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Multiscale simulation of polymeric fluids using the sparse grid combination technique

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ABSTRACT

We present a computationally efficient sparse grid approach to allow for multiscale simulations of non-Newtonian polymeric fluids. Multiscale approaches for polymeric fluids often involve model equations of high dimensionality. A conventional numerical treatment of such equations leads to computing times in the order of months even on massively parallel computers.

For a reduction of this enormous complexity, we propose the sparse grid combination technique. Compared to classical full grid approaches, the combination technique strongly reduces the computational complexity of a numerical scheme but only slightly decreases its accuracy.

Here, we use the combination technique in a general formulation that balances not only different discretization errors but also considers the accuracy of the mathematical model. For an optimal weighting of these different problem dimensions, we employ a dimension-adaptive refinement strategy. We finally verify substantial cost reductions of our approach for simulations of non-Newtonian Couette and extensional flow problems.

1. Introduction

Many fluids from the chemical industry and from nature show a non-Newtonian behavior. In the literature, the modeling of non-Newtonian fluids is usually based on an additional elastic stress tensor in the fluid equations. Then, macroscopic approaches compute the entries of this stress tensor by solving an additional differential or integral constitutive equation. An overview of macroscopic approaches is given in the book by Owens and Philips [1].

Macroscopic models have a low computational complexity but exhibit two serious drawbacks: They are prone to numerical instabilities, the so called *High Weissenberg number problem* (HWNP), and they have limited modeling capabilities. Both drawbacks can be avoided in a multiscale approach. There, the kinetic equations of the microscopic polymeric structure are directly modeled which allows for a better description of real polymers. Furthermore, immunity to the type of instability caused by the HWNP seems to result, as reported by Mangoubi et al. [2]. A more detailed explanation of multiscale models can be found in a survey by Keunings [3].

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Despite their advantages compared to macroscopic models, multiscale models are hardly used in practical applications. This is due to their enormous computational complexity. Depending on the degrees of freedom of the polymeric microstructure, the configuration space for the polymer model can be high-dimensional. For instance, it is of dimensionality fifteen for a model that consists of five spring segments. This leads to an exponential growth in the complexity of grid-based numerical approaches which is often described by the term *curse of dimensionality*.

In the following, we aim for a reduction of this multiscale model complexity. For this purpose, we employ the sparse grid combination technique to cope with the curse of dimensionality. The combination technique [4] is a specific sparse grid representation [5]. The basic idea is to linearly combine a sequence of coarse grid numerical solutions to approximate a numerical solution on a fine grid. Since an optimal balancing of the different problem dimensions is not a priori clear, we employ a dimension-adaptive refinement strategy for the combination technique. Furthermore, our novel approach balances not only errors that result from the discretization schemes but also considers the error of the modeling equation which stems from the choice of the spring-chain length.

The first application of sparse grids to non-Newtonian fluids was given by Delaunay et al. [6]. In contrast to our stochastic polymer model, the authors employ a deterministic Fokker–Planck-based approach to model the high-dimensional configuration space. Furthermore, there exist several literature results on sparse grids for Newtonian fluids, see, e.g., Griebel and Koster [7] for results on turbulent flows. An alternative approach in the literature to cope with the high complexity of multiscale non-Newtonian models is the proper generalized decomposition (PGD). The PGD is a model reduction technique that bases on a separated representation of the unknown field. An overview of the PGD for applications related to non-Newtonian fluids is given by Chinesta et al. [8].

The remainder of this article is organized as follows: First, in Section 2, we discuss the governing equations of our multiscale polymer model. Then, in Section 3 we cover techniques related to the numerical treatment of the high-dimensional equations. This includes the spatial and temporal discretization of the partial and stochastic differential equations in Section 3.1 and the dimension-adaptive combination technique in Section 3.2. Finally in Section 4, we present the resulting numerical outcomes for Couette and extensional flows. Moreover, we verify that our approach actually reduces the complexity compared to classical full grid approaches.

