Computers and Fluids 124 (2016) 190–196

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Lattice Boltzmann method for Oldroyd-B fluids

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ARTICLE INFO

Article history:
Received 17 December 2014
Revised 22 July 2015
Accepted 9 August 2015
Available online 14 August 2015

Keywords:
Lattice Boltzmann Method
Viscoelastic
Oldroyd-B fluid
Lattice Fokker-Planck Method

ABSTRACT

A lattice method for modeling a solution of dumbbells in a Newtonian fluid, introduced by Onishi et al. (2005) [1], is implemented within an existing lattice Boltzmann framework (Körner et al. (2005)) [2]. The numerical scheme is compared with the analytical solution of steady state and start up simple shear flow and an oscillating velocity field under uniform motion. Furthermore, a new transport model is introduced and validated for an oscillating velocity field under uniform motion. Both tests are in good agreement with the analytical solution. Additionally, a 4 to 1 planar contraction is simulated to test if the method is capable of reproducing complex viscoelastic flows. A lip vortex at the entrance corner is observed. A second benchmark is the four-roller setup. The overall results are in good agreement with previous studies.

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1. Introduction

The lattice Boltzmann method (LBM) is a promising tool for getting insight into fluid dynamics with especially complex boundaries. It can be used to model flow through porous media [3] or foams with free surfaces [4]. Most of these numerical studies cover Newtonian fluids. One way to introduce viscoelastic effects into LBM are multi-relaxation time (MRT) models. Giraud et al. [5] added two non propagating distribution functions to incorporate memory effects of viscoelastic fluids. This model was further analyzed by Wagner [6] and it was shown to be a non-objective Oldroyd model. The method was improved by Lallemand and Luo [7] by achieving Galilean invariance, isotropy and better stability. It was shown to reproduce the hydrodynamics of a fluid described by the Jeffreys model. A huge simplification was just recently developed by Dellar [8], removing the need of resting particles. This seems to be a very efficient method to describe linear viscoelastic effects. A class of viscoelastic fluids can be characterized by the elastic dumbbell model [9]. Malaspinas et al. [10] developed a method to include the dumbbell model into the LBM, which was further improved by Su et al. [11]. In the approach, the stress tensor is calculated using an advection–diffusion scheme on an additional lattice for each component. A comprehensive review of lattice Boltzmann methods for viscoelastic fluids is given by Phillips [12]. In this work, a numerical scheme that only needs one additional lattice, developed by Onishi et al. [1], is studied. The governing Fokker–Planck equation of the dumbbell distribution function is solved on a lattice and the components of the stress tensor are reconstructed from the distribution functions. The scheme is implemented into an existing LBM framework [2] and a new transport model for the dumbbell distribution functions is proposed. Furthermore, we test the numerical scheme not only for simple shear cases but also for planar flow.

In Section 2, an overview of the governing equations is presented, followed by the numerical implementation in Section 3. The simulation results are compared with the analytical solutions in Section 4 and benchmarks are presented in Section 5. A brief conclusion and outlook is given in Section 6.

2. Governing equations

2.1. Fluid dynamics

The hydrodynamics of a general fluid is described by the continuity and Navier–Stokes equation. The continuity equation in the incompressible limit reads as:

$$\nabla \cdot \vec{v} = 0 \tag{1}$$

Here, $\vec{v}$ is the velocity. The general form of the Navier–Stokes equation is:

$$\rho(\partial_t \vec{v} + \vec{v} \cdot \nabla \vec{v}) = -\nabla p + \nabla \cdot \mathbf{T} + \vec{f}_{ext} \tag{2}$$

With p being the pressure, ρ being the fluid density and $\vec{f}_{ext}$ being an external force. The stress tensor $\mathbf{T}$ can be separated into a Newtonian $\mathbf{T}_N$ and a non-Newtonian $\mathbf{T}_P$ contribution:

$$\mathbf{T} = \mathbf{T}_N + \mathbf{T}_P \tag{3}$$

For an incompressible fluid, the Newtonian part of the stress tensor can be written as:

$$\mathbf{T}_N = \mu_N \left(\mathbf{L} + \mathbf{L}^T\right) \tag{4}$$

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http://dx.doi.org/10.1016/j.compfluid.2015.08.004
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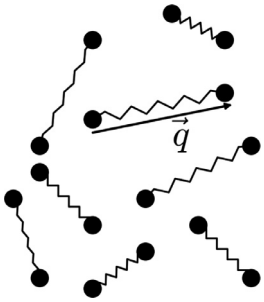

Fig. 1. Illustration of dumbbells solved in a Newtonian fluid.

