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A First Principle Approach to Rescale the Dynamics of Simulated Coarse-Grained Macromolecular Liquids IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — A first-principle approach has been developed to rescale dynamical data from mesoscopic molecular dynamics simulations of polymer liquids. We derive rescaling factors from Generalized Langevin Equations (GLE) for the coarse-grained at the monomer level representation and coarse-grained at the mesoscopic level representation of the liquid, exploiting the Mori-Zwanzig projection operator formalism. The rescaling factors explicitly depend on coarse-grained model parameters and thermodynamic parameters. Two corrections need to be accounted to compensate the acceleration effect on dynamics caused by higher level of coarse-graining: change in entropy and change in friction. After applying our rescaling to data from mesoscopic simulations of unentangled and weakly entangled polyolefin melts we observe a good agreement with data of translational diffusion measured experimentally and from UA simulations. The method is used to predict self-diffusion coefficients for systems not yet investigated experimentally.

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