Simulation of Dynamical Processes in Block Copolymer Micelles
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Micellar solutions exhibit a "fast" dynamical process associated
with single-molecular insertion and expulsion and a "slow" process associated with
birth and death of entire micelles. We report an analysis of simulations of highly
asymmetric "hairy" micelles that is designed to quantify rates of both types of pro-
cess, and to elucidate mechanisms. By modeling diffusion of the micelle aggregation
number on a well characterized free energy surface, we are able to calculate and
compare relaxation for different possible mechanisms for the slow process, which
would otherwise be computationally inaccessible. This method allows us to com-
pare the rate for step-wise association and dissociation to the rate of the competing
mechanism of micelle fission and fusion.

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