

Department of Applied Mathematics and Statistics
The Johns Hopkins University

SEMINAR

Shan Zhao
Department of Mathematics
Michigan State University

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304 Whitehead Hall
Refreshments: 3:30 p.m.
Seminar: 4:00 p.m.

**MATHEMATICAL PROBLEMS IN IMPLICIT SOLVENT APPROACHES
FOR BIOMOLECULAR MODELING**

ABSTRACT

The rapid growth of computer capability in the past few decades notwithstanding, our ability to predict the structure and dynamics of biological macromolecules such as proteins, DNAs, and RNAs is severely limited. Implicit solvent models based on the Poisson–Boltzmann equation have emerged as a promising means of investigating the structure and dynamics of biomolecules. However, there are mathematical problems in this approach that hinder its further development. First, the generation of molecular surfaces is a time-consuming task and often encounters topological singularities. Second, the numerical solution of the Poisson–Boltzmann equation suffers from poor convergence or non-convergence due to the presence of irregular molecular surfaces and singular charge distributions. In this talk, I will discuss a novel PDE-based approach for molecular surface modeling. A new higher-order convergent interface method, the matched interface and boundary (MIB) method, will be presented to solve the Poisson–Boltzmann equation with irregular dielectric interfaces and singular charges. The application of the MIB method will be briefly discussed to problems in electromagnetics, optics, fluid dynamics, and structural design.