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Direct numerical simulation of complex viscoelastic flows via fast lattice-Boltzmann solution of the Fokker–Planck equation

L. Bergamasco [a], S. Izquierdo [a,*], A. Ammar [b]

[a] Instituto Tecnológico de Aragón (ITA), María de Luna 8, 50018 Zaragoza, Spain
[b] Arts et Métiers ParisTech, Boulevard du Ronceray, BP 93525, F-49035 Angers cedex 01, France

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ABSTRACT

Micro–macro simulations of polymeric solutions rely on the coupling between macroscopic conservation equations for the fluid flow and stochastic differential equations for kinetic viscoelastic models at the microscopic scale. In the present work we introduce a novel micro–macro numerical approach, where the macroscopic equations are solved by a finite-volume method and the microscopic equation by a lattice-Boltzmann one. The kinetic model is given by molecular analogy with a finitely extensible non-linear elastic (FENE) dumbbell and is deterministically solved through an equivalent Fokker–Planck equation. The key features of the proposed approach are: (i) a proper scaling and coupling between the micro lattice-Boltzmann solution and the macro finite-volume one; (ii) a fast microscopic solver thanks to an implementation for Graphic Processing Unit (GPU) and the local adaptivity of the lattice-Boltzmann mesh; (iii) an operator-splitting algorithm for the convection of the macroscopic viscoelastic stresses instead of the whole probability density of the dumbbell configuration. This latter feature allows the application of the proposed method to non-homogeneous flow conditions with low memory-storage requirements. The model optimization is achieved through an extensive analysis of the lattice-Boltzmann solution, which finally provides control on the numerical error and on the computational time. The resulting micro–macro model is validated against the benchmark problem of a viscoelastic flow past a confined cylinder and the results obtained confirm the validity of the approach.

1. Introduction

One of the most commonly adopted practices for the simulation of dilute polymeric suspensions relies on macroscopic constitutive equations for the polymeric extra stress, derived from molecular models and solved via well-established numerical methods [1]. The advantage of this approach is the low computational cost associated, the drawback is that some kinetic models does not have a closed-form continuous counterpart. With regards to the finitely extensible non-linear elastic (FENE) model for example, a rheological law can only be derived under closure approximations, i.e. FENE-P, FENE-LS [2]. The resulting models are then able to phenomenologically describe the basic flow features but the underlying theoretical assumptions can hinder the retrieval of relevant viscoelastic phenomena.

In a more general modeling strategy, the kinetic origin of the molecular models is retained [3]. Methods using this approach are generally described as micro–macro models, due to the separated solution of the micro and macroscales. Continuity and momentum equations are solved using continuous equations (macro-scale) and kinetic equations are solved by stochastic or deterministic methods (micro-scale) [4]. In this framework, one of the most popular methodologies is the CONNFFESSIT approach, where a finite element solution of the macroscopic equations is combined with stochastic simulations for the dumbbell configuration [5]. One of the major issues concerned with this approach is the high computational expense and the embedded statistical noise, which can be filtered using variance reduction techniques [6]. Another similar and commonly used approach is the Brownian configuration field method [7]. This method already embeds efficient variance reduction, as long as individual molecules are clustered in continuous configuration fields according to their initial configuration and applied force, but the computational cost of the stochastic simulation is anyway a limit.

An alternative approach for noise reduction and faster computations consists in the solution of an equivalent Fokker–Planck equation for the probability density of the dumbbell configuration. However, a literature review reveals that due to the dimensionality of the problem and the lack of efficient numerical methods to solve the Fokker–Planck equation, little progress has been done in this framework [4] and no method prevail. Relevant recent work about the direct solution of the Fokker–Planck equation for complex

* Corresponding author.
E-mail addresses: lbergamasco@ita.es (L. Bergamasco), sizquierdo@ita.es (S. Izquierdo), amine.ammar@ensam.eu (A. Ammar).

