Poster abstract

P.09 Deriving constitutive models of polymer dynamics from thermodynamically consistent coarse-graining molecular models

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How can reliable constitutive equations for owing complex fluids be derived from their underlying microscopic dynamics? Contrary to phenomenological approaches with ad-hoc assumptions, nonequilibrium statistical mechanics provides tools to systematically derive macroscopic properties from microscopic models not only for equilibrium situations but also under ow conditions. Here, we suggest to use these tools within the framework of nonequilibrium thermodynamics in order to systematically derive a thermodynamically consistent macroscopic constitutive model from the underlying microscopic dynamics [1]. Our systematic coarse-graining method is able to efficiently bridge the time- and length scale gap between the microscopic level and macroscopic dynamics. We illustrate the proposed method for two cases: low-molecular polymer melts [1,2] and liquid crystals [3]. In both cases, the fluids are subjected to homogeneous ow fields. We use a hybrid Monte-Carlo-molecular dynamics iteration scheme in order to obtain the coarse-grained model [1]. We establish the functional form of the macroscopic constitutive model by reconstructing the thermodynamic building blocks from our simulations [2,3]. The constitutive models that we derive in this way are in agreement with reference results.

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