_{n+1} \cdot \nabla d, \frac{2\mathbf{b}_n - \frac{1}{2}\mathbf{b}_{n-1}}{\Delta t} + 2h(G_n, \mathbf{b}_n) - h(G_{n-1}, \mathbf{b}_{n-1})),
\end{equation}

with prediction $\hat{\mathbf{u}}_{n+1} = 2\mathbf{u}_n - \mathbf{u}_{n-1}$. The time integration is started with a first-order semi-implicit scheme in the first time step:

\begin{equation}
(d + \kappa \mathbf{u}_n \cdot \nabla d, \frac{\mathbf{b}_{n+1}}{\Delta t} + \mathbf{u}_n \cdot \nabla \mathbf{b}_{n+1}) = (d + \kappa \mathbf{u}_n \cdot \nabla d, \frac{\mathbf{b}_n}{\Delta t} + G_n \cdot \mathbf{b}_n - g(b_n)).
\end{equation}
The velocity \( \mathbf{u}_{n+1} \), pressure \( p_{n+1} \) and velocity gradient \( \mathbf{G}_{n+1} \) at the new time \( t_{n+1} \) are then obtained by evaluating Eqs. (19)-(21) at \( t_{n+1} \):

\[
((\nabla \mathbf{v})^T, 2\eta_s \mathbf{D}(\mathbf{u}_{n+1}) + \beta(\nabla \mathbf{u}_{n+1} - \mathbf{G}_{n+1}^T)) - (\nabla \cdot \mathbf{v}, p_{n+1}) = ((\nabla \mathbf{v})^T, \mathbf{\tau}(\mathbf{b}_{n+1})), \tag{25}
\]

\[-(q, \nabla \cdot \mathbf{u}_{n+1}) = 0, \tag{26}\]

\[(\mathbf{H}, \beta(-\nabla \mathbf{u}_{n+1} + \mathbf{G}_{n+1}^T)) = 0. \tag{27}\]

Note that Eq. (26) has been multiplied by \(-1\) and Eq. (27) by \(\beta\) to get a symmetric system matrix. Besides, the system matrix is constant in time and needs to be built only once. Linear interpolation of \( \mathbf{b}_{n+1} \) as in Eq. (18) is used for numerical integration of the viscoelastic extra stress \( \mathbf{\tau}(\mathbf{b}_{n+1}) \) by applying Eq. (4) and Eqs. (8) and (10) in the integration points. For solving Eq. (24) in the first time step, Eqs. (25)-(27) are evaluated at \( t_0 \) and solved for \( \mathbf{u}_0, p_0 \) and \( \mathbf{G}_0 \) without a contribution from \( \mathbf{\tau}(\mathbf{b}_0) \) because the fluid is assumed to be stress-free initially, i.e. the initial condition is \( \mathbf{\tau}(t = 0) = 0 \). The explicit stress formulation can be very efficient if the solvent viscosity is sufficiently large. However, time-step restriction can be very severe for small values of the solvent viscosity \( \eta_s \), and, if \( \eta_s \) is zero, the system of equations (25)-(27) even becomes singular and no unique solution for \( \mathbf{u}_{n+1} \) can be obtained. These problems can be avoided by employing the implicit stress formulation, which will be the subject of the next section.

### 3.2.2. Implicit stress formulation

For flows with a small or zero solvent contribution, the implicit stress formulation [7] is often used to decouple the momentum balance, mass balance and projection equation from the constitutive equation. In this formulation, an expression for \( \mathbf{\tau}_{n+1} \) is found which still contains unknown velocity terms \( \mathbf{\tau}_{n+1} \) so that the system in Eqs. (19)-(21) is not singular. This results in the set of
momentum balance, mass balance and projection equations

\begin{align}
(\nabla v)^T, 2\eta_s D(u_{n+1}) + \alpha(\nabla u_{n+1} - G_{n+1}^T) + G\Delta t(-u_{n+1} \cdot \nabla c_n \\
+ L_{n+1} \cdot c_n + c_n \cdot L_{n+1}^T) - (\nabla \cdot v, p_{n+1}) \\
&= -((\nabla v)^T, G(c_n - I - \Delta t f(c_n))), \\
(q, \nabla \cdot u_{n+1}) &= 0,
\end{align}

\begin{align}
(H, (-\nabla u_{n+1} + G_{n+1}^T)) &= 0,
\end{align}

which is a Stokes-like system in the unknowns \( u_{n+1}, p_{n+1} \) and \( G_{n+1} \) at the new time \( t_{n+1} \). An \( L^2 \)-projection on the discretised space defined in Eq. (18) is used to obtain \( c_n \) from \( b_n \) (see Eq. (4)):

\begin{align}
(P, c_n - b_n \cdot b_n^T) &= 0,
\end{align}

with \( P \in B_h \) a test function. After obtaining the solution of these equations, the constitutive equation (Eq. (22)) is solved using a BDF2 time-discretisation scheme with contravariant deformation \( b \) prediction:

\begin{align}
(d + \kappa u_{n+1} \cdot \nabla d, \frac{3}{2} \frac{b_{n+1}}{\Delta t} + u_{n+1} \cdot \nabla b_{n+1}) &= (d + \kappa u_{n+1} \cdot \nabla d, \frac{2b_n - 1}{2} \frac{b_{n-1}}{\Delta t} \\
+ G_{n+1} \cdot \hat{b}_{n+1} - g(\hat{b}_{n+1})),
\end{align}

with prediction \( \hat{b}_{n+1} = 2b_n - b_{n-1} \). This two-step time-stepping scheme is started by using a first-order semi-implicit scheme in the first time step:

\begin{align}
(d + \kappa u_{n+1} \cdot \nabla d, \frac{b_{n+1}}{\Delta t} + u_{n+1} \cdot \nabla b_{n+1}) &= (d + \kappa u_{n+1} \cdot \nabla d, \frac{b_n}{\Delta t} + G_{n+1} \cdot b_n - g(b_n)).
\end{align}

