Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Improving the kinetics from molecular simulations using biased Markov state models JOSEPH F RUDZINSKI, KURT KREMER, TRISTAN BEREAU, Max Planck Institute for Polymer Research — Molecular simulations can provide microscopic insight into the physical and chemical driving forces of complex molecular processes. Despite continued advancement of simulation methodology, model errors may lead to inconsistencies between simulated and experimentally-measured observables. This work presents a robust and systematic framework for reweighting the ensemble of dynamical paths sampled in a molecular simulation in order to ensure consistency with a set of given kinetic observables. The method employs the well-developed Markov state modeling framework in order to efficiently treat simulated dynamical paths. We demonstrate that, for two distinct coarse-grained peptide models, biasing the Markov state model to reproduce a small number of reference kinetic constraints significantly improves the dynamical properties of the model, while simultaneously refining the static equilibrium properties.

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Date submitted: 30 Oct 2015 Electronic form version 1.4