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A Multiscale Modeling Procedure for Simulations of Polymer Melts[1] JAMES MCCARTY, IVAN LYUBIMOV, MARINA GUENZA, Department of Chemistry, University of Oregon, Eugene, Oregon — One of the major ambitions in developing a coarse-grained model for macromolecular fluids is to provide a rigorous procedure to reintroduce the chemical details of the system. Such a scheme allows for the development of a multiscale modeling protocol. Here, a novel multiscaling scheme is presented that uses a hierarchical approach of combining mesoscopic and united atom molecular dynamic (UA MD) simulations. In this way, the multiple length and time scales of relevance to complex fluids are effectively bridged. The method is applied to various polymer melts of different architectures and chain lengths, and results are compared directly to UA MD simulations over the entire length-scale range of interest. It is shown that this approach reproduces pair correlation functions at a high computational efficiency, providing a method of extending simulations to very large length and time scales. Since the approach is analytical, it is applicable to a broad range of polymer systems.

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