

Some Unsolved Issues in the Multi-scale Modeling of Complex Fluids and the Related Forming Processes

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Keywords : Model reduction, Nano-science, Complex fluids, Numerical Modeling.

Abstract

Description of macromolecular materials involves numerous computational challenges. Accurate descriptions of such materials need for a multiscale description and the definition of pertinent bridges between the different scales. The finest description starts at the atomic level where quantum mechanics leads to molecular dynamics simulations. The next description scale introduces some molecular simplifications leading to a coarse grained molecular dynamics, the DPD being one of such approaches. Other descriptions consider molecules as interacting multi-bead-springs or multi-bead-rods. At this level Brownian dynamics simulations are usually employed. However, this level of description requires intensive computation resources with its significant unfavorable impact on the simulation performances (CPU time). For this reasons sometimes kinetic theory descriptions are preferred. In that description, the molecular conformation is described from a probability density function whose evolution is governed by the Fokker-Planck equation.

This approach, despite its mathematical simplicity, introduces a density function that is defined in a multidimensional space, and then the associated partial differential equations must be solved in a multidimensional domain. To circumvent the curse of dimensionality that these high-dimensional partial differential equations induce, stochastic techniques have been applied intensively in the last decade. Some improvements have been proposed, the Brownian Configurations Fields being one of such approaches. Recently some incipient techniques based on sparse grids or those based on separated representations have allowed solving models defined in highly multidimensional spaces.

The aim of this paper is identify the main challenges and recent advances in the multiscale modeling just described.