



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
COLLOQUIUM

Learning Transition Pathways Using Artificial Neural Networks

by



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Date: January 24, 2025 (Friday)

Time: 4:00 - 5:00 p.m.

Place: L2, Science Centre, CUHK

(Light refreshments will be served at [SCNB 1/F lobby](#) from 3:30 to 3:50 p.m.)

ALL INTERESTED ARE WELCOME

Abstract

I will present a neural-network-based strategy that simultaneously learns the committor function and committor-consistent string, providing a novel framework for uncovering transition pathways in rare-event dynamics. This approach, based on the committor time-correlation function, transcends traditional methods by accommodating diverse dynamical regimes and distinguishing competing pathways. Demonstrated on benchmark potentials and biological systems, it accurately captures dynamics, rate constants, and mechanisms. Its adaptability to collective variables and robustness across neural architectures establish it as a versatile tool for enhanced-sampling simulations, offering deep insights into complex biomolecular landscapes.

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