3.3. Rotation reinitialisation of \( b \)

Very refined meshes to resolve the small length scales due to differences in the rotation of \( b \) between different parts of the flow, see Sec. 2.3, can be omitted if \( R \) in Eq. (11) is reset to the unit tensor \( I \) by computing \( V \), which leaves the conformation unchanged, see Eq. (4). To keep the second-order accuracy of the time-discretisation schemes presented in this section, \( b \) at the discrete times
$t_n$ and $t_{n-1}$ needs to be reset by the same rotation tensor for reinitialisation. Therefore, $V_n$ is computed in the nodes for resetting the rotation of $b_n$, whereas the rotation of the nodal values of $b_{n-1}$ is reset according to:

$$b'_{n-1} = b_{n-1} \cdot R_n^{-1}$$

$$= b_{n-1} \cdot (b_n^{-1} \cdot V_n),$$

where Eq. (11) has been used.

The reinitialisation is performed whenever a measure for the skew-symmetry of $b$ in practice exceeds a critical value anywhere in the entire domain. For this we use the quantity:

$$\|b_A\| \equiv \frac{\text{tr}(b_A \cdot b_A^T)}{\text{tr}(c)},$$

which is the squared magnitude of the skew-symmetric part of the contravariant deformation, $b_A = (b - b^T)/2$, normalised with the trace of the conformation. The value of $\|b_A\|$ is limited between 0 for a symmetric $b$ and 1 for a skew-symmetric $b$, see Appendix B. Choosing this criterion for reinitialisation is preferred over a strain criterion for instance, as $\|b_A\|$ not only contains the (affine) deformation but the relaxation as well.

4. Homogeneous flows

In order to compare the numerical accuracy of the $b$- and $c$-formulation of the UCM model (Eq. (7)), their evolution equations are integrated in time for a single point in simple-shear and uniaxial-extensional flow, respectively. For simple shear, a velocity gradient $\nabla u = \dot{\gamma} e_y e_x$ is imposed with (constant) shear rate $\dot{\gamma}$, while for uniaxial extension $\nabla u = i e_x e_x - \dot{\epsilon}/2(e_y e_y + e_z e_z)$ is used with (constant) extension rate $\dot{\epsilon}$. The material parameters used are $G = 1$ and $\lambda = 1$. A second-order BDF2 time-discretisation scheme with contravariant deformation prediction in the right-hand side of Eq. (3) is applied. For showing the results of these computations, we use the following notation for the first and second normal-stress difference $N_1$ and $N_2$, and definition of the Weissenberg
number Wi:

\[
N_1 = \tau_{xx} - \tau_{yy},
\]

(36)

\[
N_2 = \tau_{yy} - \tau_{zz},
\]

(37)

\[
Wi = \lambda \dot{\gamma} \quad \text{for simple shear flow},
\]

(38)

\[
Wi = \lambda \dot{\epsilon} \quad \text{for uniaxial extensional flow}.
\]

(39)

4.1. Contravariant deformation dynamics

The relevant components of \( \mathbf{b} \) for both simple shear at Wi = 1 and uniaxial extension at Wi = 0.1 are plotted in Fig. 1 as a function of time. The chosen time step is \( \Delta t = 1.25 \cdot 10^{-2} \lambda \), which is small enough to see no difference with the analytical solution in a graph. As already stated in Sec. 2.3, it can be seen that \( \mathbf{b} \) is not necessarily constant when the flow has reached a steady state with a constant stress (see also Figs. 2(a) and 3(a)). For extensional flow, the rotation rate is \( \dot{R} = 0 \) since \( \mathbf{L} \) and \( \mathbf{V} \) are diagonal (see Eqs. (12)-(13)), and the rotation can be chosen to be \( \mathbf{R} = \mathbf{I} \) for all times. Therefore, \( \mathbf{b} \) becomes indeed steady for long times, just as \( \mathbf{c} \). The components of \( \mathbf{b} \) are oscillatory in steady shear (see also Eq. (13)), due to the rotational nature of the shear flow. Their angular frequency \( \omega \) is in agreement with the analytical result from Eq. (14).

4.2. Convergence in time

For simple shear flow, the exact solutions for the shear stress and first normal-stress difference of the UCM model are given by

\[
\tau_{xy} = G\lambda(1 - e^{-t/\lambda}), \quad N_1 = 2G(\lambda \dot{\gamma})^2 \left[ 1 - e^{-t/\lambda} \left( 1 + \frac{t}{\lambda} \right) \right].
\]

(40)

The relative error in \( \tau_{xy} \) and \( N_1 \) for simple shear at Wi = 1 obtained from the \( \mathbf{b} \)-form is plotted in Fig. 2(a) as a function of time for various time steps. It can be seen that the error becomes constant when the stress reaches a steady state, which is caused by time-discretisation errors due to rotation of \( \mathbf{b} \) in steady shear, see Eq. (13). For showing convergence of the stress approximation towards
Figure 1: Relevant components of the contravariant deformation $b$ of the UCM model as a function of time for simple shear and uniaxial extension.
(a) Relative error in $\tau_{xy}$ (solid lines) and $N_1$ (dashed lines) with the $b$-formulation as a function of time for different time steps.

