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

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\textbf{A B S T R A C T}

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 $L^\infty(W^1)$ and $L^2(W^1)$ 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.

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\section{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 \cite{1–5}, electrochemical systems \cite{6–11} and biological membrane channels \cite{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 \cite{22,23}. In \cite{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 \cite{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 \cite{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 \cite{12,13,30–32,19}. In \cite{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 \cite{33}. The use of finite difference method has certain limitation on the description of ionic channel geometry. Finite volume method was then used in \cite{34,35} to solve PNP
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 \( L^2 \) norm depend essentially on the \( L^1 \) 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-discretization 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 finite-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 discretization 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 \( W^{1,p} (\Omega) \) and their associated norms and seminorms. For \( p = 2 \), the notations \( W^{1,2} (\Omega) = H^1 (\Omega) \), \( H^1_0 (\Omega) = \{ v \in H^1 (\Omega) : v|_{\partial \Omega} = 0 \} \) 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 \( C_1, C_2 : \Omega \times (0, T) \rightarrow \mathbb{R}_0^+ \), and the electrostatic potential \( \Phi : \Omega \times (0, T) \rightarrow \mathbb{R} \),

\[
\begin{align*}
\partial_t C_i - \nabla \cdot (\nabla C_i + q_i C_i \nabla \Phi) &= F_i, \quad \text{for } i = 1, 2, \\
-\Delta \Phi &= \sum_{i=1}^{2} q_i C_i + F_3,
\end{align*}
\]  

(2.1)

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.
Denote the initial concentrations and potential by \((C^0_i, C^0_0, \phi^0)\). Either flux-free condition or Dirichlet type boundary conditions can be applied to the PNP equations [50]. For simplicity, we shall consider the homogeneous Dirichlet boundary conditions as follows:

\[ C_1 = C_2 = \phi = 0, \quad \text{on } \partial \Omega \times (0, T]. \]

The weak formulation of the system (2.1) and (2.2) is given as: find \(C_i \in L^2(0, T; H^1_0(\Omega)) \cap L^\infty(0, T; L^\infty(\Omega)), i = 1, 2, \) and \(\Phi(t) \in H^1_0(\Omega)\) such that,

\[
(\partial_t C_i, v) + (\nabla C_i, \nabla v) + (q_i C_i \nabla \phi, \nabla v) = (F_i, v), \quad \forall v \in H^1_0(\Omega),
\]

\[
(\nabla \Phi, \nabla \phi) - \sum_{i=1}^{2} q_i (C_i, \phi) = (F_3, \phi), \quad \forall \phi \in H^1_0(\Omega).
\]

In [25], it was proved that there exists a unique solution \((C_i, C_2, \Phi)\) satisfying (2.3) and (2.4) when \(F_i \in L^\infty_+(0, T; \mathbb{R}^d)\).

3. Finite element discretization

Let \(T_h\) be a quasi-uniform mesh of \(\Omega\) with mesh size \(0 < h < 1\) [51] and define the corresponding finite element space \(S_h \subset H^1_0(\Omega)\) by

\[ S_h = \{ v \in H^1(\Omega) : v|_{\partial \Omega} = 0 \text{ and } v|_K \in P_k(K), \forall K \in T_h \}, \]

where \(P_k(K)\) is the set of polynomials of degree \(k\) or less.

The semi-discretization to (2.3)–(2.4) is defined as follows: find \((C_{1,h}, C_{2,h}, \Phi_h) \in [S_h]^3\) such that,

\[
(\partial_t C_{i,h}, v_h) + (\nabla C_{i,h}, \nabla v_h) + (q_i C_{i,h} \nabla \phi_h, \nabla v_h) = (F_i, v_h), \quad \forall v_h \in S_h, \tag{3.1}
\]

\[
(\nabla \Phi_h, \nabla \phi_h) - \sum_{i=1}^{2} q_i (C_{i,h}, \phi_h) = (F_3, \phi_h), \quad \forall \phi_h \in S_h, \tag{3.2}
\]

with the initial condition \((C^0_{1,h}, C^0_{2,h}, \Phi^0_h)\) given by the interpolation of \((C^0_1, C^0_2, \Phi^0)\) in \([S_h]^3\) and the Dirichlet boundary condition \(C_{1,h} = C_{2,h} = \phi_h = 0\).

