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Reconstructing Polymer Melt Dynamics Sped up due to Large-Scale Coarse-Graining IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — A theoretical approach to rescale the artificially fast dynamics of highly coarse-grained polymer melts is extended to chains represented as soft particles. The effective pair potential derived from first-principles to represent polymer chains with soft interactions is used to perform mesoscale molecular dynamics simulations of coarse-grained melts. This potential ensures the reproduction of the correct global structure and thermodynamics, but entropic and frictional corrections are necessary to reconstruct realistic dynamics. The behavior of the system is described by generalized Langevin equations derived for different levels of coarse-graining. The explicit analytical dependence on the thermodynamic and molecular parameters enhances the predictive power of the reconstruction method. The dynamics, reconstructed from mesoscale simulation, is in quantitative agreement with experiments and atomistic simulations.

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