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Numerical simulation of the viscoelastic flow in a three-dimensional lid-driven cavity using the log-conformation reformulation in OpenFOAM®

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ABSTRACT

In this work we implement the log-conformation reformulation for viscoelastic constitutive equations as proposed by Fattal and Kupferman (2004) in the open-source CFD-software OpenFOAM®, which is based on the collocated finite-volume method (FVM). The implementation includes an efficient eigenvalue and eigenvector routine and the algorithm finally is second-order accurate both in time and space, when using it in conjunction with an adequate convection scheme such as the CUBISTA scheme (Alves et al., 2003). The newly developed solver is first validated with the analytical solution for a startup Poiseuille flow of a viscoelastic fluid and subsequently applied to the three-dimensional and transient simulation of a lid-driven cavity flow, in which the viscoelastic fluid is modeled by the Oldroyd-B constitutive equation. The results are presented for both the first-order upwind scheme and the CUBISTA scheme on four hexahedral meshes of different size in order to check for mesh convergence of the results and a tetrahedral mesh to show the applicability to unstructured meshes. The results obtained for various values of the Weissenberg number are presented and discussed with respect to the location of the primary vortex center, streamline patterns and velocity and stress profiles besides others. We are able to obtain sufficiently mesh converged results for Weissenberg numbers, which would have been impossible to obtain without use of the log-conformation reformulation. An upper limit for the Weissenberg number in terms of stability could not be found.

1. Introduction

Simulation of complex viscoelastic flows at high Weissenberg numbers is an outstanding challenge. Fortunately, the last years provided significant progress in developing stable and accurate numerical algorithms [5,10,29]. Benchmark problems used in academia to test numerical algorithms include contraction flows [28,29], flows around spheres [30,17] and cavity flows [10,11,16] besides others.

Most of the work on cavity flows done so far was solely theoretically motivated, which is mainly because remarkably complex flow patterns develop in this very simple geometry [23]. Nevertheless, predicting and understanding the flow inside cavities is also of particular industrial relevance for short-dwell and flexible blade coaters [2]. Numerical simulation of the flow of a Newtonian fluid inside a cavity is straightforward and literature on that is exhausting, e.g. Sheu and Tsai [26], who studied the steady flow topology in a three-dimensional lid-driven cavity with a finite-element method at a Reynolds number of $Re = 400$. In contrast, predicting the flow of a viscoelastic fluid in a cavity is demanding and literature about that is few so far. A reason for the little interest may partly be due to the comparatively very low Weissenberg number that can be achieved. For example, Demir [8] studied the transient flow of a viscoelastic fluid governed by the upper convected Criminale–Ericson–Filbey (CEF) equation and the maximum Weissenberg number obtained was only $We_{max} = 0.01$ for all Reynolds numbers considered. Similar to others, Demir [8] imposed a uniform velocity at the moving lid, which leads to discontinuities at the two upper corners. This limits the maximum attainable Weissenberg number typically to below 0.2 [13]. More recent works impose regularized boundary conditions in order to have a vanishing velocity and velocity gradient at the two upper corners, see for example Fattal and Kupferman [11]. However, a thin boundary layer close to the lid and a singular point for the conformation

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tensor at the downstream upper corner remain, which still leave this problem to be difficult and pose an upper limit for the Weissenberg number [16].

Fattal and Kupferman [10,11] proposed the so-called log-conformation reformulation (LCR), in which a logarithmized evolution equation for the conformation tensor is solved instead of solving the constitutive equation itself. This removes the exponential variation of the stress (and also the conformation tensor) at stagnation points. The new variable (the logarithm of the conformation tensor) can better be approximated by polynomial-based interpolation schemes than the exponentially behaving conformation tensor (or stress) itself. A beneficial side-effect of this technique is that the positive-definiteness of the conformation tensor is always preserved. Fattal and Kupferman tested this technique for a two-dimensional viscoelastic cavity flow of a FENE-CR [10] and Oldroyd-B [11] fluid and they presented stable simulations up to a Weissenberg number of 5. Oscillations in the kinetic energy show the loss of convergence and the onset of a transient flow pattern for Weissenberg numbers above 3. Pan and Hao [25] applied the log-conformation technique in operator-splitting form to their finite-element code and simulated the two-dimensional Stokes flow of a viscoelastic fluid in a cavity up to a Weissenberg number of 3. They solve the logarithmized evolution equation for the conformation tensor on a coarser grid than the velocity, similar as it was done in the work of [10,11]. This reduces the number of high frequency modes, which, in turn, further stabilizes the solution of the logarithmized equation. A first-order upwind difference scheme was used for discretizing the advection term of the constitutive equation in that work. Upwind differencing, however, is known to be least accurate as it introduces a large amount of numerical diffusion, although this helps to stabilize the solution and significantly increases the maximum achievable Weissenberg number. Oliveira [23] used a finite-volume method to simulate the steady flow and the transient recoil of a FENE-CR fluid with a regularized boundary condition and a comparatively large retardation ratio of 0.79. The maximum Weissenberg number was 10 for creeping flow conditions ($Re = 0$). The advection term of the constitutive equation was discretized with the convergent and highly accurate CUBISTA scheme, which is formally of order three [3]. Yapici et al. [33] used a finite-volume method code, in which they also use the upwind scheme for treating the convective term in the constitutive equation. They performed simulations for the flow of an Oldroyd-B fluid in a cavity at different Reynolds numbers and presented results up to a Weissenberg number of 1 for creeping flow conditions.

