School of Molecular Sciences
Arizona State University

SMS Spring 2024 Seminar Series

Friday March 1 | 3:00 pm | Biodesign Auditorium

Computer Simulations of Large-Scale, Long-Time Biomolecular Motions: Examples and Theoretical Methods

Biomolecules undergo large-scale conformational changes along pathways that are heterogeneous in time and space, and therefore this process is to be fundamentally understood at the single-molecule level. In my talk, I will present *virtual* single-molecule “experiments," i.e., computer simulation results obtained by my research team that showcase several examples of large scale rearrangements. They will include protein-induced DNA , DNA ejection from bacteriophage viruses, and dendrimer transport in the context of single-pore current measurements.

On the methodological side, two techniques we developed for these simulations will be showcased. One uses molecular-dynamics derived parameters to scale up the dynamics on the micrometer-microsecond scale via the Kirchhoff theory for elastic rods. The other allows for the enhanced calculation of long-time kinetics in complex systems and is based on the Wiener stochastic path integral formalism: assigning weights to Langevin trajectories of artificially biased dynamics allows for the calculation of time correlation functions for the unbiased system of interest via re-weighting.

Ioan Andricioaei, PhD

Professor, University of California, Irvine

Ioan Andricioaei, a native of Romania, studied physics and biophysics at the A. I. Cuza University of Iasi. He then pursued graduate studies at Boston University and completed his Ph.D. in 1999 under the supervision of Professor John Straub. He then worked as a postdoctoral fellow at Harvard with Nobel Laureate Martin Karplus. Andricioaei was then on the faculty at the University of Michigan, before moving to the University of California, Irvine in 2008, where he is Professor of Chemistry. His research explores theoretical topics at the interface between molecular biophysics and physical chemistry.

**ZOOM option available: https://asu.zoom.us/j/81517529537*