WEEKLY SEMINAR

Topic: **Multiscale Multiphysics and Multidomain Models for Biomolecules**

Speaker: **Guowei Wei**
Department of Mathematics, Michigan State University

Time: 15:30-16:30, 5 June 2014

Venue: Room 264, Geography Building, 3663 Zhongshan Road North, Shanghai
(华东师范大学中山北路校区，地理楼 264 室)

ABSTRACT OF THE TALK

A major feature of biological sciences in the 21st Century will be their transition from phenomenological and descriptive disciplines to quantitative and predictive ones. However, the emergence of complexity in self-organizing biological systems poses fabulous challenges to their quantitative description because of the excessively high dimensionality. A crucial question is how to reduce the number of degrees of freedom, while preserving the fundamental physics in complex biological systems. We discuss a multiscale multiphysics and multidomain paradigm for biomolecular systems. We describe macromolecular system, such as protein, DNA, ion channel, membrane, etc., by a number of approaches, including static atoms, molecular mechanics, quantum mechanics and elastic mechanics; while treating the aqueous environment as a dielectric continuum or electrolytic fluids. We use differential geometry to couple various microscopic and macroscopic domains on an equal footing. Based on the variational principle, we derive the coupled Poisson-Boltzmann, Nernst-Planck, Kohn-Sham, Laplace-Beltrami, Newton, elasticity and/or Navier-Stokes equations for the structure, dynamics and transport of protein, protein-ligand binding and ion-channel systems.

BIOGRAPHY

Guowei Wei, professor of Department of Mathematics at Michigan State University. He graduated from Chinese Academy of Sciences with M.S. degree in physical chemistry in 1988 and Ph.D. degree in Non-equilibrium statistical mathematical from the University of British Columbia in 1996. His current research interests include mathematical molecular biosciences, mathematical biophysics, nanofluidic systems, molecular imaging and image analysis, quantum kinetic theory, high order interface methods and matched interface and boundary (MIB) method. Over years, Prof. Wei has accumulated research experience in many disciplines, including mathematics, physics, chemistry, biology, computer science and engineering.