



Singapore-MIT Alliance for Research and Technology



Focused Seminar Series on Computational Techniques

15 Feb — 11 Apr 2016, Level 5 Seminar Room, Enterprise Wing @ UTown, S'138602

Seminar 2: Coarse-grained Molecular Modelling: Theory and Applications in Biology

Professor Lu Lanyuan

Nanyang Technological University

Date: 22 Feb 2016, Monday

Time: 4pm to 5pm

Venue: Perseverance Room, Enterprise Wing Level 5 @ UTown



Abstract

Coarse-grained models are widely used in molecular simulations to extend the temporal and spatial limits of conventional atomistic potential energy functions (aka force fields). In the first part of the presentation, various strategies of developing coarse-grained models are briefly reviewed, focusing on the multi-scale coarse-graining approach. In the multi-scale coarse-graining method, coarse-grained force fields are systematically developed from atomistic simulation data, and successful applications of this approach include simple liquids, lipid membranes, and actin filaments. Two recent applications of coarse-grained modelling on a RNA-binding protein and a dengue non-structural protein are discussed in the second part of the seminar. More specifically, coarse-grained simulations are performed to investigate the inter-domain interactions in multi-domain proteins. Coarse-grained simulation is particularly advantageous for exploring the dynamic binding interfaces between weakly interacted protein domains connected by flexible parts. The computer simulation results, combined with nuclear magnetic resonance or small angle X-ray scattering data, enable the construction of conformational ensembles for the studied protein systems.

Biography

Dr Lu Lanyuan graduated from the University of North Carolina at Chapel Hill in 2007 with a PhD in chemistry. Subsequently, he joined Professor Gregory Voth's group as a postdoctoral fellow at University of Utah (2007-2010), University of Chicago and Argonne National Laboratory (2010-2011). He is currently an assistant professor at School of Biological Sciences, Nanyang Technological University. The research interests of Lu's lab focus on 1) developing force fields and simulation methods for multi-domain proteins and protein-protein interactions; and 2) computer modelling of solution X-ray scattering and nuclear magnetic resonance data.