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EXERCISE - Explore Emerging Computing in Science and Engineering
Research Speaker Series

New Approaches in ab initio Protein Structure Modeling

Professor Yaohang Li

Date: Tuesday July 24, 2012

Time: 2:00pm-3:00pm

Location: Henson Science 101

Abstract: Accurately modeling protein or protein complex structure is considered one of the most significant grand challenges that have broad economic and scientific impact. Since Anfinsen's thermodynamic hypothesis is formulated, according to which the native structure conformation has the minimum free energy of all accessible conformations, the ab initio protein structure modeling efforts are focused on globally optimizing a scoring (energy) function to find the native conformation. However, due to insensitivity and inaccuracy of the existing scoring functions used to describe protein conformational energy, ab initio approaches have low success rate in predicting models with satisfactory resolutions. In this talk, we present new computational sampling approaches of integrating multiple physics- and knowledge-based scoring functions to improve protein structure modeling accuracy. Applications in protein loop structure modeling and implementations on emerging High Performance Computing platforms are also discussed.

Bio: Yaohang Li is an Associate Professor in the Department of Computer Science at Old Dominion University. His research interests are in Computational Biology, Markov Chain Monte Carlo (MCMC) methods and Parallel/Distributed/Grid Computing. Yaohang Li received "Rookie of the Year" young investigator award at North Carolina A&T State University in 2005 and Ralph E. Powe young faculty award in Computer Science and Mathematics from Oak Ridge Associated Universities (ORAU) in 2005. He is the recipient of an NSF CAREER Award in 2009. He received the Ph.D. and M.S. degrees in Computer Science from the Florida State University in 2003 and 2000, respectively, and the B.S. degree in Computer Science and Engineering from the South China University of Technology in 1997. After graduation, he worked at Oak Ridge National Laboratory for a short period of time. He was a Summer Research Fellow at National Center of Supercomputing Applications (NCSA) in 2007 and a Summer Faculty Research Participation member at Oak Ridge National Laboratory in 2006 and 2008. Before joining ODU, he was an associate professor in the Computer Science Department at North Carolina A&T State University.

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