UCMERCED | CHEMISTRY & BIOCHEMISTRY

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CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

Free-energy estimation at and far from equilibrium through stochastic control

Abstract:

Free energy landscapes are ubiquitous in the study of chemical and biological systems, in part because statistical mechanics teaches that the structure of systems at thermodynamic equilibrium governs their function under weak perturbations. This simple relation breaks down as the system is driven non-perturbatively or persistently, at which point dissipation couples with energetics to determining structure and stability. A precise characterization of this interplay is provided by the fluctuation theorems of stochastic thermodynamics, which relate structural deformations to generalized notions of dissipation as a system shifts away from equilibrium. The integral fluctuation theorems suggest quantifiable structure-function relations for passive, driven, and self-propelled systems, but their accurate evaluation can be challenging as it requires access to rare dissipative fluctuations that dominate the relevant averages. In this talk, we discuss our ongoing work formalizing connections between time-reversed response and statistically optimal free-energy estimation to develop a class of importance-sampling methods that render rare fluctuations typical under an optimally controlled surrogate dynamics. These methods allow for efficient nonequilibrium free-energy estimation while providing mechanistic insight into dissipative pathways in complex systems. We apply our methods to accurately resolve free energy landscapes at and away from equilibrium, achieving accurate characterizations of the free-energetic deformation of a semi-flexible filament under strong self-propulsive driving, the formation free energy of simple solids, and the solvation free energy of an isomerizing molecule in explicit solvent.

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About the Speaker:

Jorge is an NSF MPS-ASCEND postdoctoral fellow at the Department of Chemistry in UC Berkeley. He currently works in the group of David Limmer, developing free-energy estimation methods for molecular models of soft matter in and out of thermodynamic equilibrium, with the aim of studying how dissipation governs structural transitions along self-assembly protocols of active matter and along upcycling pathways of emerging materials. Jorge completed his PhD under Tom Miller at Caltech, developing path-integral methods for simulating nuclear quantum effects in condensed-phase systems, after obtaining a BSc with honors in the University of Puerto Rico's Chemical Engineering program.

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