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Using Markov State Models to Study Self-Assembly MATTHEW PERKETT, MICHAEL HAGAN, Brandeis University — In recent years, a number of algorithms have been developed to study rare events, which has resulted in paradigm shift from running a few long trajectories to gathering statistics from many shorter trajectories. Running many simulations in parallel to build a Markov State Model (MSM) is one such technique, which has been applied to protein folding with great success. We present an adaptation to the MSM framework that enables its application to a wide range of systems undergoing self-assembly. The feasibility of this approach is demonstrated on two different coarse-grained models for virus self-assembly. We find good agreement between the MSM calculations and brute force long simulations, with up to several orders of magnitude reduction in simulation time.

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