Yale Institute for Nanoscience and Quantum Engineering

Friday-March 2, 2018

12:00-1:00 PM

BECTON SEMINAR ROOM
Light lunch will be served at 11:45 a.m.

Amir Haji-Akbari
Department of Chemical and Environmental Engineering, Yale University

TOO SMALL IS NEVER TOO SMALL: USING ADVANCED SAMPLING TECHNIQUES TO STUDY RARE EVENTS, FROM ATMOSPHERIC ICE NUCLEATION TO DESALINATION

More often than not, scientists are challenged with the daunting problem of measuring or computing astronomically small quantities that are related to the occurrence of rare events. A phenomenon is called a **rare event** when the amount of time that elapses before its occurrence is orders of magnitude larger than the time needed for its completion. Rare events are ubiquitous in nature, and span a wide range of phenomena such as earthquakes, telecommunication and power grid failures, protein folding, genetic mutations, and crystallization. Capturing the statistical nature of such events is key in many applications, including materials synthesis, climate modeling, bioengineering and medicine. Unfortunately, achieving this with conventional experiments or simulations is inefficient at best as the waiting times for observing a single rare event can surpass the experimentally or computationally accessible timescales by several orders of magnitude. This becomes an almost impossible undertaking when the rate of occurrence of a rare event is astronomically small. Under such circumstances, specialized sampling techniques are necessary for capturing the statistical features of the corresponding rare event.
In this presentation, I will talk about a computational technique known as forward flux sampling (FFS) that has been specifically designed for computing such minuscule occurrence probabilities [1]. I will discuss a variant of FFS newly developed in my group particularly suited for studying phenomena such as crystallization, that can only be described using jumpy order parameters [2]. As case studies, I will talk about our recent work in using this technique to address a longstanding problem in cloud microphysics regarding the role of vapor-liquid interfaces in inducing ice nucleation. I will also discuss our recent work on using FFS to model ion selection in desalination processes.

Megan King
Department of Cell Biology, Yale University

"The Mechanics and Dynamics of the Cell Nucleus"

The organization and dynamics of chromatin within the nucleus of eukaryotic cells influences all genomic processes, including gene regulation, genome replication and DNA repair. A major barrier to a quantitative and comprehensive understanding of chromatin organization is the lack of versatile, tractable systems in which to probe and interpret chromatin dynamics. In collaboration with the Mochrie lab, my group is leveraging recently developed methods to combine observations of the dynamic behavior of specific chromatin loci in individual living cells with a systems-level image and data analysis pipeline that sorts single-particle-tracking data from a population of cells into discrete diffusive states. Using the power of the genetic model, fission yeast, we are defining the key factors that influence chromatin structure, for example the protein complexes cohesin and condensin. This project is also being driven by insights derived from simulations of chromatin organization based on looping interactions. Lastly, I will discuss new ideas for monitoring dynamic chromatin conformations through proximity-dependent recombination reactions that become encoded in the DNA sequence.

Host: Professor Corey O’Hern