Speeding Up Intrinsically Slow Collective Processes in Particle Simulations by Concurrent Coupling to a Continuum Description

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The difficulty to study intrinsically slow collective processes by computer simulation of particle- based models stems from multiple disparate time scales (e.g., stiff bonded interactions vs soft non- bonded interactions and/or small Onsager coefficients). Continuum models, which describe the system by collective density variables rather than the coordinates of the individual molecular constituents, often do not suffer from this time-scale problem because the stiff microscopic degrees of freedom have been integrated out. We propose to concurrently couple these two descriptions by a heterogeneous multiscale method, which is comprised of three steps: (i) We estimate the parameters of the continuum description from simulations of the particle model, (ii) we propagate the configuration of the parameterized con- tinuum model for a large time step, and (iii) we relax the configuration of the particle model to the new order- parameter configuration of the continuum model. Then, the simulation cycle commences again. We illustrate the technique by studying the Lifshitz-Slyozov coarsening mechanism in a binary polymer blend using a soft coarse-grained particle model and a Landau-Ginzburg-de-Gennes free energy functional, respectively. A speed-up of up to two orders of magnitudes is achieved. We expect that this heterogeneous multiscale method can speed-up collective processes that occur on time scales that are much larger than the relaxation time of a single molecule and spontaneously proceed with a single time scale in the continuum description by amplifying the collective driving forces via a restraining potential or by additionally coupling the particle system to a flow field that matches the time evolution of the densities predicted by the continuum model.