Coarse-Graining: Theory and Applications

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As an introduction, a general framework of nonequilibrium thermodynamics (GENERIC) is presented, and atomistic expressions for the building blocks of the framework are given. These expressions provide a systematic procedure for coarse-graining, and they are the basis for nonequilibrium simulations for systems of practical interest.

For this talk, I distinguish between two fundamentally different simulation approaches, "brute-force simulations" and "thermodynamically guided simulations." Brute-force simulations can be thought of as computer experiments mimicking the physical situation of interest directly on a computer; thermodynamically guided simulations rely on a nonequilibrium statistical ensemble containing the variables of some coarse-grained description of the system of interest. The availability of an appropriate coarse-grained level of description is thus crucial for thermodynamically guided simulations. Brute-force simulations require less insight, which may be considered as good or bad. For reasons to be explained in the talk, I find a negative annotation going with brute-force simulations more appropriate.

The above remarks are elaborated in the context of polymer melts. It is shown how simulations based on nonequilibrium ensembles can help to bridge the wide range of time scales from monomer motions to polymer processing. The importance of coarse-grained models for specifying an ensemble and for identifying suitable quantities of interest is illustrated.