(b) Quantification of the error in stress obtained from $b$ and $c$ as a function of the inverse of the time step.

Figure 2: Calculations of UCM stress growth in simple shear at Wi = 1.
the exact solution, a quantification of the approximation error $\epsilon$ is calculated according to

$$
\|\epsilon\|_2 = \sqrt{\frac{\sum_{i=1}^{N} (s_i - s_{e,i})^2}{\sum_{i=1}^{N} s_{e,i}^2}},
$$

(41)

with $N$ the number of time steps, $s_i$ the approximation at time $t = t_i$ and $s_{e,i}$ the exact solution at $t = t_i$. It is plotted in Fig. 2(b) for $\tau_{xy}$ and $N_1$ as a function of the inverse of the time step with both the $b$- and $c$-form. It is observed that the error decreases quadratically with the inverse of the time step, as expected for this discretisation method. Additionally, it can be seen that the error is larger if it is calculated with $b$ in comparison to $c$, probably because the rotation of $b$ in steady shear leads to an additional approximation error. Reinitialising the rotation of $b$ - as described in Sec. 3.3 - after each update of $b$ proved to have no effect on the error for this homogeneous flow. Apparently, reinitialisation does not affect the time-discretisation error. Note, that reinitialisation does not affect the rotational dynamics that is encoded in the evolution equation for $b$; reinitialisation just resets the absolute rotation after every time step. This error also results in a non-zero $N_2$ approximation ($\tau_{yy} \neq 0$) with the $b$-formulation which converges quadratically to zero. A zero $N_2$ is the exact solution that is obtained for the calculation with the $c$-formulation for all $\Delta t$.

For uniaxial extension, the exact solution for the first normal-stress difference of the UCM model reads

$$
N_1 = \frac{G\dot{\lambda}}{(1 - 2\dot{\epsilon}\lambda)(1 + \dot{\epsilon}\lambda)} \left[ 3 - 2(1 + \dot{\epsilon}\lambda)e^{-t(1 - 2\dot{\epsilon}\lambda)/\lambda} - (1 - 2\dot{\epsilon}\lambda)e^{-t(1 + \dot{\epsilon}\lambda)/\lambda} \right].
$$

(42)

The relative error in $N_1$ of the approximations obtained with the $b$-form for $Wi = 0.1$ and different time steps $\Delta t$ is plotted in Fig. 3(a) as a function of time. It can be seen that after start-up of the flow, the error keeps decreasing with time, because a steady-state $b$ will eventually be obtained for extensional flow, see Eq. (13). In Fig. 3(b) where the quantification of the approximation error is plotted, it can be seen that the slope of $-2$ corresponding to the accuracy of the time integration, is again obtained. Moreover, the approximation errors
Figure 3: Calculations of UCM first normal-stress difference growth in uniaxial extension at Wi = 0.1.
with the $b$- and $c$-formulation for this rotation-free flow are nearly equal, which supports the above-mentioned statement that the rotation of $b$ contributes to the error.

Thus, the results in this section show that within numerical errors the $b$- and $c$-formulation of the UCM model are equivalent representations of that model.

5. Time-dependent stability in planar Couette flow

A planar Couette flow of a UCM fluid is considered, as illustrated in Fig. 4, which is known to be a stable flow [29]. A horizontal velocity $u = (1,0)$ is imposed on the top wall of the unit-square problem domain, while the bottom wall is stationary. The box is periodic in $x$-direction, generating a linear velocity profile between the walls. The Weissenberg number can then be defined as $Wi = \lambda \dot{\gamma} = \lambda$. The domain is periodic in $x$-direction so that fluid leaving the domain via the boundary $\Gamma_{p,r}$ re-enters via $\Gamma_{p,l}$ and that periodic copies of the box in horizontal direction can be imagined. Therefore, periodic boundary conditions for the velocity and

Figure 4: Schematic representation of the planar Couette flow of a UCM fluid. A horizontal velocity is imposed on the top wall of the unit-square problem domain while the bottom wall is stationary. The box is periodic in $x$-direction.
contravariant deformation are used:

\[ u|_{\Gamma_{p,l}} = u|_{\Gamma_{p,r}}, \quad (43) \]

\[ b|_{\Gamma_{p,l}} = b|_{\Gamma_{p,r}}, \quad (44) \]

As initial condition for \( b \), the square root of the exact solution for \( c \) of the UCM model in steady shear flow is taken. This is not a steady-state solution for the \( b \)-formulation, since \( b \) remains time dependent in steady shear, see Eq. (13).