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flows relies on a Galerkin spectral element technique for 2D [8] and its extension to 3D [9]. Another group of promising methods are those that approximate the solution of the Fokker–Planck equation reducing the dimensionality of the problem. This order-reduction can be done *a priori*, like in the lattice-Fokker–Planck method [10], *on line* like in the proper generalized decomposition [11] or *a posteriori* like in the proper orthogonal decomposition [12]. All these techniques aim to systematically reduce the degrees of freedom and therefore the computational expense.

In this work we focus on direct deterministic numerical methods, therefore no approximation occurs beyond mesh resolution. The proposed approach relies on a previous work by Ammar [13] about a lattice Boltzmann solution of the Fokker–Planck equation for homogeneous flows. Recently this method has been also theoretically analyzed [14] and applied for the solution of a population balance equation [15] and for the Fokker–Planck equation [16]. However, none of the previous works [13–16] deals with the coupling of the kinetic solution with macroscopic fields, thus we investigate efficient ways to exploit it in multi-scale simulations.

In the proposed micro–macro model, the macroscopic equations are solved by a finite-volume method using the commercial solver ANSYS Fluent® v14.0, while the microscopic equation is solved by a lattice-Boltzmann method. The Fokker–Planck equation is solved using an operator-splitting procedure that allows to solve the configurational part by a GPU implementation of the lattice Boltzmann method and the physical convection by a finite volume method. The operator-splitting indeed allows us to transport only viscoelastic stresses instead of the whole distribution function defined in the configuration space. Consequently, algorithms with low-memory requirements can be formulated.

The outline of the paper is as follows: the governing equations for the polymeric suspension and a derivation of the stochastic equation for the FENE dumbbell model are firstly presented; successively, the equivalent Fokker–Planck equation is introduced (Section 2). In Section 3, the solution and coupling strategy is detailed together with the numerical methods. Section 4 comprises the numerical analysis of the sub-grid solution, the validation of the coupled model and its optimization. The details of the GPU implementations and the relative coupling with the macroscopic solver are reported in Appendix C. A brief summary of the results obtained and an outlook on further developments concludes the paper (Section 5).

2. Theoretical model

2.1. Hydrodynamic system

Let us consider a polymeric solution as a blend between a Newtonian and a viscoelastic fluid. Assuming the flow to be incompressible and isothermal, mass and momentum conservation reads:

$$\nabla_x \cdot \mathbf{v} = 0; \tag{1}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot (\nabla_x \mathbf{v}) = -\nabla_x p + \nabla_x \cdot \boldsymbol{\sigma}; \tag{2}$$

where ρ is the density, p the pressure, $\mathbf{v}$ the velocity vector and the subscript x denotes operators in the physical space. The total stress tensor $\boldsymbol{\sigma}$, embeds contributions from both the Newtonian solvent $\boldsymbol{\sigma}_s$ and the polymeric solute $\boldsymbol{\sigma}_p$, therefore $\boldsymbol{\sigma} = \boldsymbol{\sigma}_s + \boldsymbol{\sigma}_p$. Denoting by μ_s the dynamic viscosity of the solvent, $\boldsymbol{\sigma}_s$ is given as:

$$\boldsymbol{\sigma}_s = \mu_s(\nabla_x \mathbf{v} + (\nabla_x \mathbf{v})^\dagger) = \mu_s \dot{\boldsymbol{\gamma}}; \tag{3}$$

being $\dot{\boldsymbol{\gamma}}$ the rate of strain tensor. In order to close the hydrodynamic system, an additional material model must be solved for the viscoelastic contribution $\boldsymbol{\sigma}_p$.

