Topics in Stochastic Modeling and Simulations

Topic (2017): Rare Events: Theory and Computation

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Course Outline:

Lect01: Introduction: Formulation, examples and issues

Part 1: Zero temperature regime

Lect02: Gradient system:
Path integral and LDT (diffusion process),
Transition path: MAM, NEB, String method etc.
Lect03: Transition rate asymptotics: 1D and Multi-D
Lect04: Saddle points finding: Dimer, GAD etc.
Lect05: Non-gradient system:
Chemical reaction kinetics, large volume limit,
Path integral and LDT (jump process)
Lect06: Energy landscape and gMAM
Lect07: Non-gradient system: difficulties and unsolved issues
Lect08: Spectral theory approach
Lect09: Onsager-Machlup and Freidlin-Wentzell dilemma

Part 2: Finite temperature case

Lect10: Potential Theory for Markov processes: I
Lect11: Potential Theory for Markov processes: II
Lect12: Transition path theory: Diffusion and jump case
Lect13: Finite temperature string method
Lect14: Markov state modeling: I (Formulation and computation)
Lect15: Markov state modeling: II (Analysis and applications)

Part 3: Sampling approach

Lect16: Accelerated MD, TAMD, AFED etc.
Lect17: Umbrella sampling, meta-dynamics, replica exchange etc.

Topics to be covered: rare events on manifold, multiscale system, max-flux formulation, meta-stability theory, …