The stability is investigated by applying a small random perturbation to the contravariant deformation, after which the perturbation of the conformation is followed in time. To this end, we added to all degrees of freedom of \( b \), a distinct pseudorandom number between 0 and 1 drawn from a uniform distribution, multiplied by \( 10^{-3} \). Since \( b \) remains unsteady, there is a time-discretisation error in \( c \) and therefore, some time is required for \( c \) to become steady before applying the perturbation. This error decreases quadratically with the inverse of the time step. The implicit stress formulation from Sec. 3.2.2 is used to integrate the flow equations forward in time with second-order accuracy. The mesh used consists of \( 20 \times 20 \) square elements. Reinitialisation of \( b \) as described in Sec. 3.3 is performed after every time step, but the stability is not affected by the frequency of reinitialisation.

To examine the stability of the numerical method for the planar Couette problem, a measure for the perturbation of the flow is calculated according to

\[ \| c - c_s \|_2 = \sqrt{\frac{1}{3N} \sum_i \left( (c_{xx,i} - c_{xx,s})^2 + (c_{xy,i} - c_{xy,s})^2 + (c_{yy,i} - c_{yy,s})^2 \right)}, \quad (45) \]

with \( c_{ab,i} \) a component of \( c \) in node \( i \), \( N \) is the number of nodes and \( c_{ab,s} \) is the field-maximum steady-state value of a \( c \)-component just before applying the perturbation. Fig. 5 shows \( \| c - c_s \|_2 \) for \( Wi = 10 \) as a function of time after the perturbation. Results are shown for \( \Delta t = 0.05 \lambda \) and two different choices for the velocity gradient in Eq. (32) are made, namely the direct velocity gradient \( (\nabla u)^T \) and the projected velocity gradient \( G \). It is observed that after an initial increase of \( \| c - c_s \|_2 \), the conformation perturbation magnitude decreases with
time for $L = G$ whereas for $L = (\nabla u)^T$ it keeps growing. This verifies that the time-dependent stability in shear flow for the $c$-formulation \[21, 22\] is kept for the $b$-formulation.

6. Flow around a cylinder with walls

The numerical stability and accuracy of the FEM solution for the 2D flow around a cylinder with wall confinement, obtained with the $b$-representation, are investigated and tested against the results with the $c$- and log $c$-representations. The problem is schematically depicted in Fig. 6. A stationary cylinder with radius $R$ is placed in the middle of a rectangular channel with walls $\Gamma_w$ at a distance of $H = 2R$ from the cylinder centre and having a length of $L = 30R$. A Cartesian coordinate system is introduced in the cylinder centre. The flow is generated by imposing a constant in time flowrate $Q$ while the pressure drop $\Delta p$ over the channel is computed. The periodic boundary conditions for the velocity, contravariant deformation and traction by which the channel is periodically
Figure 6: Schematic representation of the 2D flow around a stationary cylinder of radius $R$ confined between walls. The channel is periodic in $x$-direction and a constant flowrate is imposed.

extended in the $x$-direction, are:

$$u|_{\Gamma_{p,l}} = u|_{\Gamma_{p,r}}, \quad b|_{\Gamma_{p,l}} = b|_{\Gamma_{p,r}}, \quad t|_{\Gamma_{p,l}} = -t|_{\Gamma_{p,r}} - \Delta p n, \quad (46)$$

$$- \int_{\Gamma_{p,l}} u \cdot n \, dA = Q, \quad (47)$$

where $t = \sigma \cdot n$ is the traction with $n$ the outwardly-directed unit-normal vector.

The flow is assumed to be symmetric and therefore only half of the domain $\Omega$ is considered, whereas symmetry boundary conditions for the velocity and traction on the centreline $\Gamma_{cen}$ are used:

$$u_y = 0, \quad t_x = 0 \quad \text{on} \ \Gamma_{cen}, \quad (48)$$

where $t_x$ is the $x$-component of the traction. Furthermore, no-slip boundary conditions on the channel walls $\Gamma_w$ and cylinder wall $\Gamma_{cyl}$ are assumed:

$$u = 0 \quad \text{on} \ \Gamma_w \text{ and } \Gamma_{cyl}. \quad (49)$$

Although $b$ is allowed to be an arbitrary rotation tensor at time $t = 0$ for an initially stress-free fluid (see Eq. [4] and Eqs. [8] and [10]), the initial condition for $b$ is chosen to be

$$b(t = 0) = I \quad \text{in} \ \Omega, \quad (50)$$
for simplicity. The relevant dimensionless number of this problem is the Weis-
senberg number $Wi = \lambda U/R$, with $U$ the average velocity in the channel defined
as $U = Q/2H$.

6.1. Reinitialisation of the rotation of $b$

As discussed in Sec. 3.3, large gradients in $b$ occur if solving non-homogeneous
flow problems due to the rotation of $b$ in shear. To avoid these large gradients,
a reinitialisation of the rotation of $b$ is performed whenever a measure for the
skew-symmetry of $b$, namely $\|b_A\|$ in Eq. (35), exceeds a critical value. In Fig. 7
the maximum of $\|b_A\|$ in the domain is plotted as a function of the global strain
$tU/R$, with $U/R$ a global strain rate, for the Giesekus model with $\alpha = 0.01$ and
viscosity ratio $\nu = \eta_s/\eta_0 = 0.59$ and for two different values of $Wi$ using the
implicit stress formulation. It is observed that the domain-maximum of $\|b_A\|$}

