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TITLE: Computational Polymer Science - The challenge of Mesoscale Coarse Graining"

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ABSTRACT:

In polymer science, the macroscopic properties greatly rely on the microscopic properties of a specifically investigated system. Due to the broad range of time and length scales, not all questions can be dealt with at the atomistic level in which all atoms are contained explicitly. The detailed treatment of degrees of freedom that govern small scales computationally prohibits the consideration of the longer modes that determine macroscopic properties. To solve this problem, coarse graining to mesoscopic models is often considered. At this level, "superatoms" composed of up to ten atoms replace complete-chemical repeat units.

In recent years, several methods how to pursue the problem of moving from one scale to the other have been proposed and established. The crucial problem is to maintain the chemical identity of the specific polymer system at all levels. In this talk, we shall introduce our approach to do that, the "Iterative Boltzmann Inversion Method". Examples, advantages and shortcomings of this method will be presented. Finally, we will show some recent results and discuss upcoming challenges.