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# Theoretical Characterization of Protein Folding Dynamics: Connecting Atomist Model with Time-Resolved Spectroscopy Data

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## Abstract

From a theoretician's perspective, the characterization of the protein folding process involves overcoming three formidable challenges. First, one needs to generate a statistically significant ensemble of transition pathways, which provide extremely rare fluctuations. Next, the huge amount of data contained in the reactive trajectories needs to be reduced, in order to identify the essential slow processes and meta-states. Finally, theoretical predictions have to be validated against the existing experimental data, which typically provide information on the dynamics of a limited set of collective variables.

In this talk we show how these three major steps can be undertaken by a specific combination of advanced enhanced sampling algorithms, statistical analysis and quantum chemical calculations, to provide contact with spectroscopic observables.

We present applications to specific protein folding processes, where theoretical predictions are directly compared against time resolve linear spectroscopy data.

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