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The Hong Kong University of Science and Technology

Department of Mathematics

Seminar on Applied Mathematics

Variational Implicit Solvation of Biomolecules

by

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Abstract

The structure and dynamics of biomolecules such as DNA and proteins determine the functions of underlying biological systems. Modeling biomolecules is, however, extremely challenging due to their enormous complexity. Recent years have seen the initial success of variational implicit-solvent models (VISM) for biomolecules. Central in VISM is an effective solvation free-energy functional of all possible solute-solvent interfaces, coupling together the solute surface energy, solute-solvent van der Waals interactions, and electrostatic contributions. Numerical relaxation by the level-set method of such a functional determines biomolecular equilibrium conformations and minimum free energies. Comparisons with experiments and molecular dynamics simulations demonstrate that the level-set VISM can capture multiple dry and wet states, subtle charge eects, and many other important solvation properties. This talk begins with a description of the level-set VISM and continues to present main developments around the VISM. These include: (1) The effective dielectric boundary forces within the Poisson Boltzmann theory of electrostatics; (2) A stochastic level-set VISM for the dewetting transition; (3) The dynamics of solvent fluid; and (4) The coarse-graining VISM with the Martini forceeld. Mathematical theory and numerical methods are discussed, and applications are presented. This is joint work mainly with J. Andrew McCammon, Li-Tien Cheng, Joachim Dzubiella, Jianwei Che, Zhongming Wang, Shenggao Zhou, Zuojun Guo, and Clarisse Ricci.

Date: **Friday, 30 November 2018**
Time: **3:00p.m. – 4:00p.m.**
Venue: **Room 5560, Academic Building, (Lifts 27, 28), HKUST**

All are welcome!