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Active learning of constitutive relation from mesoscopic dynamics for macroscopic modeling of non-Newtonian flows ☆

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ABSTRACT

We simulate complex fluids by means of an on-the-fly coupling of the bulk rheology to the underlying microstructure dynamics. In particular, a continuum model of polymeric fluids is constructed without a pre-specified constitutive relation, but instead it is actively learned from mesoscopic simulations where the dynamics of polymer chains is explicitly computed. To couple the bulk rheology of polymeric fluids and the microscale dynamics of polymer chains, the continuum approach (based on the finite volume method) provides the transient flow field as inputs for the (mesoscopic) dissipative particle dynamics (DPD), and in turn DPD returns an effective constitutive relation to close the continuum equations. In this multiscale modeling procedure, we employ an active learning strategy based on Gaussian process regression (GPR) to minimize the number of expensive DPD simulations, where adaptively selected DPD simulations are performed only as necessary. Numerical experiments are carried out for flow past a circular cylinder of a non-Newtonian fluid, modeled at the mesoscopic level by bead-spring chains. The results show that only five DPD simulations are required to achieve an effective closure of the continuum equations at Reynolds number $Re = 10$. Furthermore, when Re is increased to 100, only one additional DPD simulation is required for constructing an extended GPR-informed model closure. Compared to traditional message-passing multiscale approaches, applying an active learning scheme to multiscale modeling of non-Newtonian fluids can significantly increase the computational efficiency. Although the method demonstrated here obtains only a local viscosity from the polymer dynamics, it can be extended to other multiscale models of complex fluids whose macro-rheology is unknown.

1. Introduction

The main motivation for investigating non-Newtonian fluids is that no fluid is virtually Newtonian except some simple fluids such as air and water [1]. The distinguishing feature of non-Newtonian fluids is that the microstructures present in

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variable rheological conditions are not only transient but can be easily changed by the application of low stresses [2]. Consequently, non-Newtonian fluids usually have complex stress-strain rate relationships and their apparent viscosities depend on the transient shear rate. In particular, polymeric fluids are the most widely used industrial non-Newtonian fluids. Their non-Newtonian behavior stems from the chain-like molecular structure of polymers, whose length can be so long that the collective effect of structural reorganization of polymer chains affects the macroscale rheological properties [3]. Moreover, because the forces generated by the polymer relaxation depend on its original orientation, polymeric fluids can also exhibit significant memory effects, i.e., the stress tensor depends on the strain history [4]. As a result, unlike the linear constitutive relation of Newtonian fluids, the constitutive equation of non-Newtonian fluids becomes much more complicated [5], which makes the modeling of non-Newtonian fluids a challenging problem.

In continuum approaches, an expression for the stress tensor in terms of various kinematic tensors is needed in the momentum equation and also in the energy equation [6]. This problem is similar to that arising in modeling turbulent flows [7], where an empirical model is needed for computing the Reynolds stress tensor for subgrid contributions to shear stress. Under the continuum hypothesis, various phenomenological models for the constitutive relation of non-Newtonian fluids have been developed to close the continuum equations. Examples include the power-law and Bingham plastics models [8], the Oldroyd-B model [9], the finitely extensible non-linear elastic-Peterlin (FENE-P) model [10,11] and the Phan-Thien–Tanner model [12], to name but a few.

Because the non-Newtonian properties are strongly related to the dynamics of underlying microscopic structures, it is a straightforward idea to couple the rheology of non-Newtonian fluids and the microscopic physics using multiscale simulations, in which a continuum approach is used to model the bulk behavior of polymeric fluids, while a microscopic model is used to describe the dynamics of underlying microstructures. In the present work, a microscopic model refers to an atomistic approach that completely resolves all the details of atoms; a mesoscopic model refers to a coarse-grained approach that drastically simplifies the atomistic dynamics by averaging out fast atomic motions and preserving collective molecular behaviors with fluctuations at a coarse-grained level; a macroscopic model refers to a continuum deterministic approach derived from the continuum hypothesis that neglects all molecular details and stochastic effects. Many research efforts have been devoted to coupling continuum equations to micro/meso-scale simulations. Bell et al. [13] combined a spectral method and Brownian dynamics to investigate the recovery of polymeric fluids after the cessation of shear flow. Wagner and Liu [14] coupled continuum finite elements to molecular dynamics (MD) simulations, and tested their scheme on a one-dimensional lattice; Kojic et al. [15] then extended it by coupling finite elements to dissipative particle dynamics (DPD) simulations for simple fluids. Using the idea of domain decomposition, Fedosov and Karniadakis [16] developed a hybrid multiscale method (triple-decker) to concurrently couple atomistic–mesoscopic–continuum models, and Li et al. [17] coupled DPD simulations and a finite element method for the Couette flows of polymer solutions. Also, Moreno et al. [18] coupled a finite element model with smoothed DPD to capture the non-Newtonian behavior of blood flowing through arteries. Recently, Barnes et al. [19] constructed an effective equation of state for a finite element model from DPD simulations.

In general, there exist three main categories of multiscale approaches, namely sequential approaches, concurrent couplings and adaptive resolution schemes [20,21]. In concurrent coupling and adaptive resolution schemes the time step is limited by the time step used for microscopic simulations, while the sequential approach also known as message-passing is more suitable for multiscale problems with apparent scale separation between macroscopic and microscopic systems [20]. In the present work, we consider the continuum system to be much larger than its microscopic counterpart, so that a macroscale element is large enough to contain a representative sample of the micro-system. Specifically, the continuum equations are solved by the finite volume method (FVM) whose benefits are both high computational efficiency and numerical stability. The polymer fluid is modeled by bead-spring chains whose coarse-grained dynamics are computed by DPD – a method well suited for modeling mesoscopic phenomena with much greater efficiency than all-atom molecular dynamics [22–25].

In the multiscale coupling procedure, the continuum model of polymeric fluids will be constructed without a closed form of the constitutive model, which can be computed by performing DPD simulations where the dynamics of polymer chains is explicitly simulated. In this proof-of-concept study for demonstrating how to implement the active-learning scheme for multiscale simulation, we assume that the fluid is inelastic and can be descried as a generalized Newtonian fluid in the FVM system, so that the stress field can be computed from a steady shear flow in the DPD system. We note, however, that there are more rheological properties of non-Newtonian fluids beyond the shear stress that can be obtained from DPD simulations, such as the normal stress differences and the spectrum of relaxation times that can be used for modeling elasticity and fading memory in continuum approaches [26]. The on-the-fly communications between FVM and DPD solvers can be implemented *seamlessly* by using a multiscale universal interface (MUI) library [27]. In general, to obtain an accurate function of the non-Newtonian viscosity in terms of shear rate requires many DPD simulations [28], making this process computationally prohibitive as DPD simulations of polymer models are expensive. Hence, in this work we will mitigate this computational expense by employing an *active learning* strategy together with the Gaussian process regression (GPR) to obtain the fluid's non-Newtonian viscosity only when necessary. Gaussian process models are particularly useful for regression because they provide not only the mean function response but also the corresponding uncertainty, which naturally allows for an active learning paradigm so that new training points are optimally selected to minimize this uncertainty. As a result, in the proposed multiscale coupling framework, only a few expensive DPD simulations will be performed to provide the effective constitutive relation of the polymeric fluids to close the continuum equations. Consequently, the total computational efficiency will be significantly increased compared to traditional message-passing multiscale approaches.