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Moment closure for FENE models of complex fluids

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In this talk, we present some joint work with current and former colleagues at Penn State (C. Liu, P. Yu and Y. Hyon) on moment closure approximations of multiscale complex fluid models. Moment closure not only provides a computationally feasible approach to simulate many multiscale phenomena but also offers insight to the understanding of the underlying physical processes. We will discuss some of our recent works on developing systematic moment closure models for micro-macro FENE models of complex fluids and demonstrate their effectiveness for a wide range of parameter regimes.

1 Micro-macro models of FENE fluid

A popular micro-macro multiscale approach to model dilute solutions of flexible polymers (treated as dumbbells) involves solving the coupled partial differential equations consisting of the macroscopic momentum equation, the incompressible Navier-Stokes equation, and a Fokker-Planck equation describing the probability distribution function (PDF) $f = f(\vec{x}, \vec{Q}, t)$ of the dumbbell orientation $\vec{Q}$ on the microscopic level. The coupled system reads [1]

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} + \nabla p = \nabla \cdot \tau_p + \nu \triangle \vec{u} \,, \qquad \nabla \cdot \vec{u} = 0 \tag{1}$$

$$\frac{\partial f}{\partial t} + (\vec{u} \cdot \nabla) f + \nabla_{\vec{Q}} \cdot (\nabla \vec{u} \vec{Q} f) = \frac{2}{\zeta} \nabla_{\vec{Q}} \cdot (\nabla_{\vec{Q}} \Psi(\vec{Q}) f) + \frac{2kT}{\zeta} \triangle_{\vec{Q}} f \,. \tag{2}$$

In equation (1), τ_p is a tensor representing the polymer contribution to stress: $\tau_p = \lambda \int (\nabla_{\vec{Q}} \Psi(\vec{Q}) \otimes \vec{Q}) f(\vec{x}, \vec{Q}, t) d\vec{Q}$ where $\Psi(\vec{Q})$ is the elastic spring potential, and λ is the polymer density constant. This induced elastic stress τ_p can be derived from the least action principle. In the Fokker-Planck equation (2), ζ is the friction coefficient of the dumbbell beads, T is the temperature, and k is the Boltzmann's constant. The terms in (2) can be roughly explained as follows. The second and third terms on the left-hand side of (2) stem from the fact that the polymers are convected and stretched by the macroscopic flow, the first term on the right-hand side of (2) accounts for the inner force of the dumbbell due to the spring potential, and the last diffusion term on the right-hand side of (2) models the random collisions of the solvent particles with the polymers. This interpretation becomes clearer when we associate the Fokker-Planck equation (2) with the stochastic differential equation [4],

$$d\vec{Q} + \vec{u} \cdot \nabla \vec{Q} dt = (\nabla \vec{u} \vec{Q} - (2/\zeta) \nabla_{\vec{Q}} \Psi) dt + \sqrt{4kT/\zeta} d\vec{W}_t,$$

where $\vec{W}_t$ is the standard Brownian motion. This stochastic differential equation defines Brownian dynamics of the connector vector $\vec{Q}$ such as the probability distribution of dumbbell polymers evolves according to the Fokker-Planck equation (2). The simplest spring potential is given by the Hookean law $\Psi(\vec{Q}) = HQ^2/2$, where $Q = |\vec{Q}|$ and H is the elasticity constant. In fact, exploiting this simple potential, one can derive a macroscopic differential constitutive equation for the polymeric stress τ_p from the Fokker-Planck equation, which leads to the so-called Oldroyd-B fluids. However, for a more practical FENE (Finite Extendible Nonlinear Elasticity) potential that takes into account a finite-extensibility constraint, $\Psi(\vec{Q}) = -(HQ_0^2/2) \log(1 - (Q/Q_0)^2)$, there does not exist an exact macroscopic constitutive equation for τ_p, and thus the FENE model represents a truly multiscale model. Our focus regarding numerical simulation of the FENE model is on the so-called moment-closure approach [9, 3].

2 Closure approximation

To illustrate the idea of moment-closure approximations, we multiply the Fokker-Planck equation in 2D by $\vec{Q} \otimes \vec{Q}$, and perform integration by parts on the probability space $|\vec{Q}| < Q_0$. Denoting by A the conformation tensor $\langle \vec{Q} \otimes \vec{Q} \rangle$, where the brackets represent the ensemble average over the space $|\vec{Q}| < Q_0$, i.e. $\langle \vec{Q} \otimes \vec{Q} \rangle \equiv \int_{|\vec{Q}| < Q_0} \vec{Q} \otimes \vec{Q} f(\vec{x}, \vec{Q}, t) d\vec{Q}$, we get

$$\frac{\partial A}{\partial t} + (\vec{u} \cdot \nabla) A - (\nabla u) A - A (\nabla u)^T = -\frac{4}{\zeta} \int \frac{H \vec{Q} \otimes \vec{Q}}{1 - Q^2/Q_0^2} f(x, \vec{Q}, t) d\vec{Q} + \frac{4kT}{\zeta}. \tag{3}$$

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If we select the conformation tensor as the only *state variable*, to close the equation, it is necessary to find an approximate relation to represent the ensemble average term $\langle \frac{H\vec{Q}\otimes\vec{Q}}{1-Q^2/Q_0^2} \rangle$ on the right-hand side in terms of A. If done properly, this closure approach reduces the needs to resolve the probability space and thus results in dramatic savings computationally.

3 Ansatz near equilibrium

In [9], a new closure approximation, FENE-S, is presented for deriving effective macroscopic moment equations from micr-macro FENE model of viscoelastic polymeric fluids. The closure is based on restricting the otherwise general probability distribution functions (PDF) to a class of smooth distributions motivated by perturbing the equilibrium PDF. The simplified system coupling the moment equations and the Navier-Stokes equations still possesses an energy law analogous to the original micro-macro system. Some theoretical analysis and numerical experiments are presented to ensure the validity of the moment-closure system, and to illustrate the agreement of the simplified model with the original system solved using a Monte-Carlo approach, for a certain regime of physical parameters.

4 Higher order expansion

In [3], some analytical and numerical studies are presented on the FENE model of polymeric fluids. The well-posedness of the FENE model is established under the influence of a steady flow field. We further infer existence of long-time and steady-state solutions for purely symmetric or anti-symmetric velocity gradients. The stability of the steady-state solution for general velocity gradient is illuminated by the analysis of the FENE-P closure approximation. We also propose a new linear closure approximation utilizing higher moments, which is shown to generate more accurate approximations than other existing closure models for moderate shear or extension rates. An instability phenomenon under a large strain is also investigated.

5 Generalized ansatz

In [5], an enhanced moment-closure approximation to the finite extensible nonlinear elasticity (FENE) models of polymeric fluids. This new moment-closure method, named FENE-D, involves the perturbation of the equilibrium probability distribution function (PDF), which takes into account of the singularity behavior under the large macroscopic flow effects. The final resulting macroscopic system includes the moment-closure equations, the momentum (force balance) equations, as well as an auxiliary equation representing implicitly the dynamics of the singularities for the microscopic configurations. Through numerical experiments, we demonstrate the accuracy and robustness of the moment-closure system for some special external flow with a wide range of flow rates.

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