Computational Biology Seminar Series for Undergraduates

Molecular Dynamics Simulation Studies of Surface and Interfacial Phenomena in Biomolecular Systems

Dorel Moldovan, Associate Professor

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Life Sciences Annex Auditorium A101
January 22, 2014 - 05:30 pm

Abstract:

Biomolecular systems such as cell membranes, DNA, and proteins have unique attributes that make them suitable for a large number of applications of great importance in pharmaceuticals, biosciences, biomedical, and biomolecular engineering. Much of the advancements in these applications are hindered by our limited understanding of the fundamentals of these molecules structure, interaction, and transport properties in the presence of various surfaces or interfaces. In this seminar I will give a brief introduction of the molecular dynamics (MD) simulation methodology and present some of our recent MD investigations into a host of open research problems pertaining to the areas of cryopreservation, drug delivery systems, and DNA sequencing.

Speaker's Bio:

Dr. Dorel Moldovan obtained his Ph.D. from West Virginia University in Physics. Dr. Moldovan's research interests include condensed matter and materials physics focusing on various surface and interfacial phenomena such as elastic instabilities in membranes and polymers, and on microstructure evolution and thermal stability of nanocrystalline materials. Using atomistic and mesoscale simulations his recent research focuses on the development of fundamental understanding of large scale behavior of various biopolymers and lipid structures based on the interactions between atoms.

As a member of LA-SiGMA project Dr. Moldovan will explore, using atomistic and coarse grained simulations, the assembly and the interaction with lipid bilayers of various self-assembled drug delivery vehicles. In addition, he will contribute to other computational tasks such as the development of all-atom and coarse grained force field for biomaterials and the development of hybrid MD/continuum formalisms for simulation of bimolecular systems and their implementation into LAMMPS.

This lecture has a reception @ 05:00 pm

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