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Speed-Up of Dynamic Observables in Coarse-Grained Molecular Dynamics Simulations of Polymer Melts PRAVEEN DEPA, JANNA MARANAS, Pennsylvania State University, PENN STATE TEAM — We provide a prediction for the "indirect speed-up" observed in Coarse-Grained Molecular Dynamics (CGMD) simulations of chain molecules, including those of biological significance. The indirect speed-up can be advantageous in that it provides reduction in computation time, in addition to the direct speed-up obtained by coarse-graining. By moving to a coarser description of the system, the interaction energies between the particles decrease (the potential energy surface becomes shallower), leading to an apparent increase in the time-step of the CGMD simulation. We borrow from the framework of Accelerated Molecular Dynamics method to predict the time-step i.e., the observed indirect speed-up. With this prediction of indirect speed-up, we are able to accurately reproduce both static and dynamic properties from CGMD simulations.

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