1056-60-91 **Christopher P Calderon*** (calderon@rice.edu), Lawrence Berkeley National Lab, 1 Cyclotron Rd, Berkeley, CA 94720. *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)