Extracting multiscale information from time series characterizing nanoscale systems.

Single-molecule experiments and computer simulations have generated noisy data sets containing useful information about the dynamics of nanoscale systems. The many degrees of freedom present and multiple time-scale fluctuations inherent at this level of detail complicate the task of summarizing the interesting information in these data sets. I demonstrate how a collection of surrogate processes, estimated from batches of time series using new local maximum likelihood techniques, can assist in understanding these complex data sets. Both thermodynamic and kinetic information can be extracted using the collection of surrogate models. The methods are also useful when a good set of system observables is unknown or not experimentally accessible. For example, a collection of surrogate models can be used to infer information about slowly evolving degrees of freedom not directly monitored. Illustrative results obtained using various all-atom molecular dynamics simulations and atomic force microscope experiments are presented. I also discuss new penalized spline algorithms that were developed to address the ill-conditioned design matrices that can result when modeling the single-molecule time series data and outline future applications/extensions of the algorithms developed. (Received July 25, 2009)