Abstract Submitted
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Data-driven coarse-grained modeling for polymers[1] SHU WANG, WENXIAO PAN, University of Wisconsin-Madison — We present a data-driven coarse-graining method to establish coarse-grained (CG) modeling for polymers, which conserves both static and dynamic properties of the fine-grained (FG) system. The dynamics of the CG system is governed by the generalized Langevin equation (GLE) derived via the Mori-Zwanzig formalism, by which the CG variables can be directly linked to the statistics of FG data. The effect of unresolved degrees of freedom on the kinetics of polymers can be captured by the non-Markovian stochastic dynamics in GLE, where the memory kernel is determined from the FG data. To circumvent the difficulty of directly solving the GLE with memory term and colored noise, we exploit the equivalence between the non-Markovian dynamics and Markovian dynamics in an extended space. To this end, the CG system is supplemented with auxiliary variables that are coupled linearly to the momentum and among themselves, subject to uncorrelated Gaussian white noise. For several different polymer systems in melts or in solution, we demonstrate that the established CG modeling can reproduce both static and dynamic properties of the reference FG system.

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