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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(Also available remotely: https://utep-edu.zoom.us/j/86199006868)

Dr. Shan Zhao is currently a Professor of Mathematics at the University of Alabama (UA), USA. He received the BS degree in mathematics from Lanzhou University, China, in 1997, and the PhD degree in computational science from National University of Singapore, in 2003. From 2003 to 2006, he was a postdoctoral fellow with the Michigan State University. Since 2006, he has been working at UA, and was promoted to full professor in 2015. He is currently the Leadership Board Fellow of the College of Arts and Sciences at UA. With continuous grant supports from the NSF, Dr. Zhao has a track record in developing mathematical models and computational tools for molecular bioscience and biophysics. His recent research focuses on fast algorithms for solving partial differential equations, high-order finite difference methods, implicit solvent modelling, electrostatic analysis, and fast biomolecular simulation. He has published more than 70 papers, which have been cited more than 2500 times according to the Google Scholar. He served on the editorial boards of several journals in mathematical biophysics and scientific computing.