In order to give the full discretization of the system (2.3)–(2.4), we first define a uniform partition \(0 = t^0 < t^1 < \cdots < t^N = T\), with time-step size \(\Delta t = T/N\), and \(t^n = n \Delta t, n \in \mathbb{R}\). Also, for any function \(\phi\), denote \(\phi^n \equiv \phi(x, t^n)\), \(\phi^{n+\frac{1}{2}} \equiv (\phi^{n+1} + \phi^n)/2\), and \(d_t \phi^n \equiv (\phi^{n+1} - \phi^n)/\Delta t\). We use the Crank–Nicolson scheme for the time discretization, i.e., given \((C^n_{1,h}, C^n_{2,h}, \Phi^n_h)\), we seek \((C^{n+1}_{1,h}, C^{n+1}_{2,h}, \Phi^{n+1}_h) \in [S_h]^3\) such that,

\[
(d_t C^n_{i,h}, v_h) + (\nabla C_{i,h}^{n+\frac{1}{2}}, \nabla v_h) + \left( q_i C_{i,h}^{n+\frac{1}{2}} \nabla \phi_h^{n+\frac{1}{2}}, \nabla v_h \right) = (F_{i,h}^{n+\frac{1}{2}}, v_h), \quad \forall v_h \in S_h, \tag{3.3}
\]

\[
(\nabla \phi_h^{n+\frac{1}{2}}, \nabla \phi_h) - \sum_{i=1}^{2} q_i (C_{i,h}^{n+\frac{1}{2}}, \phi_h) = (F_{3,h}^{n+\frac{1}{2}}, \phi_h), \quad \forall \phi_h \in S_h. \tag{3.4}
\]

The wellposedness of (3.3) and (3.4) can be proved by a similar approach shown in [46]. In fact, the given configurations of our method match all the assumptions prescribed in [46] except the only difference between our time integration scheme (Crank–Nicolson) and theirs (backward Euler) in [46] for (3.3). Considering that Crank–Nicolson scheme is just an average of the backward Euler scheme and forward Euler scheme, fortunately, such difference does not critically affect the analytical techniques which are used in [46], we are still able to use them to prove the wellposedness of (3.3)–(3.4) in a similar fashion, which thus is omitted here.

Finally, we use the Picard’s linearization for the nonlinear term in (3.3) and obtain the following practical numerical algorithm:

**Algorithm 1.**

1. Initialization for time marching: Set time step \(n = 0\) and take the initial value \((C^0_{1,h}, C^0_{2,h}, \Phi^0_h) \in [S_h]^3\).

2. Initialization for nonlinear iteration: Let \((C^{n+1.0}_{1,h}, C^{n+1.0}_{2,h}, \Phi^{n+1.0}_h) = (C^n_{1,h}, C^n_{2,h}, \Phi^n_h)\) when \(n \geq 0\).

3. Finite element computation on each nonlinear iteration: For \(i \geq 0\), compute \((C^{n+1,i+1}_{1,h}, C^{n+1,i+1}_{2,h}, \Phi^{n+1,i+1}_h) \in [S_h]^3\), such that for all \((v_{1,h}, v_{2,h}, \phi_h) \in [S_h]^3\) and for \(i = 1, 2,\)

\[
\left( \frac{1}{\Delta t} (C^{n+1,i+1}_{i,h} - C^n_{i,h}), v_h \right) + (\nabla C^{n+1,i+1}_{i,h}, \nabla v_h) + \left( q_i C^{n+1,i+1}_{i,h} \nabla \phi^{n+1,i+1}_h, \nabla v_h \right) = (F^{n+\frac{1}{2}}_{i,h}, v_h),
\]

\[
(\nabla \phi^{n+\frac{1}{2},i+1}_h, \nabla \phi_h) - \sum_{i=1}^{2} q_i (C^{n+1,i+1}_{i,h}, \phi_h) = (F_{3,h}^{n+\frac{1}{2}}, \phi_h).
\]
4. Checking the stopping criteria for nonlinear iteration: For a fixed tolerance $\varepsilon$, stop the iteration if

