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Fully-implicit log-conformation formulation of constitutive laws

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ABSTRACT

Subject of this paper is the derivation of a new constitutive law in terms of the logarithm of the conformation tensor that can be used as a full substitute for the 2D governing equations of the Oldroyd-B, Giesekus and other models. One of the key features of these new equations is that – in contrast to the original log-conf equations given by Fattal and Kupferman (2004) – these constitutive equations combined with the Navier–Stokes equations constitute a self-contained, non-iterative system of partial differential equations. In addition to its potential as a fruitful source for understanding the mathematical subtleties of the models from a new perspective, this analytical description also allows us to fully utilize the Newton–Raphson algorithm in numerical simulations, which by design should lead to reduced computational effort. By means of the confined cylinder benchmark we will show that a finite element discretization of these new equations delivers results of comparable accuracy to known methods.

1. Introduction

Viscoelastic phenomena are important for a variety of industrial and medical applications, as, e.g., plastics profile extrusion and the design of blood pumps. Regardless of the application, the numerical simulation of flows of viscoelastic fluids often leads to difficulties, when the Weissenberg number, which relates the elastic forces to the viscous effects, is increased. This challenge has become known as the High Weissenberg Number Problem [1]. The difficulty is enhanced by the fact that it has so far not been sufficiently clarified whether the lack in simulation accuracy should be attributed to purely numerical deficiencies or is an inherent trait of the utilized constitutive models. One of the more recent approaches to resolve the former are the so-called log-conformation or shortly log-conf – formulations going back to [2].

The log-conf formulations are applicable to models of the form

$$\partial_t \boldsymbol{\sigma} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - (\nabla \boldsymbol{u})\boldsymbol{\sigma} - \boldsymbol{\sigma}(\nabla \boldsymbol{u})^T = -\frac{1}{\lambda} P(\boldsymbol{\sigma}), \tag{1}$$

where $\boldsymbol{u}$ is a d-dimensional velocity vector, $\boldsymbol{\sigma}$ the conformation tensor, λ the relaxation time and $P(\boldsymbol{\sigma})$ an analytic function. Examples are the Oldroyd-B model [3] with $P(\boldsymbol{\sigma}) = \boldsymbol{\sigma} - 1$ and the Giesekus model [4] with $P(\boldsymbol{\sigma}) = \boldsymbol{\sigma} - 1 + \alpha(\boldsymbol{\sigma} - 1)^2$ and the mobility factor $\alpha \in [0, 1]$. It has been shown in [5] that these models require that $\boldsymbol{\sigma}$ maintains positive-definiteness through time if the initial data is also positive-definite. A violation of this condition through the numerical algorithm has been observed to lead to unrecoverable failure of the simulation. The idea of the log-conf approach is to inherently respect this condition by replacing the original primal degrees of freedom, i.e., the conformation tensor $\boldsymbol{\sigma}$ or the polymeric stress $\boldsymbol{T}$, by a new field $\boldsymbol{\Psi}$ that is related to the conformation tensor by the matrix exponential function $\boldsymbol{\sigma} = \exp(\boldsymbol{\Psi})$; hence the name log-conformation formulation.

Of all possibilities, the choice of the exponential function as a means of assuring positive-definiteness can be fortified when considering the properties of Lie groups, which are manifolds with a group structure. An important class of Lie groups are the matrix groups, like the general linear group $GL(d, \mathbb{R})$, which consists of all invertible $d \times d$ matrices. In the constitutive equation, the tensorial degrees of freedom, like $\boldsymbol{\sigma}$, are part of a submanifold of $GL(d, \mathbb{R})$, which is constituted by the symmetric positive-definite matrices. This space is different as compared to the spaces containing the vectorial degrees of freedom, which are their own tangent space. The latter is not the case for general manifolds, as for example the symmetric positive-definite matrices. Nonetheless, the notion of the tangent space is important, since coordinate advancements within the tangent space of a manifold are guaranteed to remain within the manifold – an advantage when numerically advancing the coordinates. Fortunately, as $GL(d, \mathbb{R})$ is a Lie group the matrix exponential function maps the tangent

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space of the identity element – also known as the Lie algebra $\mathfrak{gl}(d,\mathbb{R}) = \mathbb{R}^{d\times d}$ – to the corresponding connected component of the Lie group. Furthermore, the subspace of the symmetric matrices of $\mathfrak{gl}(d,\mathbb{R})$ is mapped onto the symmetric positive-definite matrices, such that this particular subspace is the natural choice for a vector space for $\boldsymbol{\Psi}$. It should not be left unmentioned that one can still consider other functions than the matrix exponential function to ensure positive-definiteness, as is, e.g., done in [6] by the quadratic function.

