Stanford MEDICINE | Department of Biomedical Data Science

BIODS 260C

From coarse-grained models to conformational ensembles

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1:30PM-2:50PM

MSOB X303

Abstract:

This talk will give a detailed introduction to design principles for generative models of molecular systems. We will first discuss several relevant paradigms for building generative models, including score-based diffusion and continuous normalizing flows. We will then detail how both intramolecular and intermolecular constraints inform the architectures appropriate for modeling nanoscale materials. Finally, we will come to the crucial question of how to build scalable training strategies for systems where thermal fluctuations cannot be neglected. The talk will end with a discussion of the most pressing open problems for generative "AI" in the physical sciences.

Reading list:

- https://pubs-acs-org.stanford.idm.oclc.org/doi/full/10.1021/acs.jpcb.3c08195
- https://pubs-aip-org.stanford.idm.oclc.org/aip/jcp/article/158/12/124126/2881730