PhD Project: Memory of Protein Graphs

Computer simulations of protein dynamics are often analyzed using graphs or networks of discrete states, where each state corresponds to distinct 3D structures of the protein. To obtain a simple mechanistic description of the underlying process, transitions between states are typically assumed to be memoryless, depending only on the current state. Under this assumption, the dynamics can be represented as a random walk on the network, resulting in a Markovian state model. However, this simplifying assumption has been shown to be inadequate in many cases, particularly for nonequilibrium processes that are pervasive in biological systems. To account for memory effects in protein interaction networks, one can either derive a generalized master equation that explicitly incorporates history dependence or construct a Markovian embedding by defining a more suitable set of states.

In practice, this project focuses on the development and implementation of algorithms that infer model parameters from molecular dynamics simulations, including a range of machine learning techniques. These methods are applied to a variety of proteins, including those involved in folding and unfolding processes, signal propagation through the proteins as well as direct communication between separate domains. The project is part of the DFG Research Unit 'Reducing complexity of nonequilibrium systems', see https://www.for5099.uni-freiburg.de

We are seeking a highly motivated, creative, and collaborative Ph.D. candidate with a strong interest in interdisciplinary research. Applicants should hold a Master's degree in Physics and have a background in computational physics, along with experience in Python programming.

Please apply **until 15 July 2026** to:

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