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Towards a Fokker-Planck Rheometer

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Abstract. Models of kinetic theory provide a coarse-grained description of molecular configurations wherein atomistic processes are ignored. Kinetic theory models can be very complicated mathematical objects sometimes defined in highly multidimensional spaces including the physical space, the time and the conformational space. In the past, stochastic based simulations were preferred to circumvent or at least alleviate the curse of dimensionality that many kinetic theory models exhibit. Recently, we proposed alternative solution strategies of the kinetic theory models based on the use of model reduction and separated representations for solving generic Fokker-Planck descriptions. These strategies have been successfully applied to solve a large variety of models.

Keywords: Complex fluids; Kinetic theory description; Fokker-Planck equation; Advanced numerical modeling; Model reduction; Separated representation; Finite sums decomposition; Karhuen-Loève decomposition.

PACS: 46.15.-x; 47.11.-j; 47.50.-d; 47.57.-s; 47.61.-k

INTRODUCTION

Many natural and synthetic fluids are viscoelastic materials, in the sense that the stress endured by a macroscopic fluid element depends upon the history of the deformation experienced by that element. Notable examples include polymer solutions and melts, liquid crystalline polymers and fibre suspensions. Rheologists thus face a challenging non-linear coupling between flow-induced evolution of microscopic configurations, macroscopic rheological response, flow parameters (such as the geometry and boundary conditions) and final properties. Theoretical modelling and methods of computational rheology have an important role to play in elucidating this coupling.

Atomistic modelling is the most detailed level of description that can be applied today in rheological studies, using techniques of non equilibrium molecular dynamics. Such calculations require enormous computer resources, and then they are currently limited to flow geometries of molecular dimensions. Consideration of macroscopic flows found in processing applications calls for less detailed mesoscopic models, such as those of kinetic theory.

Models of kinetic theory provide a coarse-grained description of molecular configurations wherein atomistic processes are ignored. They are meant to display in a more or less accurate fashion the important features that govern the flow-induced evolution of configurations.

Kinetic theory models can be very complicated mathematical objects. It is usually not easy to compute their rheological response in rheometric flows, and their use in numerical simulations of complex flows has long been thought impossible. The traditional approach has been to derive from a particular kinetic theory model a macroscopic constitutive equation that relates the viscoelastic stress to the deformation history. One then solves the constitutive model together with the conservation laws using a suitable numerical method, to predict velocity and stress fields in complex flows. The majority of constitutive equations used in continuum numerical simulations are indeed derived (or at least very much inspired) from kinetic theory.

Indeed, derivation of a constitutive equation from a model of kinetic theory usually involves closure approximations of a purely mathematical nature such as decoupling or pre-averaging. It is now widely accepted that closure approximations have a significant impact on rheological predictions for dilute polymer, solutions, or fiber suspensions.

In this context, micro-macro methods of computational rheology that couple the coarse-grained molecular scale of kinetic theory to the macroscopic scale of continuum mechanics have an important role to play (see [1] and the references therein). This approach is much more demanding in computer resources than more conventional continuum simulations that integrate constitutive equation to evaluate the viscoelastic contribution of the stress tensor. On the other hand micro-macro techniques allow the direct use of kinetic theory models and thus avoid the introduction of closure approximations.

Since the early 1990's the field has developed considerably following the introduction of the CONFFESSIT method by Ottinger and Laso [2]. Being relatively new, micro-macro techniques have been implemented only for models of kinetic theory with few configurational degrees of freedom, such as non-linear dumbbell models of dilute polymer solutions and single-segment tube models of linear entangled polymers.

Kinetic theory provides two basic building blocks: the diffusion or Fokker-Planck equation that governs the evolution of the distribution function (giving the probability distribution of configurations) and an expression relating the viscoelastic stress to the distribution function. The Fokker-Planck equation has the general form:

$$\frac{d\Psi}{dt} = -\frac{\partial}{\partial \mathbf{X}} (\mathbf{A}\Psi) + \frac{\partial}{\partial \mathbf{X}} \left(\mathbf{B} \frac{\partial \Psi}{\partial \mathbf{X}} \right) \quad (1)$$

where $d\Psi/dt$ is the material derivative, vector \mathbf{X} defines the coarse-grained configuration and has dimensions D . Factor \mathbf{A} is a D -dimensional vector that defines the drift or deterministic component of the molecular model. Finally \mathbf{B} is a symmetric, positive definite $D \times D$ matrix that embodies the diffusive or stochastic component of molecular model. In general both \mathbf{A} and \mathbf{B} (and in consequence the distribution function Ψ) depend on the physical coordinates \mathbf{x} , on the configuration coordinates \mathbf{X} and on the time t .

