Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Multiresolution Modeling of Polymer Solutions: Wavelet-Based Coarse-Graining and Reverse-Mapping AHMED ISMAIL, CARL SIMON ADORF, ANIMESH AGARWAL, RWTH Aachen University, CHRISTOPHER R. IACOVELLA, Vanderbilt University — Unlike multiscale methods, which encompass multiple simulation techniques, multiresolution models uses one modeling technique at different length and time scales. We present a combined coarse-graining and reverse-mapping framework for modeling of semidilute polymer solutions, based on the wavelet-accelerated Monte Carlo (WAMC) method, which forms a hierarchy of resolutions to model polymers at length scales that cannot be reached via atomistic or even "standard" coarse-grained simulations. A universal scaling function is obtained so that potentials do not need to be recomputed as the scale of the system is changed. We show that coarse-grained polymer solutions can reproduce results obtained from the simulations of the more detailed atomistic system to a reasonable degree of accuracy. Reverse mapping proceeds similarly: using probability distributions obtained from coarse-graining the bond lengths, angles, torsions, and the non-bonded potentials, we can reconstruct a more detailed polymer consistent with both geometric constraints and energetic considerations. Using a "convergence factor" within a Monte Carlo-based energy optimization scheme, we can successfully reconstruct entire atomistic configurations from coarse-grained descriptions.

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Date submitted: 15 Nov 2013 Electronic form version 1.4