Numerical Algorithm Developments for the Poisson-Boltzmann Models in Biomolecular Electrostatics

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The Poisson-Boltzmann (PB) equation is a widely used implicit solvent model for the electrostatic analysis of solvated biomolecules. The numerical solution of this partial differential equation (PDE) is known to be challenging, due to the consideration of discontinuous coefficients, complex geometry of protein structures, singular source terms, strong nonlinearity, and unbounded domain. In this talk, I will offer a brief overview of recent studies in the math literature as well as new developments in our group for resolving the PB numerical difficulties.

(i) In treating charge singularities, several regularization methods have been developed, in which the potential function is decomposed into two or three components so that the singular component can be analytically solved using the Green's function, while other components become bounded. The source of accuracy reduction in a popular two-component regularization method has been identified, and an effective accuracy recovery has been proposed.

(ii) For treating dielectric interface and complex geometry, both finite element methods and Cartesian grid finite difference methods have been developed for delivering a second order accuracy in space.

(iii) In the framework of pseudo-time integration, we have constructed an analytical treatment to suppress the nonlinear instability.

(vi) A nonlinear PB benchmark problem has been constructed for calculating the electrostatic free energy of a Kirkwood sphere.

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