A multiscale SPH method for simulating transient viscoelastic flows using bead-spring chain model

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ABSTRACT

In this article, a multiscale smoothed particle hydrodynamics (SPH) method is proposed to simulate transient viscoelastic flows by using a bead-spring chain description of polymer molecule. This methodology couples macroscopic conservation equations for mass and momentum with a stochastic differential equation for bead-spring chain dynamics, which can be solved by a three-step semi-implicit algorithm to obtain the polymeric stress. Accordingly, a closed-form constitutive equation is not required. The multiscale SPH method is firstly verified by the plane Couette flow with Hookean and finitely extendable non-linear elastic (FENE) bead-spring chain models with the number of beads $M = 2$, which correspond to Hookean and FENE dumbbell models, respectively. Results for the velocity and shear stress are in excellent agreement with the available numerical and analytical solutions in literature. Then, the numerical method is extended to simulate the plane Couette flow and Poiseuille flow with FENE bead-spring chain model with $M > 2$. In particular, some molecular information of bead-spring chain such as the molecular stretch, the orientation angle and the mean configuration thickness are displayed. The influence of the number of beads M on the evolutions of the molecular information is also analyzed in detail. It is demonstrated that the multiscale SPH method proposed here is a promising computational tool for the multiscale simulations of transient viscoelastic flows.

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1. Introduction

Numerical simulation of transient viscoelastic flows is a well-established research field with many important practical applications such as extrusion, film-casting, blow molding, fiber-spinning, etc. To date, these simulations have been widely carried out by using a purely macroscopic approach [1], which is based on solving the conservation equations for mass and momentum in conjunction with a closed-form constitutive equation for the polymeric stress. Although the progress in macroscopic calculations of viscoelastic flows was very impressive, further developments are still needed, such as multiscale mathematical modeling of such flows.

The multiscale approach for viscoelastic flows is based on the kinetic theory, and accordingly it offers opportunity to study viscoelastic flows that are well beyond the limitations inherent to the purely macroscopic approach. The pioneering work for the multiscale calculations of viscoelastic flows was fulfilled by Laso and Öttinger [2], which combined the solution of macroscopic

conservation equations with the direct use of a kinetic theory model describing the fluid rheology. Specially, the finite element technique was employed to discretize the conservation equations of mass and momentum at the macroscopic level while a stochastic differential equation for the molecular models of polymer was solved by Brownian dynamics to obtain the polymeric stress without having to resort to a closed-form constitutive equation. This hybrid method is then termed as Calculation of Non-Newtonian Flow: Finite Elements and Stochastic Simulation Technique (CONNFFESSIT). The CONNFFESSIT method offers greater flexibility in the kinetic theory models that can be used in numerical simulations since it indeed dispenses with a closed-form constitutive equation. The molecular models of interest include the bead-spring dumbbell with Hookean or finitely extendable non-linear elastic (FENE) force laws, the bead-rod dumbbell, the bead-rod chain, the bead-spring chain, etc. Moreover, some effects such as the hydrodynamic interactions and the excluded volume can be easily incorporated into these molecular models, as stated in [2].

Another alternative multiscale approach for viscoelastic flows is the Brownian configuration fields method proposed by Hulsen et al. [3]. Specifically, in this approach, the polymeric dynamics are described by an ensemble of continuous configuration fields of spatially correlated molecules in comparison to the collection

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of individual molecules in CONNFFESSIT. Furthermore, it assumes locally correlated Brownian force which leads to tremendous spatial variance reduction. This implies that the calculated polymeric stress in Brownian configuration fields is spatially smooth. According to Bonvin and Picasso [4], this approach improves the global accuracy of the polymeric stress, which further leads to an enhanced stability in numerical calculations. Some research works using Brownian configuration fields have been reported in the literature [5–9]. Specifically, Öttinger et al. [5] reported that the concept of Brownian configuration fields can be regarded as an extremely powerful extension of variance reduction techniques based on parallel process simulation. Bonvin and Picasso [4] presented simple but efficient variance reduction method for CONNFFESSIT-like simulations, which extends the ideas of Hulsen et al. [3] and Laso and Öttinger [2] to non-equilibrium ensembles of dumbbells. Fan et al. [6] employed the discontinuous Galerkin method to discretize the equation of Brownian configuration fields, and the flow past a sphere, which forms the basis of the so-called falling ball viscometer, is tested. Phillips and Smith [8] described a spectral element method to simulate simple and complex flows of viscoelastic fluids based on Brownian configuration fields. In their work, both plane Couette flow and flow between eccentrically rotating cylinders were simulated. Recently, Mangoubi et al. [9] investigated some numerical aspects of Brownian configuration fields. More recently, Griebel and Rüttgers [10] coupled the Brownian configuration field method with their fully parallelized Navier–Stokes solver, and applied the multiscale FENE dumbbell model to a viscoelastic Poiseuille flow and square–square contraction flow problems.