$$
\sum_{i=1}^{2} \| C_{i,h}^{n+1,l+1} - C_{i,h}^{n+1,l} \|_{L^2}^2 + \| \Phi_h^{n+1,l+1} - \Phi_h^{n+1,l} \|_{L^2}^2 \leq \varepsilon,
$$

and set $(C_{1,h}^{n+1}, C_{2,h}^{n+1}, \Phi_h^{n+1}) = (C_{1,h}^{n+1,l+1}, C_{2,h}^{n+1,l+1}, \Phi_h^{n+1,l+1})$. Otherwise, set $l \leftarrow l + 1$ and go to Step 3 to continue the nonlinear iteration.

5. Time marching: Stop if $n + 1 = N$. Otherwise set $n \leftarrow n + 1$ and go to Step 2.

4. Error analysis for the semi-discretization

In this section, we give a priori error estimates for the semi-discrete solution $(C_{1,h}, C_{2,h}, \Phi_h)$. For the sake of simplicity, we sometimes drop the time dependence in $C_i(t), C_{i,h}(t), \Phi(t)$ and $\Phi_h(t)$ in the following sections. Denote $M$ as a generic constant throughout the paper.

First of all, we assume the following regularity properties hold for $C_i (i = 1, 2)$, and $\Phi$ in the semi-discretization analysis:

$$
C_i \in W^{1,\infty}(0, T; H^{k+1} \cap W^{1,\infty}(\Omega)) \quad \text{and} \quad \Phi \in W^{1,\infty}(0, T; W^{k+1,\infty}(\Omega)).
$$

(4.1)

For any $\tau \in [0, T]$, let $\tilde{\Phi} \in S_h$ be the $H^1$ projection of $\Phi(\tau)$ satisfy

$$
(\nabla(\Phi(\tau) - \tilde{\Phi}(\tau)), \nabla \phi_h) = 0, \quad \forall \phi_h \in S_h.
$$

(4.2)

We first recall the standard error estimates of the above $H^1$ projection in various norms $[52, 53]$, as shown in the following lemma.

**Lemma 4.1.** Let $(C_1, C_2, \Phi)$ be the solution of (2.3)–(2.4) satisfying the regularity assumptions (4.1). Let $\tilde{\Phi}(\tau)$ be the projection of $\Phi$ defined in (4.2), then for $\tau \in (0, T]$, we have the following error estimates:

$$
\begin{align*}
&h \| \partial_t \nabla (\Phi(\tau) - \tilde{\Phi}(\tau)) \|_{L^2}^2 + \| \partial_t (\Phi(\tau) - \tilde{\Phi}(\tau)) \|_{L^2}^2 \\
&+ h \| \nabla (\Phi(\tau) - \tilde{\Phi}(\tau)) \|_{L^2}^2 + \| \Phi(\tau) - \tilde{\Phi}(\tau) \|_{L^2}^2 \leq M h^{k+1} (\| \Phi(\tau) \|_{H^{k+1}} + \| \partial_t \Phi(\tau) \|_{H^{k+1}}),
\end{align*}
$$

(4.3)

and

$$
\begin{align*}
&\| \nabla(\Phi(\tau) - \tilde{\Phi}(\tau)) \|_{L^\infty}^2 + \| \partial_t \nabla (\Phi(\tau) - \tilde{\Phi}(\tau)) \|_{L^\infty}^2 \\
&\leq M h^k (\| \Phi(\tau) \|_{W^{k+1,\infty}} + \| \partial_t \Phi(\tau) \|_{W^{k+1,\infty}}).
\end{align*}
$$

(4.4)

In the following lemma, we prove the error estimates of $\tilde{\Phi} - \Phi_h$ and $\partial_t (\tilde{\Phi} - \Phi_h)$.

