

Abstract Submitted  
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**Multiscale Modeling of Polymer Liquids** IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — For polymer systems, the time and length scales where relevant phenomena take place encompass a large range. Theoretical approaches and computer simulations are limited. The effective way to investigate polymer systems is to coarse-grain and apply multiscaling procedure. Using the Ornstein-Zernike relation we derived an analytical way to coarse-grain the structure of polymer liquids (homopolymer melts, block copolymers, and polymer mixtures) to the different length scales. The effective pair potential between coarse-grained units is an input to the mesoscale computer simulation. Outputs from the united atom simulation and mesoscale simulation are combined in an original multiscale procedure providing information at all length scales of interest, which substantially saves computational time. Rescaling the output of mesoscale simulations allow us to describe the dynamics of a system in the complete range of timescales of interest.

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