

UNIVERSITY OF CALIFORNIA, IRVINE

THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

Is Proud to Host a Seminar by:

PRESIDENT'S POSTDOCTORAL FELLOW

JORGE L. ROSA-RAICES

Department of Chemistry
University of California, Berkeley

Thursday, June 1, 2023

2:00-3:20 PM

Location:

McDonnell Douglas Engineering Auditorium

Non-Equilibrium Free-Energetics of Active Filaments From Variational Time Reversal

Abstract: The interplay between dynamics, structure and function of active systems is central to inquiries ranging from spontaneous organization inside the cell nucleus to macroscopic collective organization of self-driven agents. In this talk, we introduce a method to estimate deviations from equilibrium of arbitrary structural properties of active systems through the solution of a stochastic optimal control problem for non-equilibrium free-energy profiles along order parameters. We find a physical interpretation for a unique optimal control policy as that which achieves a non-dissipative time reversal of the driven system, and use this knowledge to design ansätze that lead to rapid convergence in a variational reinforcement-learning implementation of the control problem. Applications of this scheme to coarse-grained models of active semi-flexible filaments swimming freely and under confinement allow us to map out non-equilibrium density enhancements of structural-dynamic motifs as functions of the distribution and intensity of active forces along the filament's backbone.

Bio: Dr. Jorge L. Rosa-Raíces obtained his Bachelor's degree in Chemical Engineering from the University of Puerto Rico, Mayagüez and his PhD degree in Caltech on path-space MCMC methods for molecular simulation under the supervision of Prof. Thomas F. Miller, III. He currently works in the research group of David Limmer at UC Berkeley on control-theoretic methods for simulating rare-events in the non-equilibrium stationary states of active materials.