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Multiscale simulations of three-dimensional viscoelastic flows in a square–square contraction

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ABSTRACT

We apply the multiscale FENE model to a 3D square–square contraction flow problem and to two 2D benchmark experiments. For this purpose, we couple the stochastic Brownian configuration field method (BCF) with our fully parallelized three-dimensional Navier–Stokes solver NaSt3DGPF. The robustness of the BCF method enables the numerical simulation of higher Deborah number flows for which most macroscopic methods suffer from stability issues. We validate our implementation by investigating the numerical error for a 2D viscoelastic Poiseuille flow that has an analytical solution. Furthermore, we compare the FENE model with the FENE-P closure for a two-dimensional 4 : 1 contraction flow. We then compare the results of our 3D simulations with that of experimental measurements from literature and obtain a very good agreement. In particular, we are able to reproduce effects such as strong vortex enhancement, streamline divergence and flow inversion for highly elastic flows. Due to their computational complexity, our simulations require massively parallel computations. To this end, we use a domain decomposition approach with MPI.

1. Introduction

The macroscopic mathematical modeling of dilute viscoelastic fluids usually involves an additional stress tensor in the Navier–Stokes equations and the solution of a differential or integral constitutive equation to compute the stress tensor entries. Here, the Oldroyd-B model can be employed. It originates from a two-bead dumbbell model with a linear Hookean spring force. Despite its shortcoming to describe extensional flows accurately, it is widely used for simulating dilute polymeric fluids. Other constitutive models for dilute polymeric fluids include the FENE-P model of Peterlin [1] and the FENE-L model of Lielens et al. [2]. Both models are simplifications, obtained with closure approximations, of a two-bead dumbbell system connected with a **f**initely **e**xtensible **n**onlinear **e**lastic (FENE) spring. In the literature, there is no known direct constitutive model for the FENE spring so far and it is widely assumed that it does not exist. An extensive description of constitutive models is given in the book by Owens and Phillips [3].

More advanced multiscale approaches have been recently developed that directly solve the kinetic equations of the microscopic system. In this case, the macroscopic stress tensor results from the internal configurations of the underlying molecular system. Using this ansatz avoids further closure errors but yields the mathematical problem of adequately modeling the internal orientations. Biller and Petruccione theoretically investigated this approach in their pioneering work in 1988 [4]. A detailed overview of micro-macro approaches is given in a general survey by Keunings [5].

Representing polymer molecules by a system of beads connected with massless springs leads to a high-dimensional diffusion equation, the Fokker–Planck equation, that describes the evolution of the configuration probability density function (cf. [6]). Then, Kramers' formula connects the stress tensor with the expectation of the instantaneous polymer configuration. Even for a simple dumbbell system, the Fokker–Planck equation for non-homogeneous, three-dimensional flow systems is six-dimensional. Three dimensions are needed for the physical space of the flow system and three dimensions are needed to describe the dumbbell's internal orientation which is referred to as configuration space. More complex multi-bead systems involve configuration spaces of higher dimensionality and require special numerical treatment to reduce the curse of dimensionality. Chauviére and Lozinski [7] proposed a first-order operator splitting of the Fokker–Planck equation to separate operator treatment in the physical space from that of the configuration space [8,9]. They applied their spectral method approach to two- and three-dimensional configuration

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spaces and non-homogeneous two-dimensional physical spaces. Recently, Knezevic and Süli [10] used a similar technique that is based on a spectral Galerkin discretization with weighted ansatz and test functions in configuration space and a three-dimensional finite element discretization in physical space. A promising new approach to deal with configuration spaces of up to twenty dimensions is the Proper Generalized Decomposition (PGD) method (cf. [11]). So far, the solution in high-dimensional configuration spaces with the PGD approach has been primarily applied to homogeneous flow problems that are simple in the flow space. The most advanced implementation which we are aware of is a two-dimensional contraction flow problem considered in Mokdad et al. [12].

A more common method for multiscale viscoelastic flow simulations is based on the theory of stochastic calculus. The main idea is to rewrite the Fokker–Planck equation as a formally equivalent stochastic differential equation in which a Wiener process models the Brownian forces acting on the polymer. Numerical treatment of stochastic differential equations normally leads to stochastic noise in the stress tensor solution. On the other hand, stochastic approaches are more adapted to higher Weissenberg or Deborah number flows than comparable methods as noted by Mangoubi et al. [13]. Furthermore, they are, due to their intrinsic Monte-Carlo method, less affected by the curse of dimensionality than deterministic Fokker–Planck based methods in high-dimensional configuration spaces.

In 1993, Laso and Öttinger [14] introduced the particle-based CONNFFESSIT method (**C**alculation **o**f **N**on-**N**ewtonian **F**low: **F**inite **E**lements and **S**tochastic **Si**mulation **T**echniques) and applied it to two-dimensional flow problems. In this approach, a large number of sample particles in the flow domain approximates the stochastic process numerically. Each particle, representing a polymeric configuration, moves within the physical flow domain. Using Monte-Carlo integration, we obtain the stress tensor as the first moment of the particle orientations. However, the method exhibits several shortcomings such as wild spatial fluctuation of the stress tensor which is caused by a non-uniform particle density and uncorrelated Brownian forces acting on individual sample particles (cf. [15]).

