Mathematical biophysics I: Basic concepts (Fall 2016)

Instructor: Professor Guowei Wei

A major feature of life sciences in the 21st century is their transformation from phenomenological and descriptive to quantitative and predictive. Revolutionary opportunities have emerged for mathematically driven advances in biological research. Experimental exploration of self-organizing molecular biological systems, such as HIV viruses, molecular motors and proteins in Alzheimer's disease, are examples of dominating driving forces in scientific discovery and innovation in the past few decades. However, the emergence of excessive complexity in self-organizing biological systems poses fundamental challenges to their quantitative description, because of the excessively high dimensionality and the complexity of the processes involved. Mathematical approaches such as multiscale modeling, manifold extraction, topological simplification, dimensionality reduction and machine learning techniques will be introduced to reduce the complexity of biomolecular systems while maintaining an essential and adequate description of biomolecular structure, function, dynamics and transport. A wide variety of basic concepts in molecular biophysics, such as solvation, binding, ion channel, protein folding, protein-DNA/RNA interaction, signal transduction, transcription, translation, and drug design and discovery, will be discussed.

Mathematical biophysics II: Mathematical models (Spring 2017)

Instructor: Professor Guowei Wei

First, we will discuss a number of deterministic and stochastic models, such as Boltzmann equation, Boltzmann-Vlasov equation, Liouville equation; Zwanzig's equation, Fokker-Planck equation, Brownian dynamics, Langevin dynamics, molecular dynamics, master equation, Poisson-Nernst-Planck equations, Kohn-Sham equation, Navier-Stokes equation, Laplace-Beltrami equation, mean curvature flow, Willmore flow, Poisson-Boltzmann equation, Maxwell's equations, wave equation, anisotropic diffusion equation, and generalized Kohn-Sham equation. Emphases will be placed on how to utilize the aforementioned models in a consistent manner for the description of biomolecular systems. We will make extensive use of fundamental laws of physics via variational approaches to derive governing equations for biomolecular systems. In additional to partial differential equations, other mathematical theories, methods and algorithms, including differential geometry, differential topology, persistent homology, Morse theory, knot theory, graph theory, algebraic geometry and geometric modeling, will be discussed for molecular biophysical modeling and computation.