UNIVERSITY OF DELAWARE

CENTER FOR BIOINFORMATICS & COMPUTATIONAL BIOLOGY

BIOINFORMATICS SEMINAR

JUAN R. PERILLA

Associate Professor Chemistry & Biochemistry

UNIVERSITY OF DELAWARE

Molecular dynamics simulations of large macromolecular complexes

Connecting dynamics to structural data from diverse experimental sources, molecular dynamics simulations permit the exploration of biological phenomena in unparalleled detail. Advances in simulations are moving the atomic resolution descriptions of biological systems into the million-to-billion atom regime, in which numerous cell functions reside. Here, I present ongoing research in my group, driven by large-scale molecular dynamics simulations, in the study of viruses, bacterial and human systems. These examples highlight the utility of molecular dynamics simulations in the critical task of relating atomic detail to the function of supramolecular complexes, a task that cannot be achieved by smaller-scale simulations or existing experimental approaches alone.

BIOGRAPHY

Principal Investigator Perilla Laboratory

Interests:
Molecular biophysics
Molecular mechanisms of HIV-1 infection

Education:
Postdoctoral Training - University of Illinois at Urbana-Champaign
Ph.D. Biophysics - Johns Hopkins University
B.S. Physics - Universidad Nacional de Colombia

Perilla Lab
Molecular biophysics of cellular processes
https://perilla.chem.udel.edu/

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