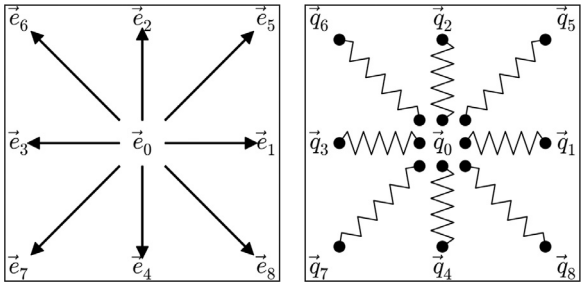

Fig. 2. Discrete velocities (left) and dumbbell connection vectors (right) on a D2Q9 lattice.

$$\mathbf{L} := (\nabla \vec{v})^T \tag{5}$$

Where μ_N is the dynamic viscosity of the Newtonian fluid. Inserting $\mathbf{T}$ into Eq. (2), the incompressible Navier–Stokes equation with the extra stress tensor becomes:

$$\rho(\partial_t \vec{v} + \vec{v} \cdot \nabla \vec{v}) = -\nabla p + \mu_N \Delta \vec{v} + \nabla \cdot \mathbf{T}_P + \vec{f}_{ext} \tag{6}$$

2.2. The elastic dumbbell model

The elastic dumbbell model describes a solution of flexible molecules in a Newtonian fluid (Fig. 1). The complex chains are simplified to elastic dumbbells, consisting of two beads connected by a spring. The probability to find a dumbbell within the volume $d\vec{x}$ at time t with the connection vector $\vec{q}$ is given by the configurational distribution function $\Psi(\vec{q}, \vec{x}, t)$. It can be shown that the time evolution of the configurational distribution function obeys [9]:

$$\partial_t \Psi = -\vec{v} \cdot \nabla \Psi - \partial_{\vec{q}}(\mathbf{L} \cdot \vec{q})\Psi + \frac{2\epsilon_{th}}{c_f} \partial_{\vec{q}} \left(\partial_{\vec{q}} \Psi + \frac{1}{\epsilon_{th}} \vec{f}_c \Psi \right) \tag{7}$$

where $\vec{f}_c$ is the connecting force between the two beads, $\epsilon_{th} = k_b T$ is the thermal energy and c_f is the friction coefficient of the solvent. The viscoelastic stress tensor can be written in Kramers form [9]:

$$\mathbf{T}_P = -n_P \left\langle \vec{q} \vec{f}^c \right\rangle + n_P \epsilon_{th} \mathbf{I} \tag{8}$$

Multiplying Eq. (7) with $\mathbf{Q} = \vec{q}\vec{q}$ and integrating over configurational space, the upper-convected Maxwell (UCM) model can be obtained:

$$\mathbf{T}_P + \lambda_1 \overset{\nabla}{\mathbf{T}}_P = \mu_P \mathbf{D} \tag{9}$$

$$\mathbf{D} = \mathbf{L} + \mathbf{L}^T \tag{10}$$

where λ_1 is relaxation time and μ_P the zero shear viscosity of the viscoelastic fluid. The upper convected time derivative is defined as:

$$\overset{\nabla}{\mathbf{T}} = \partial_t \mathbf{T} + \vec{v} \cdot \nabla \mathbf{T} - (\mathbf{L} \cdot \mathbf{T} + \mathbf{T} \cdot \mathbf{L}^T) \tag{11}$$

