

Abstract Submitted
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Exploring the Limits of the Iterative Boltzmann Inversion

ROLAND FALLER, UC Davis, BESTE BAYRAMOGLU, Izmir Institute of Technology — We explore the limits of the purely structure based coarse-graining technique, the iterative Boltzmann inversion (IBI), for confined systems using the example of polystyrene solutions. First some technical considerations and challenges encountered in the course of the optimization process are presented. The choice of the initial potentials and the cross-dependency of the interactions as well as the order of optimization are discussed in detail. Furthermore, the transferability between different degrees of confinement is examined. We investigate if a CG force field developed for a confined polymer solution by IBI is sensitive to changes in the degree of localization or arrangement of polymers near the surfaces although the concentration is kept constant. The differences in the structure and dynamics of the chains are addressed. Results are compared with those of an unconfined (bulk) system at the same concentration. The chain dimensions and orientations as a function of the distance from the surfaces are also reported. We find that the arrangement of monomers and solvent molecules near the surfaces is an important factor that needs to be paid attention to when considering the application of a CG force field developed by IBI to different degrees of confinement.

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