{\begin{figure}[h]
\centering
\includegraphics[width=0.6\textwidth]{figure7.png}
\caption{Maximum in the domain of the normalised squared magnitude of the skew-symmetric
part of the contravariant deformation as a function of the global strain at two different Weis-
senberg numbers. No reinitialisation is performed. The mesh is M3 (see Table 1) and the
time step is $\Delta t = 0.01\lambda$.}
\end{figure}

approaches 1 at a higher strain for the higher value of $Wi$. In the following, reini-
tialisation is performed whenever $\|b_A\| \geq a$, with $0 \leq a < 1$ a certain threshold
value. The effect of reinitialisation on the accuracy of the solution can clearly
be observed in Fig. 8. In this figure, the maximum of the $\tau_{xx}$-component of the
Figure 8: Maximum of component $\tau_{xx}$ of the viscoelastic extra stress tensor in the domain as a function of time at $W_1 = 0.5$ for different threshold values $a$ for reinitialisation of the rotation of the contravariant deformation. Mesh M3 (see Table 1) and a time step of $\Delta t = 0.01\lambda$ are used for which convergence is obtained (see Sec. 6.2.1). Fig. (b) gives a zoom-in on the data.
viscoelastic extra stress tensor in the domain is plotted as a function of time at
$Wi = 0.5$ for different values of $a$. It can be seen that there is a relatively large
deviation in $\tau_{xx, \text{max}}$ for $a = 0.975$ from $\tau_{xx, \text{max}}$ for $a = 0$ (1% deviation max.)
in comparison with $\tau_{xx, \text{max}}$ for $a = 0.97$ (0.3% deviation max.). Compared to
no reinitialisation at all, the improvement is even more dramatic. This is shown
in Fig. 9, where the viscoelastic extra stress components are plotted for the case
that reinitialisation is performed at each time step and for no reinitialisation at all.

This section shows that the accuracy of the solution can be retained by lim-
iting the value of $\|b_A\|$ through reinitialising the rotation of $b$. In the following,
reinitialisation will be performed after every time step, implying that after doing
so, $b$ is symmetric and thus $\|b_A\| = 0$. The extra computation time needed to
reinitialise at each time step is negligible in the simulations performed for this
paper. It involves only algebraic operations on the nodal values of $b$.

### 6.2. Flow at low $Wi$

#### 6.2.1. Convergence tests

Convergence tests in space and time have been performed for the FEM
computations using the $b$-representation of the Giesekus model with non-linear
parameter $\alpha = 0.01$ as in [10], and viscosity ratio $\nu = \eta_s/\eta_0 = 0.59$, with
$\eta_0 = \eta_s + \lambda G$ the zero-shear viscosity. Results are shown for the implicit stress
formulation (see Sec. 3.2.2), though using the explicit stress formulation (see
Sec. 3.2.1) gives similar results. The flow is solved for a Weissenberg number of
$Wi = 0.5$. Table 1 gives the numerical parameters of the meshes that are used,
which are the same meshes as in [21].

In Fig. 10, the steady-state component $\tau_{xx}$ of the viscoelastic extra stress
tensor is plotted as a function of the horizontal coordinate on part of the centre-
line and on the cylinder wall for different meshes and a time step of $\Delta t = 0.01\lambda$.
It can be seen that $\tau_{xx}$ converges for meshes M3 and M4 with both the $b$-
(Fig. 10(a)) and log $c$-representation (Fig. 10(b)). This holds for the other
stress components and field variables as well.
(a) Component $\tau_{xx}$ of the viscoelastic extra stress tensor as a function of the $x$-coordinate on the centreline and cylinder wall at $t = 20\lambda$.

(b) Domain-maximum of the stress components as a function of time.

Figure 9: Effect of reinitialisation of the contravariant deformation on the solution of the flow around a cylinder with walls for $Wi = 0.5$ compared to no reinitialisation at all. Mesh M3 (see Table 1) and a time step of $\Delta t = 0.01\lambda$ are used for which the solution converges (see Sec. 6.2.1).

For checking the time convergence of the computations with the $b$-representation, the following quantification of the error in viscoelastic extra stress on the cen-
Table 1: Characteristics of the meshes generated by Gmsh [30], used for the flow around a cylinder confined between walls. The meshes, which are the same as in [21], are more refined near the cylinder wall and element sizes $h$ are halved at each refinement. $N_{\text{elem}}$ and $N_{\text{elem,cyl}}$ mean the total number of elements and the number of elements on the cylinder wall, respectively.

|   | $h_{\text{cyl}}$ | $h_{\text{wall}}$ | $h_{|x|=15R_{\text{wall}}}$ | $h_{|x|=15R_{\text{cen}}}$ | $N_{\text{elem}}$ | $N_{\text{elem,cyl}}$ |
|---|-----------------|-----------------|----------------|----------------|-----------------|----------------|
| M0 | 0.08            | 0.4             | 1.2            | 1.2            | 953             | 40             |
| M1 | 0.04            | 0.2             | 0.6            | 0.6            | 3467            | 79             |
| M2 | 0.02            | 0.1             | 0.3            | 0.3            | 13148           | 158            |
| M3 | 0.01            | 0.05            | 0.15           | 0.15           | 52053           | 315            |
| M4 | 0.005           | 0.025           | 0.075          | 0.075          | 205951          | 629            |