Apart from the choice of a suitable transforming function, the more intricate task is the derivation of a replacement for the original constitutive equation that is formulated in terms of the new degrees of freedom. Several approaches have so far been described [2,7]. In [7], $\boldsymbol{\sigma}$ is replaced by $\exp\boldsymbol{\Psi}$ in the original constitutive equation in order to obtain the new equation. Although appealing at first sight, this approach advects $\exp\boldsymbol{\Psi}$ instead of $\boldsymbol{\Psi}$, leading to possible difficulties in the stabilization of the resulting numerical discretization [8]. [2] derives the new constitutive equation based on a decomposition of the velocity gradient $\nabla\boldsymbol{u}$. This decomposition leads to an equation with an intrinsically iterative character. In this paper we derive a new constitutive equation that has neither of these shortcomings. One of its key features is that it can be stated in a closed form together with the Navier–Stokes equations. The full derivation has so far been performed for two space dimensions, whereas the three-dimensional case is still subject to current research.

The procedure is outlined in the following fashion. The derivation of the new constitutive equation will be performed in Section 2 with the help of several lemmata, which can be found in Appendix A. Section 3 introduces the numerical implementation of this new method, which is subsequently verified by means of the well-known confined cylinder benchmark in Section 4. The results are compared to those in [9–11].

2. Log-conformation

For further calculations we will introduce the strain tensor

$$\varepsilon(\boldsymbol{u}) = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T),$$

as well as the vorticity tensor

$$\Omega(\boldsymbol{u}) = \frac{1}{2}(\nabla\boldsymbol{u} - \nabla\boldsymbol{u}^T),$$

such that we can rewrite Eq. (1) as

$$\partial_t\boldsymbol{\sigma} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{\sigma} - (\varepsilon(\boldsymbol{u}) + \Omega(\boldsymbol{u}))\boldsymbol{\sigma} - \boldsymbol{\sigma}(\varepsilon(\boldsymbol{u}) - \Omega(\boldsymbol{u})) = -\frac{1}{\lambda}P(\boldsymbol{\sigma}). \quad (2)$$

In this section we are going to show that if $\boldsymbol{\Psi}$ satisfies

$$\partial_t\boldsymbol{\Psi} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{\Psi} + [\boldsymbol{\Psi},\Omega(\boldsymbol{u})] - 2\sum_{n=0}^{\infty}\frac{B_{2n}}{(2n)!}\{\boldsymbol{\Psi},\varepsilon(\boldsymbol{u})\}_{2n} = -\frac{1}{\lambda}P(e^{\boldsymbol{\Psi}})e^{-\boldsymbol{\Psi}}, \quad (3)$$

then $\boldsymbol{\sigma} = \exp\boldsymbol{\Psi}$ satisfies the original constitutive Eq. (2). In Eq. (3), B_i denote the Bernoulli numbers, $[\boldsymbol{X},\boldsymbol{Y}] = \boldsymbol{XY} - \boldsymbol{YX}$ the usual commutator and $\{\boldsymbol{X},\boldsymbol{Y}\}_n$ the iterated commutator, which is defined as

$$\{\boldsymbol{X},\boldsymbol{Y}\}_n = [\boldsymbol{X},\{\boldsymbol{X},\boldsymbol{Y}\}_{n-1}]$$
$$\{\boldsymbol{X},\boldsymbol{Y}\}_0 = \boldsymbol{Y}.$$

Before we come to the proof we will first discuss some properties and prerequisites of this equation.

