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The Hong Kong University of Science and Technology

Scientific Computation Concentration



Modeling and simulation of complex dynamical systems

By

Prof. Frank Noe

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Abstract

In this talk, Prof. Frank Noe will focus on two aspects in the analysis and simulation of complex dynamical systems:

1) variational approximation of complex dynamical systems: A central goal in describing complex dynamical systems is to obtain simple yet accurate, low-rank models from simulation data. Prof. Frank Noe will describe a variational approach for Markov processes from which we can derive algorithms to compute optimal dynamical models of the long-time behavior from simulation data. Prof. Frank Noe will show both shallow and deep learning frameworks that exploit this approach in order to obtain low-rank models from high-dimensional molecular dynamics simulations

2) particle-based reaction dynamics (PBRD) is a natural way to embed the low-rank dynamical models obtained from (1) into a larger-scale framework in order to simulate processes in chemical reactors or signal transduction in biological cells. Prof. Frank Noe will describe simulation models and efficient computing methods to realize PBRD with interaction forces between the particles in a physically meaningful way.

Date: Wednesday, 11 April 2018

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

***Venue: Room 5510, Academic Building
(near Lifts 25 & 26), HKUST***

All are welcome!