



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
SEMINAR

Nonequilibrium Driven Processes for Equilibrium Averages and Free Energies

by

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Date: February 13, 2012 (Monday)

Time: 1:30 - 2:30 p.m.

Place: G06 Y. C. Liang Hall, CUHK

ALL INTERESTED ARE WELCOME

Abstract

In the late 1990s, the field of nonequilibrium statistical mechanics was reinvigorated by a series of discoveries that exactly relate path-ensemble averages of nonequilibrium driven processes to equilibrium averages and free energies. For a substantial part of my career, I have been working on the application of these theorems to real-life problems. I will describe how a nonequilibrium driven process can be used as a Monte Carlo trial move, combining trajectory data from forward and reverse path-ensembles, and the postprocessing of trajectories to obtain distinct path-ensemble averages. I will also describe planned applications of the Nonequilibrium Candidate Monte Carlo method to problems in computational molecular biophysics.

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