

Macroscopic information from microscopic simulation. Selected issues

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Abstract: In this talk we give an overview about methods recently improved to extract mesoscopic or macroscopic variables from the simulation of microscopic or atomistic models for polymeric fluids. Upon these are concepts for detecting entanglements between polymers, the evaluation of viscosities from stress fluctuations, the prediction of macroscopic friction behavior of polymer coatings based on microscopic models, the coarse-graining of polymers in order to obtain macroscopically relevant relaxation times from a given atomistic dynamics, and possibly spectral, grid or smooth particle methods to improve the memory costs of the CONNFESSIT (Calculation of Non-Newtonian Flow using Finite Elements and Stochastic Simulation Techniques) approach.