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Non-Markovian coarse-grained modeling of polymeric fluids based on the Mori-Zwanzig formalism[1] ZHEN LI, XIN BIAN, Brown University, XIANTAO LI, Pennsylvania State University, GEORGE KARNIADAKIS, Brown University — The Mori-Zwanzig formalism for coarse-graining a complex dynamical system typically introduces memory effects. The Markovian assumption of delta-correlated fluctuating forces is often employed to simplify the formulation of coarse-grained (CG) models and numerical implementations. However, when the time scales of a system are not clearly separated, the memory effects become strong and the Markovian assumption becomes inaccurate. To this end, we incorporate memory effects into CG modeling by preserving non-Markovian interactions between CG variables based on the Mori-Zwanzig formalism. For a specific example, molecular dynamics (MD) simulations of star polymer melts are performed while the corresponding CG system is defined by grouping many bonded atoms into single clusters. Then, the effective interactions between CG clusters as well as the memory kernel are obtained from the MD simulations. The constructed CG force field with a memory kernel leads to a non-Markovian dissipative particle dynamics (NM-DPD). Quantitative comparisons on both static and dynamic properties between the CG models with Markovian and non-Markovian approximations will be presented.

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