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Analytical rescaling of dynamics from mesoscale simulations of coarse-grained polymer melts to their atomic description IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — Mesoscale simulations of coarse-grained polymeric systems enable the description of dynamics on much longer time scales than united atom simulations. However, because the energy landscape of the coarse-grained system is artificially smooth, the dynamics from mesoscale simulations is accelerated and needs to be rescaled. Starting from our analytical coarse-graining formalism, we derive a novel rescaling approach, which allows for the direct measurement of "real" dynamics from mesoscale simulations of a coarse-grained polymer liquid. The rescaling procedure is obtained in two steps, first through the inclusion of the intramolecular vibrational degrees of freedom, which were averaged out during coarse-graining, and second through the rescaling of the friction coefficient from the approximated solution of the memory kernel. Comparison of theoretical predictions of the diffusion coefficients and rotational decorrelation of the end-to-end vectors, for polyethylene liquids of increasing molecular weights, shows quantitative agreement against united atom simulations.

Ivan Lyubimov
University of Oregon

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