Biomolecular Dynamics
Stock Lab

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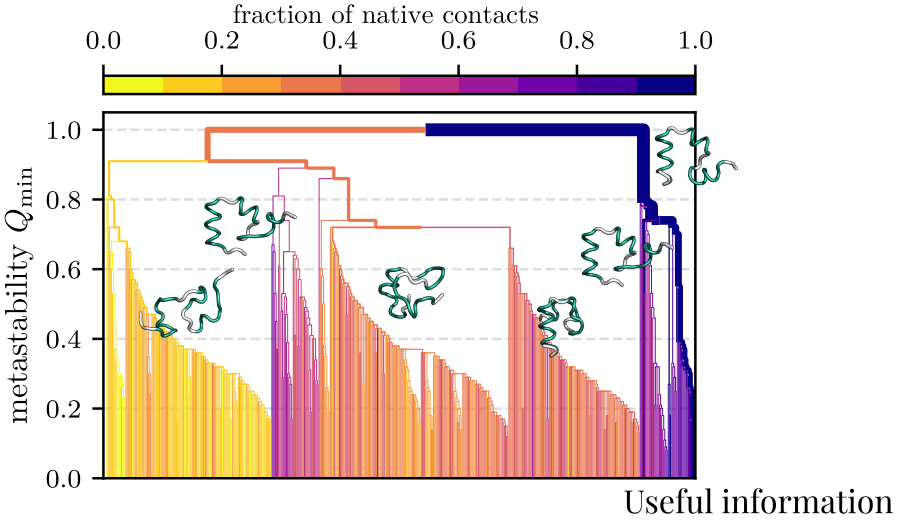
Bachelor/Master Project

Learning the structural evolution of protein function

Protein function is intimately linked to their 3D structure, such that dynamical processes are associated with transitions between different structures. Hence, by knowing the various structural states of a protein and their evolution in time, we can get a first picture on how this nanomachine works. Due to large-amplitude structural fluctuations and the huge amounts of data, however, the clustering of computer simulation data into structurally well defined and dynamically metastable states represents a formidable challenge.
Here we use machine learning strategies such as the most probable path algorithm to learn and describe protein states. The project involves the development of a smart stochastic version of the so far deterministic algorithm, which should represent a more robust model of the process.



Identifying Metastable States of Folding Proteins; Jain and Stock; Journal of Computational and Theoretical Chemisty, 2012

Perspective: Identification of collective variables and metastable states of protein dynamics; Sittel, Stock; Journal of Chemical Physics, 2018

Talk to:

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