Continuum Electrostatics, Variational Implicit Solvation, and Diffuse Interface for Cell Motion

Lecture Overview

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Winter School: Modeling, Simulation and Analysis of Biology and Physiology
Taiwan National Center for Theoretical Sciences
Taipei, Taiwan
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Biology and Physiology

- Evolution biology, population biology, ...
- Genetics and molecular biology
- Cells, tissues, organs, ...
- Neuroscience, computational neurobiology, brain research, ...
- Ecology, behavior, ...
- Biological physics, biological chemistry, mathematical biology, mathematical physiology, ...
- Computational biology, computational physiology, ...
- ...

These lectures focus on mathematical and computational studies of some biology and physiology problems at molecular and cellular levels.
Opportunities for and Roles of Mathematics and Computation in Biological Sciences

- Biological systems are highly complicated. Each one has its own unique characterization.
- Fundamental scientific questions: challenging mathematical and computational problems.
- Highly interdisciplinary research: from experiments to modeling to computation and to analysis.
- Mathematics and computation: understand biological systems and solve biological problems.
These lectures

- Some aspects of biology and physiology at the molecular and cellular levels: biological molecules, cell motion, etc.
- Mathematics and computation: partial differential equations, the calculus of variations, geometrical flow, shape derivatives, interface motion, level-set method, phase-field method, Monte Carlo simulations, molecular dynamics simulations, etc.
- Based on:
  - Topics in Mathematics and Biochemistry-Biophysics, a graduate topic course, UC San Diego, Spring 2011.
  - Lectures and talks in seminars, colloquia, meetings, etc.
- Research in recent years supported by the NSF and NIH.
Outline of Lectures

Lecture 1. The Poisson-Boltzmann Equation
(10:20–11:10, Friday, December 18)

I will introduce the classical Poisson-Boltzmann (PB) equation and a related free-energy functional of ionic concentrations. I will state and outline the proof of some properties of the functional and PB equation.

Poisson’s equation

\[ \nabla \cdot \varepsilon \varepsilon_0 \nabla \psi = -\rho \]

Work of McCammon’s group
I will present two generalized PB equations and some of the related mathematical and computational results. One of them describes ionic excluded volume (or size) effect, and the other describes the effect of ionic concentration dependent dielectric environment.
Lecture 3. Variational Implicit-Solvent Model of Biomolecules
(15:30–16:20, Tuesday, December 22)

I will start with the Born model for the solvation of an ion in water. I will then introduce the concept of dielectric boundary based implicit-solvent model for solvation of biological molecules. I will finally present a variational implicit-solvent model (VISM). I will derive the dielectric boundary force using the concept of shape derivative, and apply such boundary force to study the stability of solute-solvent (e.g., protein-water) interface for a model system. If time permits, I will describe the level-set method that implements VISM.
Lecture 4. Phase-Field Models for Molecules, Vesicles, and Cells
(16:20–17:10, Tuesday, December 22)

I will first introduce the notion of phase-field modeling and the fundamental mathematical result behind such an approach. I will then present some of our recent work on phase-field modeling and computation of charged molecules, vesicles, and moving cells.