2. Governing equations for the multiscale model

We investigate fluid flow in a bounded domain $\mathcal{O} \subset \mathbb{R}^d$ with $d = 1, 2, 3$ depending on the specific application and refer to $\mathcal{O}$ as physical space. For given position $\boldsymbol{x} \in \mathcal{O}$ and at any time $t \in \mathcal{T} = [0, T] \subset \mathbb{R}$ the current state of a non-Newtonian fluid is described by the fluid's velocity field $\boldsymbol{u} : (\boldsymbol{x}, t) \in \mathcal{O} \times \mathcal{T} \mapsto \boldsymbol{u}(\boldsymbol{x}, t) \in \mathbb{R}^d$, the hydrodynamic pressure field $p : (\boldsymbol{x}, t) \in \mathcal{O} \times \mathcal{T} \mapsto p(\boldsymbol{x}, t) \in \mathbb{R}$ and the polymeric stress tensor field $\boldsymbol{\tau_p} : (\boldsymbol{x}, t) \in \mathcal{O} \times \mathcal{T} \mapsto \boldsymbol{\tau_p}(\boldsymbol{x}, t) \in \mathbb{R}^{3\times 3}$ with corresponding initial and boundary conditions.

The dimensionless conservation of mass and momentum is given by the coupled system

$$\frac{\partial \boldsymbol{u}(\boldsymbol{x}, t)}{\partial t} + (\boldsymbol{u}(\boldsymbol{x}, t) \cdot \nabla)\boldsymbol{u}(\boldsymbol{x}, t) = -\nabla p(\boldsymbol{x}, t) + \frac{\beta}{Re}\Delta \boldsymbol{u}(\boldsymbol{x}, t) + \frac{1}{Re}\nabla \cdot \boldsymbol{\tau}_p(\boldsymbol{x}, t) \tag{1}$$

$$\nabla \cdot \boldsymbol{u}(\boldsymbol{x}, t) = 0 \tag{2}$$

Eq. (1) contains the dimensionless parameters Re (Reynolds number) and β (viscosity ratio). They are defined as

$$Re = \frac{\rho_c U_c L_c}{\eta_s + \eta_p}, \qquad \beta = \frac{\eta_s}{\eta_s + \eta_p} \tag{3}$$

with the characteristic units $L_c \in \mathbb{R}^+$ (characteristic length in macroscopic flow), $U_c \in \mathbb{R}^+$ (characteristic fluid velocity), $\rho_c \in \mathbb{R}^+$ (fluid density, scaling pressure term with $1/(\rho {U_c}^2)$), $\eta_s \in \mathbb{R}^+$ (Newtonian dynamic viscosity) and $\eta_p \in \mathbb{R}^+$ (zero shear rate polymer dynamic viscosity).

These equations are coupled with the initial conditions $\boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0(\boldsymbol{x})$, $p(\boldsymbol{x}, 0) = p_0(\boldsymbol{x})$ and $\boldsymbol{\tau}_p(\boldsymbol{x}, 0) = \boldsymbol{\tau}_0(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathcal{O}$. Furthermore, one of the conditions

$$\boldsymbol{u}|_{\Gamma_1} = \boldsymbol{u}_0 \qquad \text{on the inflow boundary } \Gamma_1, \tag{4a}$$

$$\boldsymbol{u}|_{\Gamma_2} = 0 \qquad \text{on the no-slip boundary } \Gamma_2, \tag{4b}$$

$$\partial_{\boldsymbol{n}}(\boldsymbol{u} \cdot \boldsymbol{n})|_{\Gamma_3} = 0,\ \partial_{\boldsymbol{n}}(\boldsymbol{u} \cdot \boldsymbol{t})|_{\Gamma_3} = 0 \qquad \text{on the outflow boundary } \Gamma_3 \tag{4c}$$

holds for the velocity field on the boundary $\partial\mathcal{O} = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ with $\boldsymbol{n}$ as outward pointing unit normal and $\boldsymbol{t}$ as tangential vector on $\partial\mathcal{O}$.

The polymeric stress tensor $\boldsymbol{\tau}_p$ reflects the elastic stress contribution from the underlying polymeric structure. In a multiscale approach, the microscopic structure is modeled as an arrangement of $N + 1$ beads that are connected with N elastic springs. We illustrate the resulting multi-bead spring-chain in Fig. 1. A chain is fully described by its center position $\boldsymbol{x} \in \mathcal{O}$

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