Multiscale Modeling of Viscoelastic Flows

Modeling and Algorithmic Approaches to Constitutively-Complex, Micro-Structured Fluids

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Abstract

Our goal is the modeling of macroscopic viscoelastic behavior originating in the dynamics of dissolved polymers and their coupling to the fluid solvent. We decompose this multiscale problem into three layers. (1) The continuum (macroscopic) layer, where flow will be modeled by the macroscopic momentum equation and an extra stress gradient to be derived from the microstructure. (2) The microscopic layer where individual polymer molecules may be modeled directly. We use Kramers' bead-rod representation and model solvent effects through drag and Brownian motion terms. (3) A mesoscale layer is used to model statistical properties of polymers as a probability density function (PDF), whose dynamics is governed by a Fokker-Plank equation. A Fokker-Plank representation of the exact microscale dynamics could be written – our implementation is simplified by assumptions of scale, e.g., adiabatic elimination of momentum coordinates. The result is that the three models are hierarchical in scale and in fidelity to the molecular physics.

The miscroscale solver uses a new second-order strong algorithm with a Duhamel formulation. The stability of this method by itself helps close the gap between molecular and macroscopic time scales to within ≈ 3 orders of magnitude. The mesoscale solver is a simple advection (in real space) diffusion (in the space of particle coordinates) scheme based on Lagrangian transport and statistical sampling with variance reduction.

A key challenge has been the modeling of the probability density function characterizing the mesoscale layer. The PDF has a large number of degrees of freedom, and is subject to internal constraints. We use a representation based on rod angles relative to a fixed frame, and the resulting constraints concern angle symmetry. In 2D, we use the von Mises distribution to respect the symmetry constraints. Mixtures of von Mises distributions provide additional degrees of freedom. The significance of fits is assessed with the Akaike and Bayesian criteria.

Results will be presented demonstrating macroscopic flow with extra stress derived from the microscale.

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