treline and cylinder wall with respect to a reference approximation is used,

$$\|\tau - \tau_{\text{ref}}\|_2 = \sqrt{\frac{\sum_{i=1}^{N} (\tau_i - \tau_{\text{ref},i})^2}{\sum_{i=1}^{N} \tau_{\text{ref},i}^2}}$$  \hspace{1cm} (51)$$

where $\tau_i$ and $\tau_{\text{ref},i}$ are the nodal values of a stress component for the approximation and the reference solution, respectively, and $N$ is the number of nodal points on the centreline and cylinder wall. The convergence is quadratic as is shown in Fig.11(a) where the steady-state $\|\tau - \tau_{\text{ref}}\|_2$ is plotted as a function of $\Delta t$, with $\tau_{\text{ref}}$ the approximation for $\Delta t = 0.0005\lambda$. This is a result of the second-order time discretisation of the constitutive equation. Fig.11(b) shows the same time-convergence plot as in Fig.11(a), but here for the explicit stress formulation. It can be seen that the rate of convergence is the same but the error is somewhat smaller than with the implicit stress formulation, shown in Fig.11(a).

A quantification of the difference in stress of the $b$-formulation with respect to the log $c$-formulation is plotted in Fig.12 as a function of $\Delta t$. As can be seen, convergence of the approximation with the $b$-form towards that with the log $c$-form is quadratic for larger $\Delta t$. However, a plateau in $\|\tau - \tau_{\text{ref}}\|_2$ is obtained at smaller values of $\Delta t$ since for these values of $\Delta t$ the time-discretisation error
Figure 10: Steady-state component $\tau_{xx}$ of the viscoelastic extra stress tensor as a function of the $x$-coordinate on the centreline and cylinder wall at $Wi = 0.5$ for both representations with the implicit stress formulation. Different meshes and a constant time step of $\Delta t = 0.01\lambda$ are used.

becomes of the same order of magnitude as the space-discretisation error. The plateau is due to the numerical difference between the $b$- and log $c$-formulation.

From the results in this section it can be concluded that the solutions for the explicit and for the implicit stress formulation using the $b$- as well as the
Figure 11: Quantification of the error in the steady-state viscoelastic extra stress components at the centreline and cylinder wall as a function of the inverse time step using the $b$-representation for $Wi = 0.5$ and mesh M3. The error is calculated with respect to a converged approximation for the implicit as well as the explicit stress formulation.
Figure 12: Quantification of the difference in steady-state viscoelastic extra stress components between the $b$- and $\log c$-representation at the centreline and cylinder wall as a function of the inverse time step $\Delta t$ for $Wi = 0.5$ and mesh M3 with the implicit stress formulation.

The $\log c$-representation converge to the same solution upon mesh and time-step refinement.

### 6.2.2. Comparison with literature

The accuracy of our numerical implementation of the $b$-representation using the explicit-stress formulation (see Sec. 3.2.1) has been tested against results from the literature obtained with various numerical techniques. For this purpose, the flow around a cylinder with wall confinement at low to moderate $Wi$ is solved for an Oldroyd-B fluid with viscosity ratio $\nu = 0.59$. Since for moderate $Wi$ the stress wake downstream of the cylinder extends along the centreline with respect to that obtained at the low $Wi = 0.5$, the mesh is refined near the entire centreline apart from the refinement near the cylinder wall. The characteristics of the meshes, which are comparable to the meshes in Table 1 and that are also used in [21], are given in Table 2.

Fig. 13 shows the $\tau_{xx}$-component as a function of the path length $s$ along the cylinder and centreline for $Wi = 0.5$ using different wake-refined meshes. The front and rear stagnation points are at $s = 0$ and $s = \pi R$, respectively. Convergence on the cylinder and in the wake are clearly visible. The same
Table 2: Characteristics of the meshes generated by Gmsh [30], used for the flow around a cylinder confined between walls at moderate and high Weissenberg number. The meshes, which are the same as in [21], are refined near the cylinder wall and the entire centreline. Element sizes \( h \) are halved at each refinement. \( N_{\text{elem}} \) and \( N_{\text{elem,cyl}} \) mean the total number of elements and the number of elements on the cylinder wall, respectively.

|     | \( h_{\text{cyl}} \) | \( h_{\text{wall}} \) | \( h_{|x|=15R,\text{wall}} \) | \( h_{|x|=15R,\text{cen}} \) | \( N_{\text{elem}} \) | \( N_{\text{elem,cyl}} \) |
|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| M0r | 0.08 | 0.4 | 1.2 | 0.08 | 3415 | 40 |
| M1r | 0.04 | 0.2 | 0.6 | 0.04 | 11491 | 79 |
| M2r | 0.02 | 0.1 | 0.3 | 0.02 | 42482 | 158 |
| M3r | 0.01 | 0.05 | 0.15 | 0.01 | 165097 | 315 |

Figure 13: Steady-state component \( \tau_{xx} \) of the viscoelastic extra stress as a function of the path length along the cylinder and centreline at \( Wi = 0.5 \). The front and rear stagnation points are at \( s = 0 \) and \( s = \pi R \), respectively. Different meshes are used (see Table 2) and the time step is \( \Delta t = 0.01 R/U \).
stress profile obtained with mesh M3r is compared to results from different studies in Fig. 14(a) and good graphical agreement is found. This becomes even more apparent in Fig. 14(b), where a zoom-in on the profile of Fig. 14(a) in the wake is shown.

