REVIEW ARTICLE

Recent Progress in Numerical Methods for the Poisson-Boltzmann Equation in Biophysical Applications

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Abstract. Efficiency and accuracy are two major concerns in numerical solutions of the Poisson-Boltzmann equation for applications in chemistry and biophysics. Recent developments in boundary element methods, interface methods, adaptive methods, finite element methods, and other approaches for the Poisson-Boltzmann equation as well as related mesh generation techniques are reviewed. We also discussed the challenging problems and possible future work, in particular, for the aim of biophysical applications.

Contents

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1   Introduction

Poisson-Boltzmann (PB) theory has been a well-established model in a broad range of scientific research areas. In electrochemistry, it is known as Gouy-Chapman (GC) theory [1,2]; in solution chemistry, it is known as Debye-Hückel theory [3]; in colloid chemistry, it is known as the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory [4,5]; and in biophysics, it is known as PB theory [6,7]. The Poisson-Boltzmann equation (PBE) represents a typical implicit solvent model, and provides a simplified continuum description of the discrete particle (e.g., water, ion, and protein molecule) distributions in solution. In particular, the PBE describes the electrostatic interaction and ionic density distributions of a solvated system at the equilibrium state. Since the first application of the PBE in a biomolecular system [8], a large amount of literatures and many solution techniques have been produced in this area and directed to studies of diverse biological processes.

A number of excellent review papers can be found that focus on the physical fundamentals, methodologies, and applications of PB electrostatics to molecular structure and dynamics. Here we only list some of recent references. The underlying physics and theories of implicit solvent models are discussed in [9,10]; a brief history of PB can be found in [11]; the PB methodology and applications in biomolecular modeling was summarized briefly in [12,13]; the methodological developments in both generalized Born (GB) and PB models was given by [14]. Ref. [15] focused on the GB models, which are another type of dielectric continuum model with further approximations. This review will focus on the numerical aspects of PB methodology covering several major numerical methods.

The challenges in biomolecular physical applications include macromolecular computations applied to biomolecular binding/association/assembly, (implicit) molecular dynamics (MD) simulations, and multiscale modeling in space and time. Efficiency and accuracy are two central issues in applying the PBE to biophysical modeling. For instance, a typical macromolecule may consist of tens of thousand to millions of atoms (point charges in the PBE), which significantly challenges the current computer memory and speed. Secondly, in order to incorporate the PB electrostatics (on the fly) in a typical MD simulation or Brownian dynamics (BD) simulation for molecular association/dissociation which could involve tens of millions of steps, a single solution of the