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An integrated lattice Boltzmann and finite volume method for the simulation of viscoelastic fluid flows

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ABSTRACT

A novel integrated scheme for modeling incompressible polymer viscoelastic fluid flows is proposed. Lattice Boltzmann method (LBM) is incorporated into finite volume method (FVM) to solve the incompressible Navier–Stokes equations and the constitutive equation respectively, and is implemented using open source CFD toolkits to predict nonlinear dynamics of polymer viscoelastic fluid flows. The hybrid numerical scheme inherits the efficiency and scalability of LBM and maintains the accuracy and generality of FVM. It has been critically validated using the Oldroyd-B model and linear PTT model under Poiseuille flow, Taylor-Green vortex flow and 4 : 1 abrupt planar contraction flow, respectively. The results from the integrated scheme have good agreement with the analytical solutions and the numerical results of other FVM schemes in previous publications.

1. Introduction

The dynamics of polymer solution depends not only on instant flow conditions at present, but also on the entire deformation history experienced by the fluid, hence exhibits complex non-Newtonian dynamics and viscoelastic effects. Mathematically, polymer viscoelastic fluid flows are usually studied by solving the Navier–Stokes equations and the constitutive equation, which preserve the mass and momentum conservation laws in the macroscopic flow, and account for the microstructure evolution of polymers, respectively. Given the diversity of viscoelastic liquids, various constitutive models have been developed to capture nonlinear behavior of viscoelastic fluid flows. Constitutive models are commonly classified into two categories, namely continuum models such as Oldroyd-B model [1] and PTT model [2], and microscopic models, e.g., dumbbell type models [3,4].

In order to carry out numerical simulations of viscoelastic fluid flows, the Navier–Stokes equations and the constitutive equation are usually discretized by one of the numerical schemes such as finite difference method (FDM, e.g. [5]), finite element method (FEM, e.g. [6]), finite volume method (FVM, e.g. [7,8]), spectral method (SM, e.g. [9]), smoothed particle hydrodynamics (SPH, e.g. [10]), etc., and solved numerically. Finite volume method is a well-established numerical technique in CFD research, and available in many commercial software such as CFX/ANSYS, FLUENT, PHOENICS and STAR-CD due to its advantages in preserving the conservation laws and in handling the non-regular geometric boundary. Simulation of viscoelastic fluid flows (e.g. [11]) is usually implemented by the so-called discrete elastic-viscous split stress (DVESS) numerical strategy with one of the commonly used pressure correction algorithms such as SIMPLE and PISO. Given certain initial and boundary conditions, the complex coupled partial differential equation system could be discretized into simple linear systems and solved by an iterative procedure as shown in details e.g. [11]. Although the iterative process for solving the linear systems could guarantee the accuracy of numerical solution, it will reduce computational efficiency and scalability.

With a reputation of mesoscopic scheme, Lattice Boltzmann method (LBM) is still mainly used for solving the incompressible or weakly compressible continuum Navier–Stokes equations [12,13]. Further modified LBM models can be utilized for simulation of multicomponent [14] and multiphase complex fluids. Compared to the continuum approach, LBM is constructed upon molecular statistical mechanics. Distinguished from FDM, FEM, FVM, and SM, LBM consists of only integration of the ordinary differential equation coupled with simple collision rules. Due to its good locality and simplicity, LBM scheme is suitable for parallel computing, therefore it has attracted increasing attention in CFD

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simulations. Some attempts have already been made to apply LBM scheme in simulation of viscoelastic fluid flows. But there are only limited successes because of the improper incorporation of the viscoelastic stress. In works by Onishi et al. [15,16], the evolution of polymer configuration is simulated by LBM scheme, and the Oldroyd-B and FENE-P model can be reconstructed from the polymer configuration. However, only numerical results in simple shear flows and under relatively weak viscoelastic effects are obtained. Malaspinas [17,18] proposed a LBM scheme for the simulation of viscoelastic fluid flows, by incorporating the classic LBM scheme to simulate incompressible Navier–Stokes equations with a convection-diffusion LBM mechanism for mimicking the viscoelastic stress. Unfortunately it also produce unphysical error. Su et al. [19] eliminated a part of this unphysical error in Malaspinas's works. However, both of them fail to reasonably explain the unphysical diffusive term of viscoelastic stress. Their discretization scheme for incorporating viscoelastic stress into LBM is dependent on constitutive models, and are not general either.

By taking the advantages of LBM and FVM, an **I**ntegrated **L**attice Boltzmann and **F**inite volume technique for simulation of isothermal and incompressible **V**isco**E**lastic fluid flows (**ILFVE**) is proposed here. The lattice Boltzmann-BGK scheme is used for solving the incompressible Navier–Stokes equations, in which the external force term is computed by viscoelastic stress tensor from any arbitrarily specified constitutive equation; and the constitutive equation is integrated in the framework of FVM with implicit or explicit time schemes, using the solution of the velocity field at any instant obtained from the lattice Boltzmann-BGK scheme. In order to integrate these two numerical schemes, a specific coupling scheme is constructed to ensure a seamless data transformation between the two schemes. By incorporating LBM, the iterative procedures for solving the Navier–Stokes equations with FVM scheme are eliminated, and the efficiency and scalability are considerably improved, moreover, explicit time integration schemes could also be introduced into FVM to obtain good locality when solving the constitutive equation, and therefore the hybrid numerical scheme could inherit the efficiency and scalability of LBM and maintain the accuracy and generality of FVM. ILFVE scheme is implemented using two open source CFD toolkits, namely OpenFOAM® and OpenLB. Additional coupling modules are constructed to ensure a full integration of OpenFOAM® and OpenLB libraries. The new simulation platform for modeling viscoelastic fluid flow is validated under benchmark flow problems. Although as an illustration only the Oldroyd-B model and the linear PTT model are presented here, the proposed scheme is completely general and suitable for using other constitutive models. To the best of our knowledge, it is the first attempt to construct a numerical scheme to integrate LBM and FVM in the simulation of viscoelastic fluid flows.