Using the incompressible viscoelastic stress tensor (Eq. (3)), the total viscosity μ_0 and the retardation time λ_2, the UCM model can be transformed to the Oldroyd-B constitutive equation:

$$\mathbf{T} + \lambda_1 \overset{\nabla}{\mathbf{T}} = \mu_0 \left(\mathbf{D} + \lambda_2 \overset{\nabla}{\mathbf{D}} \right) \tag{12}$$

$$\mu_0 = \mu_N + \mu_P \tag{13}$$

$$\lambda_2 = \frac{\mu_N}{\mu_0} \lambda_1 \tag{14}$$

In summary, an Oldroyd-B fluid is fully described by the equation system:

$$\nabla \cdot \vec{v} = 0 \tag{15}$$

$$\rho(\partial_t \vec{v} + \vec{v} \cdot \nabla \vec{v}) = -\nabla p + \mu_N \Delta \vec{v} + \nabla \cdot \mathbf{T}_P + \vec{f}_{ext} \tag{16}$$

$$\mathbf{T}_P + \lambda_1 \overset{\nabla}{\mathbf{T}}_P = \mu_P \mathbf{D} \tag{17}$$

3. Numerical methods

Instead of solving the Navier–Stokes equations directly, the lattice Boltzmann method is used. The basic idea of the LBM is to solve the microscopic Boltzmann equation for the particle distribution function $f(\vec{\xi}, \vec{x}, t)$, where $\vec{\xi}$ is the microscopic velocity at $(\vec{x}, t)$. The macroscopic properties of the fluid can be recovered as moments of the distribution function [13]. To solve the Boltzmann equation on a lattice, the continuous velocity space is discretized to a set of velocity vectors $\vec{e}_i$. For a lattice in two dimensions and with nine discrete velocities (Fig. 2), $\vec{e}_i$ can be defined as:

$$\vec{e}_i = \begin{cases} (0,0), & i \in 0 \\ \left(\cos\left(\frac{\pi}{2}(i-1)\right), \sin\left(\frac{\pi}{2}(i-1)\right) \right), & i \in \{1,3,5,7\} \\ \sqrt{2}\left(\cos\left(\frac{\pi}{2}(i-1)\right) + \frac{\pi}{4}, \sin\left(\frac{\pi}{2}(i-1)\right) + \frac{\pi}{4} \right), & i \in \{2,4,6,8\} \end{cases} \tag{18}$$

Therefore, there are discrete particle distribution functions $f_i(\vec{x}, t)$ at each lattice site $\vec{x}$ and the macroscopic properties can be calculated by:

$$\rho(\vec{x}, t) = \sum f_i(\vec{x}, t) \tag{19}$$

$$\vec{v}(\vec{x}, t) = \frac{1}{\rho(\vec{x}, t)} \sum f_i(\vec{x}, t) \vec{e}_i \tag{20}$$

$$\mathbf{T}(\vec{x}, t) = \sum f_i(\vec{x}, t) \vec{e}_i \vec{e}_i \tag{21}$$

Using the BGK-approximation [14], the Boltzmann equation can be solved on a lattice with the numerical scheme [13]:

$$f_i(\vec{x} + \delta t \cdot \vec{e}_i, t + \delta t) = f_i(\vec{x}, t) - \frac{\delta t}{\tau_N + 0.5 \delta t} \left(f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t) \right) \tag{22}$$

where $\tau_N = 3\nu$ is the relaxation time of the Newtonian fluid and ν is the kinematic viscosity. With a Chapman–Enskog expansion the continuity equation and the Navier–Stokes equations can be recovered. Eq. (22) is solved in two steps. The first step is the stream step, where the distribution functions propagate to the neighboring lattice sites they point at. Followed by the collide step, in which the collision operator is applied and the distribution function relaxes to its equilibrium state, given by Eq. (30). Similar to the discrete velocity space, the configurational space $\vec{q}$ of the dumbbell distribution function can be represented by a set of discrete connection vectors $\vec{q}_i$ (Fig. 2).

$$\vec{q}_i = \vec{e}_i \tag{23}$$

To solve the time evolution of the configurational distribution function (Eq. (7)) on a lattice, Onishi et al. [1] propose:

$$\Psi_i(\vec{x}, t + \delta t) = \Psi_i(\vec{x}, t) + \delta \Psi_i - \frac{\delta t}{\tau_P + 0.5\ \delta t} \left(\Psi_i(\vec{x}, t) - \Psi_i^{eq} \right) + \frac{\tau_P}{\tau_P + 0.5\ \delta t}\ \Phi_i\ \delta t \tag{24}$$

with $\tau_P = \lambda_1$. Eq. (24) is connected through two terms with Eq. (22), $\delta \Psi_i$ being responsible for the convection of the dumbbells and Φ_i

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