A different stochastic approach, the Brownian configuration field (BCF) method by Hulsen et al. [16], significantly reduces the drawbacks of CONNFFESSIT by using an Eulerian particle description. The BCF method uses a uniform number of configuration fields at fixed spatial positions to ensure a homogeneous polymeric density in physical space. Furthermore, it assumes locally correlated Brownian forces which leads to a uniform stress tensor field in the flow space. According to Bonvin and Picasso [17], this simplification might reduce the global accuracy of the stress tensor field. On the other hand, the spatial smoothness of the BCF method leads to a considerably increased stability of the numerical scheme.

Multiscale simulations involve an increased computational effort compared to purely macroscopic approaches. Therefore, most micro-macro simulations are so far restricted to homogeneous flow fields or two-dimensional physical spaces (cf. [18], Prieto et al. [19], Koppol et al. [20,21] and Smith and Sequeira [22]). To the best of our knowledge, Ramírez and Laso [23] performed the first three-dimensional stochastic BCF simulations and only recently Knezevic and Süli [10] accomplished the first three-dimensional simulation for a coupled Fokker–Planck and Stokes flow system. In both cases, the authors parallelized their algorithms to reduce computing time.

In the following, we present the first 3D multiscale FENE simulations using the BCF approach for square–square contraction flows and compare our results with that from laboratory experiments. Our multiscale simulations are more stable than comparable macroscopic flows with high Deborah numbers.

The remainder of this article is organized as follows: First, we consider the governing equations on the macro- and micro-scale in Section 2. We then describe adequate initial conditions for the stochastic equations in the case of a Hookean and a FENE dumbbell system. In Section 3 we discuss spatial and temporal discretization schemes of the Navier–Stokes, Oldroyd-B and stochastic differential equations. Furthermore, we describe our domain decomposition approach to enable parallel computation using MPI and consider variance reduction techniques. In Section 4.1, we investigate the numerical error for a 2D viscoelastic Poiseuille flow that has an analytical solution in the Oldroyd-B/Hookean dumbbell case. We then consider two-dimensional contraction flows for the FENE and FENE-P model in Section 4.2 for which published simulation results are available. Moreover, we present the results of 3D square–square contraction flows in Section 4.3 and compare them with those from literature. At last, we evaluate our findings and discuss possible extensions.

2. Governing equations for the micro-macro model

Throughout this article, we consider fluid flow in a bounded domain $\Omega \subset \mathbb{R}^3$ and refer to Ω as physical space. For any position $\boldsymbol{x} \in \Omega$ and any time $t \in (0, T] \in \mathbb{R}$, the fluid velocities $\boldsymbol{u}(\boldsymbol{x}, t) \in \mathbb{R}^3$ and the hydrodynamic pressure $p(\boldsymbol{x}, t) \in \mathbb{R}$ combined with appropriate boundary conditions fully describe the current state of a purely Newtonian system. We first give the Navier–Stokes and the stress tensor equations on the macro-scale. Subsequently, we specify the alternative stress tensor approaches on the micro-scale that either involve a Fokker–Planck or a stochastic differential equation.

2.1. Macroscopic equations

On the macroscopic scale, conservation of momentum and mass for an incompressible and isothermal viscoelastic one-phase flow is given by the coupled system of equations

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla p + \eta_s \Delta \boldsymbol{u} + \nabla \cdot \boldsymbol{\tau}_p, \tag{1}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{2}$$

with $\rho \in \mathbb{R}^+$ as the fluid density, $\eta_s \in \mathbb{R}^+$ as solvent viscosity, and $\boldsymbol{\tau}_p$ as the second-order tensor for the polymeric stress contribution.

These equations are coupled with initial conditions

$$\begin{aligned} &\boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0(\boldsymbol{x}), \\ &p(\boldsymbol{x}, 0) = p_0(\boldsymbol{x}), \\ &\boldsymbol{\tau}_p(\boldsymbol{x}, 0) = \boldsymbol{\tau}_0(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega, \end{aligned}$$

with one of the following conditions for the velocity field on the boundary $\partial\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$

$$\begin{aligned} &\boldsymbol{u}|_{\Gamma_1} = \boldsymbol{u}_0 \qquad \text{inflow boundary } \Gamma_1, \\ &\boldsymbol{u}|_{\Gamma_2} = 0 \qquad \text{no-slip boundary } \Gamma_2, \\ &\partial_{\boldsymbol{n}}(\boldsymbol{u} \cdot \boldsymbol{n})|_{\Gamma_3} = 0,\ \partial_{\boldsymbol{n}}(\boldsymbol{u} \cdot \boldsymbol{t})|_{\Gamma_3} = 0 \qquad \text{outflow boundary } \Gamma_3. \end{aligned}$$

Here, $\boldsymbol{n}$ denotes the outward pointing unit normal and $\boldsymbol{t}$ denotes the tangential vector on $\partial\Omega$, respectively.

On the macro-scale we consider the Oldroyd-B model. It is equivalent to a Hookean dumbbell system on the micro-scale. First, for an arbitrary second-order tensor $\boldsymbol{A}$ we define the upper convected derivative or Oldroyd derivative as

$$\overset{\triangledown}{\boldsymbol{A}} \equiv \frac{\partial \boldsymbol{A}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{A} - \nabla \boldsymbol{u} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot (\nabla \boldsymbol{u})^T.$$

Then, the Oldroyd-B model takes the form

$$\boldsymbol{\tau}_p + \lambda \overset{\triangledown}{\boldsymbol{\tau}}_p = 2\eta_p \boldsymbol{D}, \tag{3}$$

with the symmetric deformation tensor