**Lemma 4.2.** Let $(C_1, C_2, \Phi)$ be the solution to (2.3) and (2.4), $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution to (3.1) and (3.2), and $\tilde{\Phi}$ be defined by (4.2). Then for $\tau \in (0, T]$,

$$
\| \tilde{\Phi}(\tau) - \Phi_h(\tau) \|_{L^2} + \| \nabla (\tilde{\Phi}(\tau) - \Phi_h(\tau)) \|_{L^2} \leq M \sum_{i=1}^{2} \| C_i(\tau) - C_{i,h}(\tau) \|_{L^2},
$$

(4.5)

and

$$
\| \partial_t (\tilde{\Phi}(\tau) - \Phi_h(\tau)) \|_{L^2} + \| \partial_t \nabla (\tilde{\Phi}(\tau) - \Phi_h(\tau)) \|_{L^2} \leq M \sum_{i=1}^{2} \| \partial_t (C_i(\tau) - C_{i,h}(\tau)) \|_{L^2}.
$$

(4.6)

**Proof.** Subtract (3.2) from (2.4), use (4.2), and let $\phi_h = \tilde{\Phi} - \Phi_h$, we have for $\tau \in (0, T]$,

$$
(\nabla(\Phi - \Phi_h), \nabla(\tilde{\Phi} - \Phi_h)) - \sum_{i=1}^{2} q_i (C_i - C_{i,h}, \tilde{\Phi} - \Phi_h) = 0.
$$

By Poincaré inequality,

$$
\| \nabla (\tilde{\Phi} - \Phi_h) \|_{L^2}^2 \leq \sum_{i=1}^{2} \| C_i - C_{i,h} \|_{L^2} \| \tilde{\Phi} - \Phi_h \|_{L^2} \leq \tilde{M} \sum_{i=1}^{2} \| C_i - C_{i,h} \|_{L^2} \| \nabla (\tilde{\Phi} - \Phi_h) \|_{L^2},
$$

where $\tilde{M}$ is a constant depending on the size of the domain $\Omega$. Hence, we get

$$
\| \nabla (\tilde{\Phi} - \Phi_h) \|_{L^2} \leq M \sum_{i=1}^{2} \| C_i - C_{i,h} \|_{L^2}.
$$
Use Aubin–Nitsche duality argument, we can get that
\[
\| \tilde{\Phi} - \Phi_h \|_{L^2} \leq M h \| \nabla (\tilde{\Phi} - \Phi_h) \|_{L^2} + M \sum_{i=1}^2 \| C_i - C_{i,h} \|_{L^2}.
\]

Thus we get (4.5).

Differentiating (3.2) and (4.2) with respect to time, and following the similar process we can obtain the \( L^2 \) and \( H^1 \) error estimate of \( \partial_t (\tilde{\Phi} - \Phi_h) \). Thus we get (4.6).

By (4.3), (4.5), (4.6) and Poincaré inequality, we can easily get the error estimates of \( \Phi - \Phi_h \) and \( \partial_t (\Phi - \Phi_h) \) in \( L^2 \) and \( H^1 \) norms, as shown in the following lemma.

**Lemma 4.3.** Let \( (C_1, C_2, \Phi) \) be the solution of (2.3)–(2.4) satisfying the regularity assumptions (4.1) and \( (C_{1,h}, C_{2,h}, \Phi_h) \) be the solution of (3.1)–(3.2). Then for \( \tau \in (0, T) \), we now have the following error estimates:

\[
\| \Phi (\tau) - \Phi_h (\tau) \|_{L^2} \leq M h^{k+1} \| \Phi (\tau) \|_{H^{k+1}} + M \sum_{i=1}^2 \| C_i (\tau) - C_{i,h} (\tau) \|_{L^2},
\]

\[
\| \nabla (\Phi (\tau) - \Phi_h (\tau)) \|_{L^2} \leq M h^k \| \Phi (\tau) \|_{H^{k+1}} + M \sum_{i=1}^2 \| \nabla C_i (\tau) - \nabla C_{i,h} (\tau) \|_{L^2},
\]

\[
\| \partial_t (\Phi (\tau) - \Phi_h (\tau)) \|_{L^2} \leq M h^{k+1} \left( \| \Phi (\tau) \|_{H^{k+1}} + \| \partial_t \Phi (\tau) \|_{H^{k+1}} \right)
+ M \sum_{i=1}^2 \left( \| C_i (\tau) - C_{i,h} (\tau) \|_{L^2} + \| \partial_t C_i (\tau) - \partial_t C_{i,h} (\tau) \|_{L^2} \right),
\]

