The University of Chicago
Departments of Computer Science,
Mathematics, and Statistics

Scientific and Statistical Computing Seminar

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Modeling and Simulation of Reactive Events

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133 Eckhart Hall, 5734 S. University Avenue (unless announced otherwise).

ABSTRACT

The dynamics of a wide range of systems involve reactive events, aka activated processes, such as conformation changes of macromolecules, nucleation events during first-order phase transitions, chemical reactions, bistable behavior of genetic switches, or regime changes in climate. The occurrence of these events is related to the presence of dynamical bottlenecks of energetic and/or entropic origin which effectively partition the phase-space of the dynamical system into metastable basins. The system spends most of its time fluctuating within these long-lived metastable states and only rarely makes transitions between them. The reactive events often determine the long-time evolution of the system one is primarily interested in. In simple settings the Freidlin-Wentzell theory of large deviations provides a complete picture of how and when rare events occur. However, large deviation theory is valid in a parameter range where the random noise affecting the system is very small, which is often an inadequate assumption in complex systems. In addition, it becomes cumbersome to build numerical tools directly on Freidlin-Wentzell large deviation theory when the rare reactive events involves intermediates states, multiple pathways, etc. which is also the typical situation in high-dimensional systems. In this talk, I will explain why and describe a framework which allows to go beyond large deviation theory and can be used to identify the pathways and rate of rare reactive events in situations where the noise is not necessarily small, there are multiple pathways, etc. I will also describe numerical tools that can be built on this framework. Finally I will illustrate these tools on a selection of examples from molecular dynamics and material sciences.

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