Systematic and thermodynamically consistent coarse graining the flow of complex fluids

From 2014-03-01 to 2018-02-28, closed project

Objective

The overall aim of this project is to develop a systematic and thermodynamically consistent method to derive macroscopic constitutive equations from molecular models of polymeric and anisotropic fluids. Since the constitutive equations describe the transport and flow behavior of the material on a coarse-grained level, many phenomenological approaches have been proposed in the past. The method we will develop here combines projection operator techniques and simulations within a nonequilibrium thermodynamics framework. Novel, thermodynamically guided simulations will allow us to identify building blocks of the macroscopic model and thereby establish the macroscopic constitutive equations in a thermodynamically consistent form. The systematic coarse-graining approach is therefore well-founded and applicable to a wide variety of systems. The systematic nature of the proposed method allows us to investigate different levels of coarse graining where different amounts of information are kept in the coarser model. For each of the coarse-grained models we will determine their range of validity and thereby identify the appropriateness of the chosen level of description. The result of these works is a hierarchy of models - a truly multi-scale modelling of the system - which includes only the relevant set of variables needed on the chosen level of description.

We will develop and illustrate the method for the important case of polymeric and anisotropic fluids like liquid-crystals and ferrofluids. Many concepts of soft matter physics have been established for these systems. Moreover, transport and flow properties of polymeric and anisotropic fluids are also very interesting for industrial and food processing, as well as in biological environments. In view of these applications, we also plan to develop multi-scale simulations where we combine a finer and coarser model that we have already consistently related before, e.g. to study interface effects on bulk transport behavior.

Related information

Report Summaries

Final Report Summary - CGCOMPLEXFLUIDFLOW (Systematic and thermodynamically consistent coarse graining the flow of complex fluids)
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Subjects

Life Sciences

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