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Error analysis of finite element method for Poisson–Nernst–Planck equations

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ABSTRACT

In this paper we study the a priori error estimates of finite element method for the system of time-dependent Poisson–Nernst–Planck equations, and for the first time, we obtain its optimal error estimates in $L^\infty(H^1)$ and $L^2(H^1)$ norms, and suboptimal error estimates in $L^\infty(L^2)$ norm, with linear element, and optimal error estimates in $L^\infty(L^2)$ norm with quadratic or higher-order element, for both semi- and fully discrete finite element approximations. Numerical experiments are also given to validate the theoretical results.

1. Introduction

In this paper, we study the a priori error estimates of the finite element approximation to a type of time-dependent Poisson–Nernst–Planck (PNP) equations. PNP equations provide a mean-field continuum electrodiffusion model for the flows of charged particles in terms of the average density distributions and the electrostatic potential. This model has been widely used to describe the transport of charged particles in semiconductors [1–5], electrochemical systems [6–11] and biological membrane channels [12–21].

The mathematical analysis and numerical approximation of the PNP equations have attracted considerable interests. The existence of solutions to the PNP equations has been shown in [22,23]. In [24], the existence and local uniqueness of a solution to the one-dimensional steady-state PNP systems with multiple ion species have been shown. In [25,26], the existence and uniqueness of temporally global solutions have been proved for PNP systems based on maximum principle and compactness arguments. Analytic solutions have been found for one-dimensional case [27–29].

Due to the nonlinearity of the coupled system of partial differential equations (PDEs), in general, it is mathematically challenging to find the analytic solution of PNP equations. Therefore, numerical methods are often employed to find the approximate solutions. There are many existing studies on the numerical techniques for solving PNP equations. Finite difference method has been widely used to solve PNP equations [12,13,30–32,19]. In [19], a lattice relaxation scheme is used together with the finite difference scheme to solve three-dimensional PNP equations. A second-order finite difference method has been designed to solve PNP equations in ion channels [33]. The use of finite difference method has certain limitation on the description of ionic channel geometry. Finite volume method was then used in [34,35] to solve PNP

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equations in the irregular domains, but was still limited by the low convergence rate because of the difficulty of the design of high-order control volume. Finite element method has the advantage of handling ion channels with irregular surfaces [36,20,37–41], and its convergence rate only depends on the regularity of the solution. In [41,1], a convergence theory has been established for the finite element method by defining a fixed point mapping T, termed Gummel's map [42], solving each of the decoupled PNP equations and substituting these solutions in successive PDEs in a Gauss–Seidel fashion. The fixed points of the mapping T then coincide with solutions to the PNP system, however, no convergence rate was given for this finite element approximation. Spectral element method [43] and boundary element method [40] have also been studied for three-dimensional PNP equations, but their convergence analyses were not conducted.

Recently, an error estimate of the standard finite element method was given in [44] for a type of steady-state PNP equations modeling the electrodiffusion of ions in a solvated biomolecular system, however, their error estimates for the potential and concentration in H^1 norm depend essentially on the L^2 error of the concentration, which was only numerically shown to be second order. Another recent work about the error estimates of the spatial semi-discrete finite element method for a type of time-dependent PNP equations was done in [45], where, the suboptimal convergence rates on account of the quadratic finite element for the electric potential and the linear finite element for the charge densities are obtained in both L^2 and H^1 norm. And, due to the insufficient global regularity of the solutions of the PNP equations, which arises from the discontinuous electric diffusion coefficient for a particular case of the ion diffusion phenomenon existing in ion channels [45], the obtained suboptimal convergence rates lack one half order for all finite element solutions in both L^2 and H^1 norm in contrast with the normal optimal convergence rate when the quadratic element is used. Moreover, there is an critical incorrectness existing in the convergence proof of [45]: the constant C in the final error estimate depends on the numerical solution instead of the real solution, which is unallowable for a priori error estimate. Due to such flaw, their convergence proof is thus incomplete although the final error estimates seem correct in [45].

Two types of temporal semi-dicretization schemes for the time-dependent PNP equations are introduced in [46] and employed to prove the existence and uniqueness of the solutions of the discretized PNP equations. An optimal error estimate for a fully discrete finite element discretization of the time-dependent Navier–Stokes–Poisson–Nernst–Planck system using linear element is claimed in [47] without a complete proof. In fact, the techniques used in [47] for the error analysis of the temporal semi-discretization cannot be simply carried over to either spatial semi-discretization or full discretization of the time-dependent PNP equations. The authors in [47] state that the proof of optimal error estimates for either spatial semi- or full discretization follows by applying the same techniques used for the temporal semi-dicretization scheme. Nevertheless, they neglect a crucial fact that the convergence theory of finite element scheme in terms of the spatial variables is based upon a variational form defined in a finite-dimensional discretized space, which is different from the stability/convergence analysis of a temporal semi-discretization scheme in which the terms involving spatial variables are all associated with the infinite-dimensional continuous spaces. Such severe omission results in a failure of the derivation on their optimal error estimates in space. Thus their results may be only valid for the temporal semi-discretization scheme but unproved for the either spatial semi-discretization scheme or fully discretization scheme of the time-dependent PNP equations. So far, we have not seen a priori error estimate of finite element method for the time-dependent PNP equations with either semi- or full discretization schemes in a completely accurate fashion.

The main purpose of this paper is to provide a complete a priori error analysis for the finite element discretization of the time-dependent PNP equations. We obtain optimal error estimates in $L^\infty(H^1)$ and $L^2(H^1)$ norms and a sub-optimal error estimate in the $L^\infty(L^2)$ norm for both semi- and fully discrete finite element discretization using linear elements. In addition, we also give an optimal error estimate in $L^\infty(L^2)$ norm for the quadratic or higher-order finite element discretization.

The rest of this paper is organized as follows. Section 2 introduces the model problem. Section 3 describes the semi- and full discretization of the problem. The main error estimates for semi-discretization and full dicretization are given in Section 4 and Section 5, respectively. Numerical experiments are reported in Section 6.

2. PNP system and its variational form

Let $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$, be a bounded Lipschitz domain. We use the standard notation for Sobolev spaces $W^{l,p}(\Omega)$ and their associated norms and seminorms. For $p = 2$, the notations $W^{l,2}(\Omega) = H^l(\Omega)$, $H_0^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$ and the standard L^2 inner product $(\cdot, \cdot)$ are adopted.

The classic PNP system was introduced by W. Nernst [48] and M. Planck [49]. It describes the mass concentration of ions $C_1, C_2 : \Omega \times (0, T] \to \mathbb{R}_0^+$, and the electrostatic potential $\Phi : \Omega \times (0, T] \to \mathbb{R}$,

$$\partial_t C_i - \nabla \cdot (\nabla C_i + q_i C_i \nabla \Phi) = F_i, \quad \text{for } i = 1, 2 \tag{2.1}$$

$$-\Delta \Phi = \sum_{i=1}^{2} q_i C_i + F_3, \tag{2.2}$$

where $\partial_t = \partial/\partial t$. The index i corresponds to the different ionic species, and q_i is the charge of the species i, for simplicity, in the following we choose $q_1 = 1, q_2 = -1$. F_i $(i = 1, 2, 3)$ denote the reaction source terms. Note that the convection terms given in (2.1) are in divergence form.