and

\[
\| \partial_t \nabla (\Phi (\tau) - \Phi_h (\tau)) \|_{L^2} \leq M h^k \left( \| \Phi (\tau) \|_{H^{k+1}} + \| \partial_t \Phi (\tau) \|_{H^{k+1}} \right)
+ M \sum_{i=1}^2 \left( \| C_i (\tau) - C_{i,h} (\tau) \|_{L^2} + \| \partial_t C_i (\tau) - \partial_t C_{i,h} (\tau) \|_{L^2} \right).
\]

Next we move our focus to \( C_i \) and introduce its \( H^1 \) projection first. Define the finite element solution \( \tilde{C}_i \in S_h \) to satisfy the following variational problem at any given time \( \tau \in [0, T] \) as

\[
\left( \nabla \left( C_i (\tau) - \tilde{C}_i (\tau) \right), \nabla v_h \right) + q_i \left( \left( C_i (\tau) - \tilde{C}_i (\tau) \right) \nabla \Phi (\tau), \nabla v_h \right) = 0, \quad \forall v_h \in S_h.
\]

Now we give the error estimates of \( C_i - \tilde{C}_i \) in \( L^2 \) and \( H^1 \) norms in the next lemma.

**Lemma 4.4.** Let \( (C_1, C_2, \Phi) \) be the solution of (2.3)–(2.4) satisfying the regularity assumptions (4.1), and \( \tilde{C}_i \) defined in (4.11). We have the following error estimates for \( \tau \in [0, T] \):

\[
\| C_i (\tau) - \tilde{C}_i (\tau) \|_{L^2} + h \| \nabla \left( C_i (\tau) - \tilde{C}_i (\tau) \right) \|_{L^2} \leq M h^{k+1} \| C_i (\tau) \|_{H^{k+1}},
\]

and further,

\[
\| \partial_t \left( C_i (\tau) - \tilde{C}_i (\tau) \right) \|_{L^2} + h \| \partial_t \nabla \left( C_i (\tau) - \tilde{C}_i (\tau) \right) \|_{L^2} \leq M h^{k+1} \left( \| C_i (\tau) \|_{H^{k+1}} + \| \partial_t C_i (\tau) \|_{H^{k+1}} \right).
\]

**Proof.** Let \( \Pi_h C_i \in S_h \) be the finite element nodal interpolation of \( C_i \), use (4.11) we get

\[
\left( \nabla \left( C_i - \tilde{C}_i \right), \nabla \left( C_i - \tilde{C}_i \right) \right) + q_i \left( \left( C_i - \tilde{C}_i \right) \nabla \Phi, \nabla \left( C_i - \tilde{C}_i \right) \right)
= \left( \nabla \left( C_i - \tilde{C}_i \right), \nabla \left( C_i - \Pi_h C_i \right) \right) + q_i \left( \left( C_i - \tilde{C}_i \right) \nabla \Phi, \nabla \left( C_i - \Pi_h C_i \right) \right).
\]

Use Cauchy–Schwarz inequality and Young’s inequality,

\[
\| \nabla (C_i - \tilde{C}_i) \|_{L^2}^2 \leq \| \nabla (C_i - \Pi_h C_i) \|_{L^2}^2 + \| \nabla \Phi \|_{L^\infty} \| \nabla (C_i - \Pi_h C_i) \|_{L^2} \| C_i - \tilde{C}_i \|_{L^2}
+ \| \nabla \Phi \|_{L^\infty} \| \nabla (C_i - \tilde{C}_i) \|_{L^2} \| C_i - \tilde{C}_i \|_{L^2}
\leq \left( \frac{1}{4 \epsilon} + \frac{1}{2} \right) \left( \| \nabla (C_i - \Pi_h C_i) \|_{L^2}^2 + \| \nabla \Phi \|_{L^\infty}^2 \| C_i - \tilde{C}_i \|_{L^2}^2 \right) + 2 \epsilon \| \nabla (C_i - \tilde{C}_i) \|_{L^2}^2.
\]
hence
\[ \| \nabla (C_i - \tilde{C}_i) \|_{L^2} \leq M \left( \| \nabla (C_i - \Pi_h C_i) \|_{L^2} + \| C_i - \tilde{C}_i \|_{L^2} \right) \]
\[ \leq M \left( h^k \| C_i \|_{H^{k+1}} + \| C_i - \tilde{C}_i \|_{L^2} \right). \] (4.15)

