

Multiscale modeling of proteins

MURPA Seminar Friday 16th April 2010 at 10am

Speaker: Robert Konecny, Director of The Keck Center for Integrated Biology at University California in San Diego.

Venue: Seminar Room 135/26 at Monash Clayton

Abstract

The biological activity within living cell encompasses interaction of molecules from the nano to macroscale, both in length and time. To gain a comprehensive insight into these interactions it is necessary to use tools which allow to span multiple length and time scales.

This talk will cover our research into large scale motions of viral capsid particles (Cowpea Chlorotic Mottle Virus, CCMV) upon maturation and the role of electrostatics in this process. To investigate long time scale interactions techniques like Brownian dynamics are used. We have employed this approach to perform long time-scale simulations of an important enzyme, protein kinase A (PKA).

All these methods rely heavily on state of the art computational technology and sophisticated programming algorithms including massive parallel schemes. An outline of how we are using these methods in our applications will also be presented.

Bio

Robert Konecny is Director of The Keck Center for Integrated Biology at University California in San Diego. He received his PhD in Physical Chemistry from University of Delaware in 1997 where he computationally studied reactivity of solid surfaces with organic substrates.

He then spent a year as a postdoctoral researcher at The Scripps Research Institute, La Jolla, CA with Lou Noodleman working on theoretical description of biological activity of enzymes. From 1998 to 1999 he was postdoctoral researcher in the group of Nobel Prize winner Roald Hoffmann at Cornell University, Ithaca NY, where he was investigating formation of organic layers on semiconductor surfaces. In 1999 he became Senior Service Fellow at the Centers for Disease Control and Prevention where he explored biological implications of radical reactivity with the pulmonary system. In 2001 he joined the UCSD Center for Research on Biological Systems. He is now senior researcher at the Center of Theoretical Biological Physics (CTBP) and at the National Biomedical Computational Resource (NBCR).

His current research interests include among others electrostatics and Brownian dynamics of large protein systems, multiscale modeling and software development of applications for biological simulations.