The rest part of the paper is organized as follows: In Section 2, general mathematical models for viscoelastic fluid flows are described. In Section 3 the main idea of ILFVE scheme is explained in detail. In Section 4, comprehensive validations are carried out by comparing the numerical solutions with ILFVE scheme with the analytical solution of Oldroyd-B model in Poiseuille flow, the numerical results of Taylor-Green vortex with FVM PISO scheme [11], and the qualitative and quantitative results of $4:1$ contraction flow from literature [20]. Finally, a conclusion is presented in Section 5.

2. Viscoelastic constitutive models

In this work, we focus on the simulation of isothermal and incompressible viscoelastic fluid flows. The typical composition of the homogeneous polymer solution can be described as polymers uniformly dissolved in incompressible Newtonian solvent. The solvent dynamics is modeled by the Navier–Stokes equations derived from the mass and momentum conservation laws:

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

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot (2\eta_s \mathbf{S} + \boldsymbol{\tau} - p\mathbf{I}) \tag{2}$$

where $\mathbf{u}, \rho, \eta_s, p$ represent the velocity, the density, the dynamic viscosity, and the pressure of the viscoelastic fluid respectively. $\mathbf{S} = 1/2(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$ is the strain rate tensor. $\boldsymbol{\tau}$ is the contribution of polymer solute to the total stress, which is defined by different constitutive models.

Oldroyd-B model [1] is a relatively simple but widely used viscoelastic constitutive model, which is a tensorial extension of Maxwell model. The relationship between the viscoelastic stress tensor $\boldsymbol{\tau}$, the time and the strain rate is given by:

$$\boldsymbol{\tau} + \lambda \overset{\nabla}{\boldsymbol{\tau}} = 2\eta_p \mathbf{S} \tag{3}$$

where η_p is the polymer contribution to the total viscosity of the solution. $\overset{\nabla}{\boldsymbol{\tau}}$ is the upper convected derivative of viscoelastic stress tensor, mathematically defined as:

$$\overset{\nabla}{\boldsymbol{\tau}} = \frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u} \cdot \nabla\boldsymbol{\tau} - \boldsymbol{\tau} \cdot \nabla\mathbf{u} - (\nabla\mathbf{u})^T \cdot \boldsymbol{\tau} \tag{4}$$

PTT model [2,21] is more realistic than Oldroyd-B model, which could explain the effects of elongational viscosity, especially some transient effects. PTT model with single relaxation time could be written as:

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} + f(tr(\boldsymbol{\tau}))\boldsymbol{\tau} + \xi\lambda(\mathbf{S} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \mathbf{S}) = 2\eta_p \mathbf{S} \tag{5}$$

in which ξ is the slip parameter, which introduces a non-affine response of polymer chains to an imposed deformation. λ is the characteristic relaxation time of the fluid. Two different PTT models, namely the linear PTT model and exponential PTT model, could be defined with a scalar function of the trace of viscoelastic stress tensor $f(tr(\boldsymbol{\tau}))$. The function of f for linear PTT model [2] is given by:

$$f(tr(\boldsymbol{\tau})) = \frac{\varepsilon\lambda}{\eta_p} tr(\boldsymbol{\tau}) + 1 \tag{6}$$

The function of f for exponential PTT model [21] is given by:

$$f(tr(\boldsymbol{\tau})) = \exp\left[\frac{\varepsilon\lambda}{\eta_p} tr(\boldsymbol{\tau})\right] \tag{7}$$

where ϵ is a parameter controlling elongational viscosity. If defining ϵ and ξ as 0, Eq. (5) would reduce to Oldroyd-B model.

FENE model [4] is built upon molecular dynamics mechanics, which directly relates the macroscopic viscoelastic response of fluid to the microscopic dynamics of polymer. In the microscopic viewpoint, polymer dynamics could be characterized by the conformation tensor $\mathbf{A} = \langle \mathbf{rr} \rangle$ statistically, where $\mathbf{r}$ is the end-to-end vector of a polymer molecule and $\langle\cdot\rangle$ is an ensemble average. Among diversified FENE models, the FENE-P model [22] proposed by Peterlin is most popular, the conformation tensor of which is given by:

$$\overset{\nabla}{\mathbf{A}} = -\frac{1}{\lambda}(a\mathbf{A} - b\mathbf{I}) \tag{8}$$

where Perterlin function a and parameter b are defined as:

$$a = \frac{1}{1 - tr(\mathbf{A})/L^2}, \quad b = \frac{1}{1 - 3/L^2} \tag{9}$$

L is the dumbbell extensibility parameter. The viscoelastic stress tensor can be obtained from the conformation tensor with following equation:

$$\boldsymbol{\tau} = \frac{\eta_p}{\lambda}(a\mathbf{A} - b\mathbf{I}) \tag{10}$$