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Rescaling the Molecular Dynamics Simulation of Coarse-Grained Polymer Liquids[1] IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — Due to the limitations of theoretical approaches and computer simulations, coarse-graining of polymer systems facilitates the investigation of their dynamical and structural properties. A multiscaling description provides information at the whole range of time and length scales at which relevant phenomena take place. We use our analytical procedure to coarse-grain polymer liquids and produce mesoscale molecular dynamics simulations. Mesocalse simulations enable much longer times to be reached than in united atom simulations. However, the accelerated dynamics in mesoscale simulations need to be rescaled in order to correctly describe real time processes. We propose a rescaling procedure for mesoscale simulations of polymer liquids to allow for comparison it with united atom simulations. As a part of the rescaling procedure the friction coefficients for units of both mesoscale and united atom simulations were derived from the first principles. The rescaling procedure enhances the multiscaling modeling approach, substantially saving computational time.

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