For Wi = 0.6 a similar convergence of $\tau_{xx}$ on the cylinder as for Wi = 0.5
is observed in Fig. 15. In the wake, convergence is visible as well, yet $\tau_{xx}$ is somewhat more mesh dependent compared to $Wi = 0.5$ and it has not yet converged for the second-most refined mesh M2r. A comparison of the stress profile computed with mesh M3r for $Wi = 0.6$ with results from the literature is made in Fig. 16(a) and in Fig. 16(b), which gives a zoom-in on the profile of Fig. 16(a) in the wake. It can be seen that the results overlap quite well, even though [35] predicts a lower maximum on the cylinder. The differences are conjectured to be due to mesh dependency of the solutions.

A lack of convergence in the wake emerges when inspecting $\tau_{xx}$ on the cylinder wall and centreline for $Wi = 0.7$, which is revealed in Fig. 17(a) despite convergence on the cylinder. Nevertheless, a comparison is made between our computation of the stress profile with the most refined mesh M3r and in some cases mesh-dependent results from the literature for the most refined mesh, presented in Fig. 17(b). Good agreement between the calculated values is obtained on the cylinder while a relatively wide variety of values is noticed in the wake.

Figure 15: Steady-state component $\tau_{xx}$ of the viscoelastic extra stress as a function of the path length along the cylinder and centreline at $Wi = 0.6$. The front and rear stagnation points are at $s = 0$ and $s = \pi R$, respectively. Different meshes are used (see Table 2) and the time step is $\Delta t = 0.01R/U$. 
Figure 16: Comparison of $\tau_{xx}$ as a function of the path length along the cylinder and centreline with results from the literature for $Wi = 0.6$. The front and rear stagnation points are at $s = 0$ and $s = \pi R$, respectively. Fig. (b) gives a zoom-in on the profile in the wake. Mesh M3r is used (see Table 2) and the time step is $\Delta t = 0.01 R/U$.
Figure 17: Steady-state component $\tau_{xx}$ of the viscoelastic extra stress tensor as a function of the path length along the cylinder and centreline for $Wi = 0.7$. The front and rear stagnation points are at $s = 0$ and $s = \pi R$, respectively. The time step used is $\Delta t = 0.01 R/U$. 
6.3. Flow at higher $Wi$

The numerical stability of the solution of the flow around a confined cylinder at higher $Wi$ is checked by employing the explicit and implicit stress formulations for the Giesekus model, see Secs. 3.2.1, 3.2.2. The non-linear material parameter is set to $\alpha = 0.01$ and the viscosity ratio is chosen to be $\nu = 0.59$. Since for higher $Wi$ the stress wake downstream of the cylinder extends along the centreline with respect to that obtained at $Wi = 0.5$, the mesh is refined near the entire centreline apart from the refinement near the cylinder wall. The characteristics of the meshes, which are comparable to the meshes in Table 1 and that are also used in [21], are given in Table 2.

The solution will be called stable for a certain $Wi$ if it does not diverge, leading to breakdown of the simulation, during a simulation time of $t = 20\lambda$. Note that the solution can be unsteady yet still stable at higher $Wi$, although this fluctuating solution is probably a numerical artefact. The performance of the $b$- and log $c$-representations have been compared to that of the standard $c$-formulation for which the HWNP instability is known to occur at $Wi = \mathcal{O}(1)$. Different meshes and time steps have been used to validate the results.

The stability results are shown in Table 3 and are the same for the explicit and the implicit stress formulations. It seems that there is no limit for stability

|               | $Wi_{crit}$ | Mesh   | $\Delta t$ [R/U] |
|---------------|------------|--------|------------------|
| $c$           | 1.3-1.4    | M2r    | 0.02             |
| $c$           | 1.5-1.6    | M3r    | 0.02             |
| log $c$       | 50+        | M1r, M2r | 0.02            |
| $b$           | 50+        | M1r, M2r | 0.02            |

(we tested up to $Wi = 50$) when using the $b$- and log $c$-representations with the DEVSS-G/SUPG method, while the simulations with the $c$-representation
break down at \( Wi = 1.4 \) or 1.6 depending on the mesh. This indicates that the \( b \)-representation for this problem shows similar stability behaviour as the log \( c \)-representation. Fig. [18] shows \( \tau_{xx} \) as a function of the horizontal coordinate on the centreline and cylinder wall in steady state (although small fluctuations in the solution remain) at \( Wi = 50 \) for both the \( b \)- and log \( c \)-formulation. Note, that convergence has been obtained for neither of the formulations. Convergence would require very refined meshes to resolve the thin boundary layers if a physical solution even exists [37].

![Graph showing \( \tau_{xx} \) as a function of \( x/R \) for Wi = 50 for both representations.](image)

Figure 18: Steady-state component \( \tau_{xx} \) of the viscoelastic extra stress tensor as a function of the \( x \)-coordinate on the centreline and cylinder wall at \( Wi = 50 \) for both representations.

7. Conclusions

The new formulation for conformation-tensor based constitutive models for viscoelastic fluids, expressed in terms of the contravariant deformation, has been implemented in a numerical framework using the finite element method combined with DEVSS-G/SUPG stabilisation.

