Using an Ensemble of Surrogate Process Approximations (SPAs) to Assist Computing Quantities Depending on Rare Events

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In both MD and single-molecule experiments, the detailed dynamics are typically believed to be governed by a complex high-dimensional system of equations (e.g. Nose-Hoover dynamics). The vast range of time-scales often present in the full system complicates the task of accurately summarizing the information in these complex systems. Statistical mechanics has provided a variety of useful techniques for describing the salient features of some complex systems; e.g. when a "good" set of reaction coordinates is known, the potential of mean force (PMF) along this set is often computed because the PMF summarizes useful thermodynamic properties. I demonstrate how a collection of surrogate processes, estimated from a relatively small number non-equilibrium time series, can assist some PMF and diffusion coefficient computations. The so-called surrogate process approximation (SPA) [1] can be used to both refine average estimates and also provide the corresponding uncertainty bands (characterizing randomness at multiple scales) in various computations depending on the tails of a non-equilibrium work distribution [2,3]. A collection of SPA models can also be used to infer information about slowly evolving degrees of freedom not directly monitored. Illustrative results obtained using steered MD simulation of gramicidin A [3] and AFM pulling experiments [4,5] are presented.

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