Biomolecular Dynamics
Stock Lab

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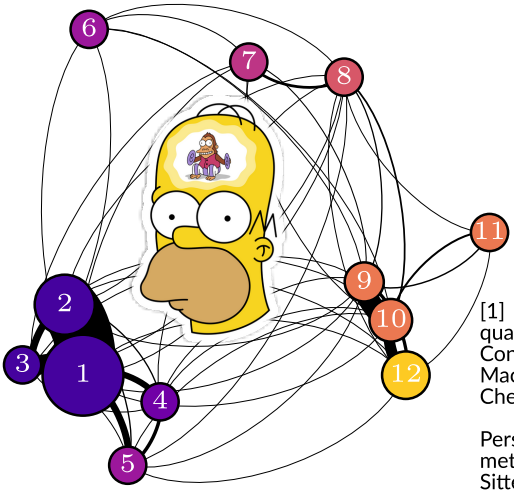
Bachelor/Master Project

Memory in Protein Graphs

Computer simulations of protein dynamics are commonly interpreted in terms of a graph or a network of discrete states, which reflect distinct 3D structures of the protein. To provide a simple mechanistic understanding of the considered process, it is usually assumed that transitions between the states exhibit no memory. This means that they depend only on the last step, thus constituting a random walk on the graph. As this naive assumption has been found largely incorrect in recent studies, we aim to construct a protein interaction network including the effects of memory. From a theoretical point of view, this leads to a so-called generalized master equation, which needs to be derived for a given process to be described.
Practically speaking, the project involves the development and implementations of algorithms that determine the parameters of the model from a molecular dynamics simulations. Applications include protein folding and the signal transport or communication between proteins.



Useful information

[1] A Step-by-step Guide on How to Construct quasi-Markov State Models to Study Functional Conformational Changes of Biological Macromolecules; Yik, Qiu, Unarta, Cao, Huang; ChemRxiv, 2022

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

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