Remark 1 (*Sobolev spaces and Banach algebras*). The analysis of partial differential equations (PDEs) is highly entangled with the theory of Sobolev spaces. Therefore, we will assume that $\boldsymbol{\Psi}$ is contained in a Sobolev space. The first thing one realizes when looking at $\boldsymbol{\sigma} = \exp\boldsymbol{\Psi}$ is that one needs to make sense of the exponential mapping, which should also map, if possible, into the same Sobolev space. Mathematically speaking we need a Sobolev space that becomes, equipped with the pointwise matrix multiplication, a Banach algebra, such that we can define an analytical functional calculus (cf. [12, Theorem 10.27]). Restricting ourselves for the moment to the stationary problem and assuming that $\boldsymbol{\Psi} \in H^n\left(\mathbb{R}^d, \mathbb{R}^{\frac{d(d+1)}{2}}\right)$ it turns out to be sufficient to demand $n > d/2$ to make the components of $\boldsymbol{\Psi}$ lie within a Banach algebra [13, Theorem 4.39]. $\boldsymbol{\sigma}$, as well as $P(\boldsymbol{\sigma})$, would then also be contained in $H^n\left(\mathbb{R}^d, \mathbb{R}^{\frac{d(d+1)}{2}}\right)$.

Moving to the time-dependent setting, we are going to introduce the spaces

$$\begin{aligned}\mathcal{H} &= C^1([0,T], H^{s-1}(\Omega)) \cap C^0([0,T], H^s(\Omega))\\ \mathcal{H}' &= C^0([0,T], H^{s-1}(\Omega)),\end{aligned} \quad (4)$$

with $s > d/2$ and Ω being a Lipschitz-bounded domain. Here, the fact that the multiplications $H^{s-1}(\Omega)\times H^s(\Omega) \to H^{s-1}(\Omega)$ and $H^s(\Omega)\times H^s(\Omega)\to H^s(\Omega)$ are continuous [14, Corollary 1.1.1] lets us conclude that $\mathcal{H}$ denotes a Banach algebra. Furthermore, this multiplication can be extended to a continuous multiplication $\cdot : \mathcal{H}'\times\mathcal{H}\to\mathcal{H}'$. Now deriving the Banach algebra $H = \mathcal{H}^{d\times d}$ and Banach space $H' = \mathcal{H}'^{d\times d}$, as well as symmetrized variants thereof

$$H_{sym} = \{\boldsymbol{X}\in H | \boldsymbol{X}^T = \boldsymbol{X}\}$$
$$H'_{sym} = \{\boldsymbol{X}\in H' | \boldsymbol{X}^T = \boldsymbol{X}\},$$

we are going to search for solutions of Eq. (3) in H_{sym}. The space H' will serve as the Banach space containing the derivatives, since from $\boldsymbol{\Psi}\in H_{sym}$ it follows that $\partial_t\boldsymbol{\Psi}, \nabla\boldsymbol{\Psi} \in H'_{sym}$. Moreover, requiring $\varepsilon(\boldsymbol{u}) \in H'_{sym}$ lets us interpret all summands in Eq. (3) as elements of H'.

Allowing to formulate the theory in a Sobolev space setting is, from the theoretical point of view, one of the key advantages of our method compared to the original log-conf formulation [2], although one has to add that it is not restricted to the choice in (4) and there are other spaces that fulfill the requirements on $\mathcal{H}$ and $\mathcal{H}'$, fully listed in Appendix A. Examples are the smooth function spaces, in which all equations can be thought of as pointwise evaluations of the specific degrees of freedom. The latter is especially helpful for comprehension since most of the following proofs are purely algebraic in their nature.

Remark 2 (*Well-definedness of the series*). We have already outlined in the last paragraph that all summands of the series are elements of H'. What is left to consider is the absolute convergence of the series. It can be analyzed using the generating function definition of the Bernoulli numbers. Together with $B_1 = -\frac{1}{2}$ as the only non-zero odd Bernoulli number it can be stated as

$$\sum_{n=0}^{\infty}\frac{B_{2n}}{(2n)!}x^{2n} = \frac{x}{2} + \frac{x}{e^x - 1} \quad \forall |x| < 2\pi. \quad (5)$$

Furthermore, the inequality $\|[\boldsymbol{\Psi},\varepsilon(\boldsymbol{u})]_{2n}\|_{H'} \leqslant 2^{2n}\|\boldsymbol{\Psi}\|_H^{2n}\|\varepsilon(\boldsymbol{u})\|_{H'}$ and the fact that the Bernoulli numbers are alternating ($(-1)^{n+1}B_{2n} > 0$ if $n \geqslant 1$) guarantee that formula (3) is well-defined at least for $\|\boldsymbol{\Psi}\|_H < \pi$. Later we will alleviate this condition for the two-dimensional case.