

Dr. Joseph F. Rudzinski

Joseph received a Bachelors in chemistry and mathematics from the University of California, Santa Barbara in 2009. In 2014, he completed his Ph.D. in theoretical chemistry at The Pennsylvania State University in the group of Professor Will Noid, studying statistical-mechanics-based methods for constructing coarse-grained simulation models. Joseph moved to Mainz in 2015 to work on the interpretation of coarse-grained dynamics at the Max Planck Institute for Polymer Research, under the supervision of Kurt Kremer and Tristan Bereau. He received a Humboldt Postdoctoral Fellowship in 2016 to develop methods for constructing kinetically-consistent coarse-grained models for peptides. Joseph has been working as a group leader since January 2020, with a focus on developing multiscale simulation methodologies and investigating the interactions and conformational dynamics of disordered biological polymers.

Research Interests

Structurally- and Kinetically-consistent Coarse-grained Simulation Models

Coarse-grained (CG) models can provide computationally efficient and conceptually simple characterizations of soft matter systems. While generic models probe the underlying physics governing an entire family of free-energy landscapes, bottom-up CG models are systematically constructed from a higher-resolution model to retain a high level of chemical specificity. We develop methods for tackling the many challenges that arise when coarse-graining, including reproducing relevant higher-order structural correlations as well as recovering the connection to the true underlying dynamics.

Automated Analysis of Molecular Simulation Trajectories

Extracting insight from the enormous quantity of data generated from molecular simulations requires the identification of a small number of collective variables whose corresponding low-dimensional free-energy landscape retains the essential features of the underlying system. Data-driven techniques provide a systematic route to constructing this landscape, without the need for extensive a priori intuition into the relevant driving forces. We apply existing methods and develop new methods for extracting the essential features from molecular simulation data, including the construction of kinetic models and performing dimensionality reduction and clustering using deep learning. Applications include characterizing conformational dynamics of disordered proteins, diffusion kinetics in glassy liquids, and polymorphism in polymer crystallization.

Interactions and Conformational Dynamics of Disordered Proteins

The interactions of intrinsically disordered proteins (IDPs) play an important role in biological processes but present a number of fundamental challenges for computational modeling. While single chain conformational dynamics can be described by coarse-grained models with near-atomic resolution and specialized implicit solvent interactions, much simpler models are often adopted for investigating interactions between multiple IDPs. We apply sophisticated methods for multiscale modeling and simulation analysis to help probe the essential driving forces in these challenging, biologically-relevant disordered systems.

Publications

Interpretable embeddings for molecular kinetics using Gaussian mixture variational autoencoders, Y. Bozkurt Varolgüneç, T. Bereau, J.F. Rudzinski, Machine Learning: Science and Technology, arXiv ... (2019)

Recent Progress towards Chemically-Specific Coarse-Grained Simulation Models with Consistent Dynamical Properties, J.F. Rudzinski, Computation 7(3), 42 (2019)

Accurate Structure-Based Coarse Graining Leads to Consistent Barrier-Crossing Dynamics, T. Bereau, J.F. Rudzinski, Physical Review Letters 121, 256002 (2018)

Consistent interpretation of molecular simulation kinetics using Markov state models biased with external information, J.F. Rudzinski, K. Kremer, K., T. Bereau, Journal of Chemical Physics 144, 051102 (2016)

Personal webpage

<http://www.RudzinskiResearch.com>

Highlight projects

Surface-hopping models for reproducing structural cross-correlations and barrier crossing dynamics with coarse-grained models

Gaussian mixture variational autoencoder for performing dimensionality reduction and clustering of metastable states in a single unified framework

Investigating the polymeric properties of intrinsically-disordered proteins

Cooperations

Prof. Tristan Bereau (University of Amsterdam) - Molecular Kinetics

Dr. Grazia Gonella (MPIP) - Peptide Aggregation on Surfaces

Prof. Mehmet Sayar (Koç University) - Peptide Conformational Dynamics