Machine Learning and Data Science for Understanding and Design in Colloidal Assembly and Protein Folding

Date : Friday, January 18, 2019

Time : 4:00 pm – 5:00pm

Location : Neckers 240

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Abstract:

Data-driven modeling and machine learning have opened new paradigms and opportunities in the understanding and design of soft and biological materials. The automated discovery of emergent collective variables within high-dimensional computational and experimental data sets provides a means to understand and predict materials behavior and engineer properties and function. I will describe our recent work in the use of two machine learning techniques for collective variable discovery within molecular simulation – nonlinear manifold learning using diffusion maps, and nonlinear dimensionality reduction using autoencoding neural networks ("autoencoders"). First, I will describe our applications of graph matching and diffusion maps to determine low-dimensional assembly landscapes for self-assembling patchy colloids. These landscapes connect colloid architecture and prevailing conditions with emergent assembly behavior, and we use them to perform inverse building block design by rationally sculpting the landscape to engineer the stability and accessibility of desired aggregates. Second, I will describe our use of autoencoders to perform automated discovery of collective variables in protein folding. We interleave deep learning variable discovery and enhanced sampling directly within the discovered variables to perform simultaneous on-the-fly variable discovery and accelerated sampling of protein folding funnels.

Bio:

Dr. Ferguson is an Associate Professor of Molecular Engineering at the University of Chicago. He received an M.Eng. in Chemical Engineering from Imperial College London in 2005, and a Ph.D. in Chemical and Biological Engineering from Princeton University in 2010. From 2010 to 2012 he was a Postdoctoral Fellow of the Ragon Institute of MGH, MIT, and Harvard in the Department of Chemical Engineering at MIT. He was a faculty member in the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign from 2012 to 2018. He joined the Institute for Molecular Engineering in July 2018. He is the recipient of a 2017 UIUC College of Engineering Dean's Award for Excellence in Research, 2016 AIChE CoMSEF Young Investigator Award for Modeling & Simulation, 2015 ACS OpenEye Outstanding Junior Faculty Award, 2014 NSF CAREER Award, and 2014 ACS PRF Doctoral New Investigator.