The second building block of a kinetic theory model is an expression relating the distribution function and the stress. It takes the form:

$$\boldsymbol{\tau}(\mathbf{x}, t) = \int_C \mathbf{g}(\mathbf{X}, \mathbf{x}, t) d\mathbf{X} \quad (2)$$

where C represents the configuration space and \mathbf{g} is a model-dependent tensorial function of configuration. In a complex flow, the velocity field is a priori unknown and the previous model must be completed with the momentum and mass balances. The generic form (1)-(2) allows describing a large variety of kinetic theory models [3][4].

In the present work we are considering complex kinetic theory models (sometimes defined in highly dimensional spaces) in simple rheometric flows, in which the microscopic configuration is assumed to be the same everywhere within the flow domain, and then, the microstructure evolution does not perturb the flow kinematics, which is assumed to correspond with well known rheometric kinematics. In some of our former works we explored the use of reduced approximation bases (based on the use of the Karhunen-Loève decomposition) for addressing kinetic theory models defined in moderate dimensions [5]. However, models defined in high-dimensional spaces deserve further considerations.

NUMERICAL SOLVER

Sometimes Eq. (1) is defined in a multidimensional space that in some cases involves hundreds of dimensions. Thus, for example, multi-bead-spring models are defined in a conformation space of dimension $D = 3N_c$, being N_c the number of connectors used to describe the molecule. Until now, the only possibility for treating this kind of models was the stochastic simulations (that exploits the equivalence between the Fokker-Planck and the Ito stochastic equation), where the complexity scales linearly with the dimension of the space. However, several difficulties remain when using stochastic simulations, being the most relevant: (i) the inevitable statistical noise, that

is reduced by evaluating a large number of trajectories of the stochastic process or by using more or less sophisticated variance reduction techniques (the Brownian Configuration Fields being one of these alternatives); (ii) the necessity of evaluating the transient model even when one is only interested in the steady state; (iii) the possibility of computing with a reasonable computing time some moments of the distribution function but not the distribution function itself that will require the evaluation of a prohibitive number of trajectories of the associated stochastic process, ... For this reason, the solution of Eq. (1) using deterministic approaches seems an appealing choice if one is able of addressing its multidimensional character.

The brut force approach cannot be considered as a possibility for treating this kind of models. We can understand the catastrophe of dimension by assuming a model defined in a hyper-cube Ω of dimension D : $\Omega =]-L, L[^D$. Now, if we define a grid to discretize the model, as it is usually performed in the vast majority of numerical methods (finite differences, finite elements, finite volumes, spectral methods etc.), consisting of N nodes on each direction, the total number of nodes will be N^D . If we assume that for example $N = 10$ (an extremely coarse description) and $D = 80$ (lower than the dimensions required in some statistical mechanics models) the number of nodes in Ω reaches the value of 10^{80} that represents the presumed number of elementary particles in the universe!

For addressing models defined in highly multidimensional spaces, new reduction strategies whose computational complexity should scale linearly with the dimension of the space should be proposed and checked. For this purpose, we proposed in some of former works writing the approximation of a generic function $\Psi(\mathbf{x}) = \Psi(x_1, x_2, \dots, x_D)$ in the whole domain as:

$$\Psi(\mathbf{x}) \approx \sum_{i=1}^{i=I} \Psi_1^i(x_1) \times \dots \times \Psi_D^i(x_D) = \sum_{i=1}^{i=I} \prod_{k=1}^{k=D} \Psi_k^i(x_k) \quad (3)$$

It is well known that several model solutions can be approximated by a finite, and sometimes quite reduced, number of functions products. Expression (3) involves $I \times N \times D$ degrees of freedom instead of the N^D required by the mesh-based discretization techniques. The functions involved in (3) are build-up iteratively (until reaching convergence) by introducing the approximation (3) within the weak form of the Fokker-Planck equation, as described in [6]-[7]. This procedure made possible the efficient treatment of many models (polymer solutions – FENE, MBS, ...[6][7]- and melts [8]), liquid crystalline polymers, associative polymers, short fiber suspensions (including aggregating effects) [9], kinetic theory description of mixing [10], ...

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