Discontinuous Bubble Immersed Finite Element Method for Poisson-Boltzmann Equation

In Kwon[1] and Do Y. Kwak[1,*]

[1] *Department of Mathematical Science, KAIST, 291 Daehak-ro (373-1 Guseong-dong), Yuseong-gu, Daejeon 305-701, Republic of Korea.*

Abstract. We develop a numerical scheme for nonlinear Poisson-Boltzmann equation. First, we regularize the solution of PBE to remove the singularity. We introduce the discontinuous bubble function to treat the nonhomogeneous jump conditions of the regularized solution. Next, starting with an initial guess, we apply linearization to treat the nonlinearity. Then, we discretize the discontinuous bubble and the bilinear form of PBE. Finally, we solve the discretized linear problem by IFEM. This process is repeated by updating the previous approximation.

We carry out numerical experiments. We observe optimal convergence rate for all examples.
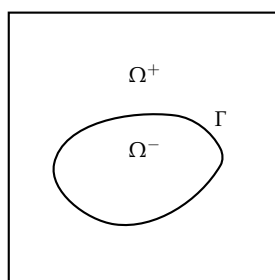
1 Introduction

Poisson-Boltzmann (PB) theory is a well-established theory in various disciplinary areas. It is known as Gouy-Chapman theory in electrochemistry [3,12], as Debye-Huckel theory in solution chemistry [9], as the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory in colloid chemistry [10,36] and as PB theory in biophysics [8,17]. The Poisson-Boltzmann equation (PBE) is applied mainly as a modeling tool to make approximations for applications such as charged biomolecular interactions, dynamics of electrons in semiconductors or plasma. For example, PBE can be used to obtain the electrostatic potential and free energy of charged molecule like tRNA in an ionic solution with diverse number of bound ions.

---

*Corresponding author. *Email addresses:* `kiki3568@kaist.ac.kr` (I. Kwon), `kdy@kaist.ac.kr` (D. Y. Kwak)

Figure 1: A domain Ω with interface.

The fundamental physics and theories of implicit solvent models are discussed in [33,34]. The PBE represents a typical implicit solvent model, and gives a simplified continuum description of the discrete particle (e.g., water, molecule) distributions in solution. The PBE expresses the electrostatic interaction and ionic density distributions in a solvated system at the equilibrium state. The equation has singular charges at discrete particles. It makes a solution singular and interrupts general approaches to solve the equation. Also, solvated biomolecular systems are usually modeled by dielectrically distinct areas with singular charges distributed in the molecular areas. The PBE has dielectric coefficient dependent on these distinct areas. It results in the discontinuity of solution on each areas.

Many numerical methods were developed for the Poisson-Boltzmann equation. Finite difference methods (FDM) have been the most popular numerical methods for the PBE in biomolecular simulations, most likely due to their simpler implementation than other methods. DelPhi [20], GRASP [32], MEAD [1], UHBD [31] are the most popular and successful traditional FDM based solver for obtaining biomolecular electrostatics. Since several features of the PBE were untreated in these traditional PBE solver, there is a loss of accuracy and convergence rate [39]. These untreated features are the approximated position of molecular surface and the continuity condition of electric displacement on the molecular surface. Later, Jump Condition capturing scheme (JCCS) [37] for structured meshes, Matched Interface and Boundary method (MIB) [38,40,41,44], and Newton algebraic multigrid (AMG) [13,15,16] for nonlinear PBE have been developed [45].

On other hand, Finite Element methods (FEM) have been developed for Poisson type of PDE in many different ways. Compared with the FDM, FEM provide more flexibility for fitting curved domain and local refinement, and more rigorous convergence analysis. Also more choices of efficient iterative solvers for the resultant linear systems and more schemes for solving nonlinear equations are allowed. Because the PBE has singular partial charges, rigorous theory for the solution and approximation theory were not well-developed until recently. In [4], first rigorous a priori error estimates and rigorous convergence results were established using a decomposition scheme. This article provides a number of fundamental technical results. Also, Newton-AMG iterations [14–16]