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Transferability of Coarse Grained Models: a Challenge for Simulation of Phase Transitions or Phase Separation Processes

CHRISTINE PETER, Max Planck Institute for Polymer Research, Mainz

Upon developing a coarse grained (CG) model, representability and transferability limitations are a problem that is inherent to the process of reducing the number of degrees of freedom. In this context, representability refers to the question which structural or thermodynamic properties of a higher resolution reference are reproduced by the CG model, and transferability refers to the question to which extent a CG model is applicable at a state-point that differs from the one where it was parametrized. This is naturally a highly relevant problem in simulations that involve phase transitions or structure formation processes driven by phase separation, for example in liquid crystalline systems or in biomolecular aggregation. I will show with a few examples how one can achieve and rationalize state-point transferability for CG models that have been parameterized in a bottom-up procedure from atomistic reference simulations, for example by choosing an appropriate reference state point.