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An Error Analysis for the Finite Element Approximation to the Steady-State Poisson-Nernst-Planck Equations

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Abstract. Poisson-Nernst-Planck equations are a coupled system of nonlinear partial differential equations consisting of the Nernst-Planck equation and the electrostatic Poisson equation with delta distribution sources, which describe the electrodiffusion of ions in a solvated biomolecular system. In this paper, some error bounds for a piecewise finite element approximation to this problem are derived. Several numerical examples including biomolecular problems are shown to support our analysis.

AMS subject classifications: 65N30, 92C40

Key words: Poisson-Nernst-Planck equations, finite element method, error bounds.

1 Introduction

In this paper, we shall analyze the finite element approximation for a widely used mathematical model-Poisson-Nernst-Planck (PNP) equations in the biomolecular modeling area as follows:

$$\begin{cases} \nabla\cdot D^i(\nabla p^i+\beta q^i p^i\nabla\phi)=0, & \text{in } \Omega_s,\ 1\le i\le n,\\ -\nabla\cdot(\epsilon\nabla\phi)-\lambda\sum_{i=1}^{n} q^i p^i=\rho^f, & \text{in } \Omega, \end{cases} \tag{1.1}$$

where ϕ is the electrostatic potential and p^i is the concentration of the *i-th* ion species. This model is used to describe the electrodiffusion of mobile ions in a solvated biomolecular system. The model and its application have been discussed by authors such

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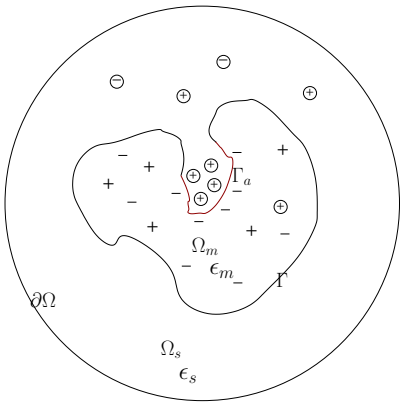

Figure 1: 2-D illustration of the computational domain modeling a solvated biomolecular system.

as [14, 16, 17]. Here the electrostatic potential is induced by the mobile ions and the fixed charges carried by biomolecules. Fig. 1 illustrates a solvated biomolecular system in an open domain $\Omega \subset \mathbb{R}^3$. The domain $\Omega_m \subset \Omega$ represents the biomolecule(s) and the remain domain $\Omega_s = \Omega \setminus \bar{\Omega}_m$ shows a solvent surrounding the biomolecule(s). The molecular surface Γ interfaces domains Ω_m and Ω_s. Charged ligands in this model are also treated as diffusive species, and might react with the biomolecules on a part of the molecular surface Γ_a. The dielectric ϵ is a piecewise constant and the permanent (fixed) charge distribution $\rho^f = \sum_{j=1}^{N_m} q_j \delta(x - x_j)$ is a combination of Dirac distributions at singular points x_j, $j = 1, 2, \cdots N_m$. The diffusive particles are distributed in Ω_s.

Since the analytic solutions of the PNP equations only exist in very few cases for simple shape molecules with continuous dielectric coefficient ϵ, numerical solutions of the PNP equations become natural. A variety of numerical methods such as finite element method, finite difference method and boundary element method etc. have been applied to solving the PNP and PNP-like systems (cf. [6, 9, 10, 13–15, 19, 20, 27] etc). Among those approaches, the finite element method is considered to be very promising in which irregular shapes can be fitted more easily. Moreover, the finite element method allows fine meshes to be put where they are needed, such as at interfaces, and coarser meshes to be put far from the molecule, where spatial changes in electrostatic potential are small.

In contrast to amount of work on the numerical computations of PNP equations, the work of mathematical analysis of PNP equations seems very limited, especially for finite element method. The existence and stability for the solutions of PNP equations are established by [12] for 1-D PNP model for electron flows in semiconductors. Singular perturbation methods and asymptotic analysis are applied to study the solution properties of 1-D PNP equations in [5]. We are not aware of any mathematical analysis for the finite element approximation of the PNP equations.

The main difficulties for mathematical analysis for the PNP equations (1.1) are Dirac distribution sources and nonlinear coupling. To deal with the Dirac distribution sources,