In this work, the log-conformation reformulation is implemented in the collocated finite-volume based open-source software OpenFOAM®. Results are presented for the flow of an Oldroyd-B fluid in a startup Poiseuille flow and a three-dimensional cavity at creeping flow conditions. The remaining of this work is organized as follows: in Chapter 2 the governing equations are presented and the theory of the log-conformation approach is explained. In the following Chapter 3 the numerical implementation in OpenFOAM® is described. In Chapter 4 the results for the startup of Poiseuille flow and the three-dimensional lid-driven cavity are presented and discussed. Finally, in Chapter 5 this work ends with a summary.

2. Mathematical background

2.1. Governing equations

We consider the flow of an incompressible and isothermal viscoelastic fluid, which is governed by the Oldroyd-B constitutive equation [22]. The balance equations are the mass and momentum balance

$$\nabla \cdot \mathbf{U} = 0 \tag{1}$$

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

where $\mathbf{U}$ is the velocity, ρ is the density, t is time, p is pressure and $\boldsymbol{\tau}$ is the extra stress tensor, which can be written as the sum of a solvent and polymer contribution

$$\boldsymbol{\tau} = \boldsymbol{\tau}_S + \boldsymbol{\tau}_P \tag{3}$$

For the solvent contribution the Newtonian law holds

$$\boldsymbol{\tau}_S = \eta_S\left[\nabla \mathbf{U} + (\nabla \mathbf{U})^T\right] \tag{4}$$

where η_S is the solvent viscosity. For the polymeric contribution $\boldsymbol{\tau}_P$, the Olroyd-B equation may hold in this work, although it should be noted here that numerous other constitutive equations, such as the Giesekus, SPTT or FENE-type models as well as multi-mode models are forthcoming within this framework. The Oldroyd-B equation is defined as follows

$$\boldsymbol{\tau}_P + \lambda \overset{\triangledown}{\boldsymbol{\tau}}_P = \eta_P\left[\nabla \mathbf{U} + (\nabla \mathbf{U})^T\right] \tag{5}$$

where λ is the relaxation time and η_P is the polymer viscosity. $\overset{\triangledown}{\boldsymbol{\tau}}_P$ denotes the upper-convected time derivative

$$\overset{\triangledown}{\boldsymbol{\tau}}_P \equiv \frac{\partial \boldsymbol{\tau}_P}{\partial t} + \nabla \cdot (\mathbf{U}\boldsymbol{\tau}_P) - (\nabla \mathbf{U})^T \cdot \boldsymbol{\tau}_P - \boldsymbol{\tau}_P \cdot \nabla \mathbf{U} \tag{6}$$

The retardation ratio β is defined as the ratio between solvent viscosity η_S and total viscosity $\eta_0 = \eta_S + \eta_P$

$$\beta = \frac{\eta_S}{\eta_0} = \frac{\eta_S}{\eta_S + \eta_P} \tag{7}$$

The Oldroyd-B equation may be rewritten in terms of the conformation tensor $\mathbf{c}$

$$\boldsymbol{\tau}_P = \frac{\eta_P}{\lambda}(\mathbf{c} - \mathbf{I}) \tag{8}$$

where $\mathbf{I}$ is the identity matrix. Using Eq. (8) the constitutive equation Eq. (5) becomes

$$\frac{\partial \mathbf{c}}{\partial t} + \nabla \cdot (\mathbf{U}\mathbf{c}) - (\nabla \mathbf{U})^T \cdot \mathbf{c} - \mathbf{c} \cdot \nabla \mathbf{U} = \frac{1}{\lambda}(\mathbf{I} - \mathbf{c}) \tag{9}$$

Instead of Eq. (9) can be solved and subsequently the polymeric stress obtained with use of Eq. (8).

2.2. Log-conformation approach

The conformation tensor $\mathbf{c}$ is required to be strictly positive definite for the evolution equation Eq. (9) to be well-posed. In flows of high elasticity, this property may be violated, which often results in the numerical computation to fail. The main issue was shown for a 1-D problem [11]: in areas of high deformation rates the stretching and relaxation terms exhibit exponential growth. The only term to balance this growth is the convection term. However, since the convection term is based on polynomial interpolations, the convection term fails to balance the exponential amplification, which then results in the numerical simulation to blow up. To cope with this instability, Fattal and Kupferman [10] suggested a logarithmic transformation of Eq. (9), which became known as the 'log-conformation approach' and will shortly be outlined in the following.

Since the conformation tensor $\mathbf{c}$ is a symmetric positive-definite (SPD) matrix, it can be diagonalized according to

$$\mathbf{c} = \mathbf{R} \cdot \boldsymbol{\Lambda} \cdot \mathbf{R}^T \tag{10}$$

$\boldsymbol{\Lambda}$ is a diagonal matrix consisting of the three eigenvalues of $\mathbf{c}$ on the diagonal and $\mathbf{R}$ is an orthogonal matrix, which is formed by the three eigenvectors of $\mathbf{c}$. Any diagonal matrix can be logarithmized