

Computer Science Seminar Series, 2012

National Capital Region

Probabilistic Methods for Structural Characterization of Protein Systems

Speaker: Prof. Amarda Shehu

George Mason University

Friday, March 16, 2012

1:00PM- 2:00PM, NVC 325

Abstract

Detailed characterization of physics-based systems often requires addressing search and optimization problems for complex high-dimensional non-linear solution spaces. Characterizing the structures and motions that protein molecules, these ubiquitous and central biological molecules in living cells, employ for their biological function is a fundamental issue in our understanding of biology and treatment of disease. Protein systems are inherently flexible, have complex geometry, and numerous inter-related degrees of freedom. Understanding proteins in silico involves searching a vast high-dimensional conformational space that is associated with a complex energy surface rich in local minima.

This talk will present our latest work on novel and powerful computational frameworks that enhance the sampling of biologically-active protein conformations. In particular, novel probabilistic algorithms inspired from robotics and evolutionary computing are introduced to handle the high-dimensionality of the conformational space and ruggedness of the protein energy surface. Extensive applications on a growing diverse list of proteins suggest the proposed efforts greatly enhance the sampling of the protein conformational space and efficiently recover functionally-relevant conformations. Interesting insight is obtained on how to tackle the dimensionality challenge in larger protein systems with possibly diverse functional states.

Biography

Amarda Shehu is an Assistant Professor in the Department of Computer Science at George Mason University. She holds affiliated appointments in the Department of Bioinformatics and Computational Biology and the Department of Bioengineering at George Mason University. She received her B.S. in Computer Science and Mathematics from Clarkson University in Potsdam, NY and her Ph.D. in Computer Science from Rice University in Houston, TX, where she was an NIH fellow of the Nanobiology Training Program of the Gulf Coast Consortia. Shehu's research contributions are in computational structural biology, biophysics, and bioinformatics with a focus on issues concerning the relationship between sequence, structure, dynamics, and function in biological molecules. Her research is funded by the National Science Foundation. Shehu is also the recent recipient of a CAREER award from the National Science Foundation for her research on probabilistic search algorithms for protein conformational spaces.