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Structure and Transport in Soft Materials Studied by Multiscale Simulation

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The mapping across length scales is now an established method in particle-based simulations of polymers and other soft-matter systems. Concepts known as coarse-graining and the inverse procedures known as reverse mapping, backmapping or fine-graining allow the bridging of scales from the electronic to the mesoscopic level. They use as basic building blocks or degrees of freedom anything from the electron (quantum chemistry), the atom (atomistic models), larger groups of atoms or superatoms (coarse-grained models), up to large sections of polymer chains (soft particle models such as dissipative particle dynamics). To devise such models which are simple enough for faster computation and yet complex enough to be material specific, a number of coarse-graining techniques have been devised. This talk covers the so-called Iterative Boltzmann Inversion, which has the reproduction of polymer structure as its primary target, its successes in the prediction of structural and thermodynamic properties, and the remaining challenges. One of them is the prediction of dynamic and transport properties.