The molecular models employed in the works mentioned above are mostly the bead-spring dumbbell model with Hookean or FENE force laws, and there are few works on developing more complex micro-structural models, *e.g.*, bead-spring chain model, to represent the polymer molecules. Actually, the bead-spring dumbbell model is an inexpensive and fairly crude representation of polymer molecules (two Brownian beads connected by a spring). Therefore, the bead-spring dumbbell model is widely adopted. However, the dumbbell model might be limited by its inability to represent the broad distribution of timescales that the real polymers possess. Consequently, for viscoelastic flows involving small polymer extensions and kinked conformational states, the predictions of dumbbell model often deviate from the experimental data [11–13]. Fortunately, the bead-spring chain model provides a more satisfactory description of polymer molecules in viscoelastic flows involving a wide range of polymer configurational states. Moreover, according to Zhou and Akhavan [14], the bead-spring chain model is able to represent the broad distribution of timescales that the real polymers possess. Therefore it is necessary to develop the bead-spring chain model as the molecular model of interest to represent the polymer solution.

The smoothed particle hydrodynamics (SPH) method is a particle-based Lagrangian method which is originally proposed by Gingold and Monaghan [15] and Lucy [16] in 1977 to deal with astrophysical problems. Since then, the application of SPH has been expanded in many areas of solid and fluid dynamic involving free surface flows [17,18], fluid–structure interactions [19, 20], multiphase flows [21,22], non-Newtonian fluid flows [23–26] and heat transfer problems [27]. Over the last decade, some attempts have been conducted to study the feasibility and fidelity of the SPH method in handing with viscoelastic fluid flows. Ellero et al. [28] presented the results for the isothermal viscoelastic Jaumann–Maxwell model by considering a basic 2D channel flow test. Then, Ellero and Tanner [29] presented an SPH formulation for transient viscoelastic flows, and the Poiseuille flows of a Newtonian and an Oldroyd-B fluids were simulated. Their results indicated that there were no particular difficulties to handle very large values of Weissenberg number. Fang et al. [30] extended the SPH method for the

numerical simulation of viscoelastic free surface flows, and found that an artificial stress is required to be added into the momentum equation so that the tensile instability is removed. Vázquez-Quesada and Ellero [31] presented the performance of SPH in solving the flow of a viscoelastic liquid around a linear array of cylinders confined in a channel, and compared the dimensionless drag force acting on the cylinder with the available numerical results. Xu et al. [32] developed SPH to simulate transient viscoelastic flows based on the concept of Brownian configuration field. In that work, both Hookean and FENE dumbbell models were considered, and their ability in solving transient viscoelastic flows was evaluated. Moreover, it should be noted that Litvinov et al. [33] performed the 2D simulations of a semi-dilute polymer solution in a microchannel following extensional flow by using dissipative particle dynamics. In that work, mesoscopic particle simulations of multi-beads FENE chains have predicted the inhomogeneous relaxation of a Poiseuille velocity profile in a channel from an inlet state where suspended polymers are fully stretched toward equilibrium configuration downstream.

The motivation of the present work is to develop a multiscale SPH method to simulate transient viscoelastic flows by using a bead-spring chain description of polymer molecule based on Brownian configuration field method. This can be recognized as an important step of SPH towards the multiscale calculations of transient viscoelastic flows. This paper is organized as follows: in Section 2, the governing equations and stochastic differential equation for bead-spring chain dynamics are introduced. In Section 3, the SPH method and some important issues for bead-spring chain model, which include some molecular information at the mesoscopic scale, parameter selection and algorithm development, are elaborated in detail. The time marching procedure of multiscale SPH algorithm is also described. Afterwards, the applications of the method to transient viscoelastic flows are presented in Section 4. Specifically, the plane Couette flow with the Hookean and FENE bead-spring dumbbell models is firstly investigated. Results for the velocity and shear stress are in excellent agreement with the available numerical and analytical solutions in literature. The numerical method is then extended to simulate the plane Couette flow and Poiseuille flow with FENE bead-spring chain model with $M > 2$. In particular, some molecular information, *i.e.*, the molecular stretch, the orientation angle, and the mean configuration thickness, is displayed. The influence of the number of beads M on the time evolutions of macroscopic and molecular information is also analyzed in detail. Finally, the concluding remarks are provided in Section 5.

2. Governing equations

The governing equations for the viscoelastic flow of an isothermal, transient, weakly compressible fluid can be written in a Lagrangian frame as

$$\frac{d\rho}{dt} = -\rho \, \nabla \cdot \mathbf{u}, \tag{1}$$

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \tag{2}$$

where ρ, t, $\mathbf{u}$, p and $\boldsymbol{\tau}$ are the density, the time, the velocity vector, the fluid pressure and the deviatoric stress tensor, respectively. The symbol d/dt denotes the material derivative, i.e., $d/dt = \partial/\partial t + \mathbf{u} \cdot \nabla$.

As is common in viscoelastic flow simulations, the deviatoric stress is split into the stress contribution from the solvent and the polymer:

$$\boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_p. \tag{3}$$