The \( b \)-formulation is proven to be stable in the perturbed planar Couette problem, tested at \( Wi = 10 \) for an UCM fluid. For the flow around a confined cylinder at low Weissenberg number (we tested \( Wi = 0.5 \)), the solution obtained with the \( b \)-representation and the log \( c \)-representation of the Giesekus model...
with $\alpha = 0.01$ and $\nu = 0.59$ converges to the same solution upon mesh and time-step refinement. Using the Oldroyd-B model, convergence of the solution is obtained until $Wi = 0.6$ and good agreement is found between our computations with the most refined mesh and results from the literature. Furthermore, the $b$-formulation of the same Giesekus model allows to simulate the flow way beyond the Weissenberg number at which the numerical instability occurs that causes the high Weissenberg number problem when using the standard $c$-formulation (we tested until $Wi = 50$), same as with the log $c$-formulation. The results obtained with the explicit and implicit stress formulations are the same in terms of stability, though the error with the implicit scheme is somewhat larger for the $b$-formulation.

The implementation of the $b$-formulation is similar to that of the standard $c$-formulation. Fully-implicit time integration of the flow equations using for example Newton-Raphson or other iteration methods, is straightforward and far less cumbersome than for the log $c$-representation [11, 12], the latter involving a spectral decomposition. Nevertheless, since $b$ remains unsteady in general flows, it is unclear how to search for a steady-state solution with Newton-Raphson iteration. Apart from that, application of the $b$-formulation to linear stability analysis, which generally requires a linearisation of the equations around a steady-state solution, might not be straightforward; this requires further study.

There are a few remarks to make concerning the application of the $b$-representation in numerical simulations. Firstly, it entails additional time-discretisation errors in a steady-state solution compared to the log $c$-formulation, since $b$ keeps rotating in shear. Reinitialisation of the rotation of $b$ in a field is needed to prevent the occurrence of large gradients in $b$ due to the rotation, retaining accuracy of the solution at negligible extra computational cost. Note that reinitialisation has no effect on the time-discretisation error, however, and for this reason it is not at all required for homogeneous flows.

Our results show that the $b$-formulation has a lot of potential in simulating viscoelastic flows due to a simpler implementation than the log $c$-formulation, yet providing similar stability.
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Appendix A. Rotation frequency of $b$ for the UCM model in steady shear

For determining the frequency of the rotation of the contravariant deformation tensor $b$ for the UCM model in steady shear from Eq. (13), an eigen decomposition of $V = \sqrt{c}$ is used according to

$$V = QDQ^T,$$

written in matrix notation. The columns of the orthogonal matrix $Q$, for which it holds that $QQ^T = I$, are the orthogonal eigenvectors of $V$, being the eigenvectors of the symmetric conformation matrix $c$. The matrix $D$ is diagonal with on its diagonal the corresponding eigenvalues of $V$, which are the square root of the eigenvalues of $c$, the latter being positive definite. Then, using a Cartesian coordinate system and defining $L_{xy} = \dot{\gamma}$ and $L_{xx} = L_{yx} = L_{yy} = 0$ for 2D simple shear flow, with $\dot{\gamma}$ the constant shear rate, Eq. (13) is written as

$$\dot{R}R^T = \frac{\dot{\gamma}}{2} \begin{pmatrix} 0 & v_y^2 \lambda_1/\lambda_2 + v_x^2 \lambda_2/\lambda_1 \\ -v_y^2 \lambda_1/\lambda_2 - v_x^2 \lambda_2/\lambda_1 & 0 \end{pmatrix},$$

where $\lambda_1, \lambda_2$ are the eigenvalues of $V$ and $v_x, v_y$ are, respectively, the $x$- and $y$-component of the eigenvector of unit length corresponding to the larger eigenvalue $\lambda_1$. Computing the eigenvalues and eigenvectors of $c$ for the UCM model in steady shear ($\dot{c} = 0$) and defining the Weissenberg number as $Wi = \lambda \dot{\gamma}$, the
angular frequency $\omega$, being the only independent non-zero component of $\dot{R}R^T$ in Eq. (A.2), can be expressed as

$$\frac{\omega}{\gamma} = \frac{1}{2\sqrt{W_1^2 + 1}}.$$  \hspace{1cm} (A.3)

**Appendix B. Quantification of skew-symmetry of $b$**

Any second-order tensor can be written as the sum of a symmetric part and a skew-symmetric part. Applying this to the contravariant deformation $b$ gives:

$$b = b_S + b_A = \frac{1}{2}(b + b^T) + \frac{1}{2}(b - b^T),$$  \hspace{1cm} (B.1)

with $b_S$ the symmetric part of $b$ and $b_A$ the skew-symmetric part. Substituting this, the quantity in Eq. (35) can be rewritten as:

$$\|b_A\| = \frac{\text{tr}(b_A \cdot b_A^T)}{\text{tr}(b_S^2) + \text{tr}(b_A \cdot b_A^T)},$$  \hspace{1cm} (B.2)

making use of $\text{tr}(b_S \cdot b_A^T) = \text{tr}(b_A \cdot b_S) = -\text{tr}(b_A \cdot b_S) = 0$ since $b_A^T = -b_A$. It can now be seen that $0 \leq \|b_A\| \leq 1$ for $b \neq 0$ as $\text{tr}(b_S^2) \geq 0$ and $\text{tr}(b_A \cdot b_A^T) \geq 0$. 

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