

Applied Dynamical Systems seminar

Dr. Chunhua Ou, Memorial University

Monday, November 18, 2013

HH-3017 @ 3 p.m.

Asymptotic Analysis of the Perturbed Poisson Boltzmann Equation on Unbounded Domains

Abstract:

The Poisson Boltzmann equation is a model that describes electrostatic interactions between molecules in ionic solutions. As the mathematical base for the Gouy Chapman double layer (interfacial) theory, it was first proposed by Gouy in 1910 and then complemented by Chapman in 1913. The equation is extraordinarily important in the fields of molecular dynamics and biophysics, because it can be used in modeling implicit solvation, an approximation of the effects of solvent on the structures and interactions of proteins, DNA, RNA, and other molecules in solutions of different ionic strength. It is often difficult to solve the Poisson Boltzmann equation for complex systems, but several computer programs have been created to solve it numerically. Recently there have been considerable investigations on the analysis and applications of this type of equations. In particular, the Poisson-Boltzmann equation can also be derived from the Poisson-Nernst-Planck system. In this talk, we study the existence, uniqueness and asymptotic expansions to perturbed Poisson Boltzmann equations on an unbounded domain. A shooting method is applied to prove the existence and uniqueness of the exact solution. As to the approximation to the regularly perturbed Poisson Boltzmann equation, we convert it into an integral equation and a uniformly convergent asymptotic expansion based on the iteration of successive approximations is provided with a rigorous proof. For the singularly perturbed problem, since the typical Poincare-type outer solution is the constant zero, we then use the inner-layer asymptotic formula to approximate the true solution in the whole domain. Our proof verifies that these expansions do give a valid approximation globally. A further discussion on the exponentially-matched asymptotic expansions is also presented.

Coffee and cookies will be served.

Seminar website: <http://www.math.mun.ca/~shuz/seminars.html>

—————All are welcome—————