2.2. Viscoelastic model

In the simplest micro-mechanical approach for polymer rheology, molecular chains are modeled by two beads and a spring connector, that is by a non-rigid dumbbell immersed in a fluid. A general kinetic model can then be derived considering the equations of motion of the beads in the dumbbell, namely the equilibrium of inertial, frictional, Brownian and connector forces [17]. For a jth bead located in $\mathbf{r}_i$, the equilibrium yields the so called *Langevin* equation:

$$m_j \frac{d}{dt}\left(\frac{d\mathbf{r}_j}{dt} - \mathbf{v}(\mathbf{r}_j)\right) = \zeta_j\left(\frac{d\mathbf{r}_j}{dt} - \mathbf{v}(\mathbf{r}_j)\right) + \sigma\frac{d\mathbf{W}_j}{dt} + \mathbf{F}_j^c; \tag{4}$$

with m being the mass of the bead, ζ a drag coefficient, σ a coefficient for the standard Wiener process $\mathbf{W}$ and $\mathbf{F}^c$ the connector force. Indicating with k_B the Boltzmann constant and T the absolute temperature, $\sigma = \sqrt{2k_B\zeta T}$ from the principle of equipartition of energy [1]. Assuming high friction regime and thus over-dumped Brownian dynamics [18], the inertial term on the left-hand side can be dropped and, indicating with $\boldsymbol{\xi} = \mathbf{r}_2 - \mathbf{r}_1$ the end-to-end vector of a dumbbell, yields the following (Itô) stochastic differential equation:

$$\frac{d}{dt}\boldsymbol{\xi} = \boldsymbol{\kappa}\cdot\boldsymbol{\xi} - \frac{2}{\zeta}\mathbf{F}^c(\boldsymbol{\xi}) + \sqrt{\frac{4k_BT}{\zeta}}\frac{d}{dt}\mathbf{W}; \tag{5}$$

where $\mathbf{W}$ is a standard Brownian motion $(\mathbf{W}_2 - \mathbf{W}_1)/\sqrt{2}$ and the symbol $\boldsymbol{\kappa}$ has been adopted for the transpose of the velocity gradient tensor $(\nabla_x\mathbf{v})^\dagger$. The peculiarity of the dumbbell model lies in the expression of the connector force law $\mathbf{F}^c(\boldsymbol{\xi})$. In this work we are concerned with the finitely extensible non-linear elastic model, therefore indicating with h the spring constant and ξ_0 a finite extensibility parameter, the connector force reads:

$$\mathbf{F}^c(\boldsymbol{\xi}) = \frac{h}{1 - \|\boldsymbol{\xi}\|^2/\xi_0^2}\boldsymbol{\xi}; \tag{6}$$

with $\|\cdot\|$ indicating vector norm. This entropic force law, originally proposed by Warner [19], exhibits linear behavior for small extensions and the finite length ξ_0 in the limit of an infinite force. In a stochastic approach, Eq. (5) should then be stochastically solved for the dumbbell configurations in the random process $\mathbf{W}$ with the spring force law (6).

Using stochastic analysis, the ordinary differential Eq. (5) can be associated with a partial differential equation for a probability density function (PDF), which can then be deterministically solved instead of a large number of realizations for the Brownian driver. In this case the resulting probability density function $\psi(\mathbf{x},\boldsymbol{\xi},t)$ satisfies the Fokker–Planck equation [20]:

$$\frac{\partial\psi}{\partial t} + \mathbf{v}\cdot(\nabla_x\psi) + \nabla_\xi\cdot\left[\left(\boldsymbol{\kappa}\cdot\boldsymbol{\xi} - \frac{2}{\zeta}\mathbf{F}^c(\boldsymbol{\xi})\right)\psi\right] = \frac{2k_BT}{\zeta}\nabla_\xi^2\psi; \tag{7}$$

which is also called *Smoluchowski* equation in polymer science. Index ξ on operators indicates that they act in the configuration space. Due to its dimensionality, the solution of Eq. (7) is non-trivial and we proceed as detailed in the next section.

3. Numerical methods

3.1. Solution strategy

In order to solve the Fokker–Planck equation directly, we consider a time-splitting-like procedure similar to that proposed by Lozinski and Chauvière [8]. Following this idea, the operators acting in the configuration space are separated from those acting in the physical space. In this way Eq. (7) can be firstly solved in the configuration space for an intermediate distribution function ψ^{n^*},