THE CHINESE UNIVERSITY OF HONG KONG

Department of Physics

COLLOQUIUM

Modeling Rare Events: Discovering Reaction Pathways, Slow Variables, and Committor Probabilities with Machine Learning

by



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Date: September 29, 2023 (Friday)
Time: 3:00 - 4:00 p.m.
Place: L2, Science Centre, CUHK

(Light refreshments will be served at SCNB 1/F lobby from 2:30 to 2:50 p.m.)

ALL INTERESTED ARE WELCOME
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Abstract

Atomistic simulations face a formidable challenge in tracking transitions between metastable states in slow molecular processes. To accelerate the underlying dynamics, importance-sampling methods are used, relying on compact reaction-coordinate (RC) models. Traditionally, researchers reduce dimensionality based on intuition. However, modern machine-learning (ML) algorithms now offer powerful alternatives. In this lecture, I will compare two ML methods, state-free reversible variational approach for Markov processes networks, or SRVs, and variational committor-based neural networks, or VCNs, in discovering meaningful RCs for slow molecular processes. Both can be incorporated into importance-sampling schemes, enhancing our understanding of transition kinetics.

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