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A DECOUPLING TWO-GRID METHOD FOR THE STEADY-STATE POISSON-NERNST-PLANCK EQUATIONS *

Ying Yang[1)]
School of Mathematics and Computing Science, Guangxi Colleges and Universities Key Laboratory of Data Analysis and Computation, Guilin University of Electronic Technology, Guilin 541004, China
E-mail: yangying@lsec.cc.ac.cn

Benzhuo Lu
LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, the National Center for Mathematics and Interdisciplinary Sciences, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China
E-mail: bzlu@lsec.cc.ac.cn

Yan Xie
LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China

Abstract

Poisson-Nernst-Planck equations are widely used to describe the electrodiffusion of ions in a solvated biomolecular system. Two kinds of two-grid finite element algorithms are proposed to decouple the steady-state Poisson-Nernst-Planck equations by coarse grid finite element approximations. Both theoretical analysis and numerical experiments show the efficiency and effectiveness of the two-grid algorithms for solving Poisson-Nernst-Planck equations.

Mathematics subject classification: 65N30, 65N15.
Key words: Poisson-Nernst-Planck equations, Two-grid finite element method, Decoupling method, Error analysis, Gummel iteration.

1. Introduction

Electrodiffusion plays an important role in many fields such as biological ion channels, cellular electrophysiology and semiconductors. For the biological processes, the kinetic properties of them are mainly governed by the electrodiffusion of charged molecules in aqueous solution. The numerical methods for deriving the kinetic parameters usually include discrete methods (such as Monte Carlo, Brownian dynamics and Langevin dynamics) and continuum methods. The latter is more efficient for simulating large systems and easier to be modified to include more physical functions. The electrodiffusion processes in biomolecular systems are usually described by a continuum model called Poisson-Nernst-Planck (PNP) equations, which is regarded as one of the most efficient theoretical methods for studying electrodiffusion.

The PNP equations are a coupled system of nonlinear partial differential equations consisting of the Nernst-Planck equation and the electrostatic Poisson equation. The steady-state PNP

[1)] Corresponding author.
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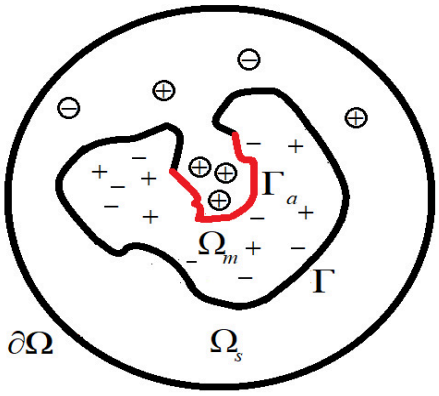
equations in the biomolecular modeling are as follows [21]:

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

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 (see Fig. 1.1). Since the analytic solutions of the PNP equations only exit in very few cases for simple shape molecules, a variety of numerical methods have been proposed to solve them [8, 10, 21, 35, 44]. For example, the finite difference method has been widely used to solve the PNP equations describing electrodiffusion in biological ion channels or other transmembrane pores [3,16,20,43], but the accuracy is not so high when it is applied to the biomolecular models with highly irregular surfaces. The finite element method is considered to be very promising in which irregular shapes can be fitted more easily when applying to the PNP equations. [18, 21, 22, 31, 32, 41].



(a)

Fig. 1.1. 2-D illustration of the computational domain modeling a solvated biomolecular system. The domain $\Omega_m \subset \Omega$ represents the biomolecule(s) and the remaining 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 diffusive particles are distributed in Ω_s.

In general, there are two types of approaches to solve such a multimodel problem like PNP equations. One is to consider the equations as a large system and solve the overall system together. The other is to first decouple the system and then solve the equations respectively. The latter can be implemented more easily and efficiently since the computational systems are smaller. It can also effectively exploit the existing computing softwares and result in parallelism in some cases. The Gummel iteration [15] is such a type of decoupling approach which may be the most commonly used decoupling method for solving PNP equations [2, 5, 17, 23]. Lu and Zhou [23] presented a size-modified PNP model which is able to treat arbitrary particle species. The Gummel iteration is applied to solve the discretized system for this strong nonlinear model. Recently, Bousquet and Hu et al. [2] designed an efficient Newton solver for drift-diffusion and