The last inequality comes from the interpolation error estimate in $H^1$ norm [52].

Now we shall use Aubin–Nitsche duality argument to obtain the $L^2$ error estimate of $C_i - \tilde{C}_i$. We define the adjoint problem of (4.11) as below,
\[
\begin{cases}
-\Delta u_i + q_i \nabla \Phi \cdot \nabla u_i = C_i - \tilde{C}_i, & \text{in } \Omega \\
 u_i = 0, & \text{on } \partial \Omega.
\end{cases}
\]

By the regularity theory of partial differential equations [54], it is well known that $\| u_i \|_{H^2} \leq M \| C_i - \tilde{C}_i \|_{L^2}$ for $\Phi(\tau) \in W^{1,\infty}(\Omega)$.

Let $\Pi_h u_i \in S_h$ be the finite element nodal interpolation of $u_i$, and use (4.11), Cauchy–Schwarz inequality and Poincaré inequality, we have
\[
\| C_i - \tilde{C}_i \|_{L^2} = (\nabla (C_i - \tilde{C}_i), \nabla u_i) + q_i (C_i - \tilde{C}_i, \nabla \Phi \cdot \nabla u_i)
\leq (\nabla (C_i - \tilde{C}_i), \nabla (u_i - \Pi_h u_i)) + (\nabla (C_i - \tilde{C}_i), \nabla \Pi_h u_i)
\leq \| \nabla (C_i - \tilde{C}_i) \|_{L^2} \| \nabla (u_i - \Pi_h u_i) \|_{L^2} + M \| \nabla \Phi \|_{L^\infty} \| \nabla (C_i - \tilde{C}_i) \|_{L^2} \| \nabla (u_i - \Pi_h u_i) \|_{L^2}
\leq M h \| \nabla (C_i - \tilde{C}_i) \|_{L^2} \| u_i \|_{H^2}
\leq M h \| \nabla (C_i - \tilde{C}_i) \|_{L^2} \| C_i - \tilde{C}_i \|_{L^2},
\]
where $M$ is the Poincaré constant. Therefore,
\[
\| C_i - \tilde{C}_i \|_{L^2} \leq M h \| \nabla (C_i - \tilde{C}_i) \|_{L^2}.
\]

Thus when $h$ is sufficiently small, use (4.15), we get (4.12).

Take derivative with respect to $t$ in (4.11), and similar to (4.14), for any $v_h \in S_h$, we have,
\[
(\partial_t \nabla (C_i - \tilde{C}_i), \nabla (C_i - \tilde{C}_i)) + q_i (\partial_t ((C_i - \tilde{C}_i) \nabla \Phi), \partial_t (C_i - \tilde{C}_i))
= (\partial_t \nabla (C_i - \tilde{C}_i), \partial_t \nabla (C_i - \Pi_h C_i)) + q_i (\partial_t ((C_i - \tilde{C}_i) \nabla \Phi), \partial_t (C_i - \Pi_h C_i)).
\]

Therefore, by Poincaré inequality and Young’s inequality,
\[
\| \partial_t \nabla (C_i - \tilde{C}_i) \|_{L^2}^2 \leq \frac{1}{4\epsilon} \| \nabla \Phi \|_{L^\infty}^2 \| \partial_t (C_i - \tilde{C}_i) \|_{L^2}^2 + \frac{1}{4\epsilon} \| \partial_t \nabla (C_i - \tilde{C}_i) \|_{L^2}^2 + \frac{1}{2} \| \partial_t \nabla (C_i - \Pi_h C_i) \|_{L^2}^2 + \frac{1}{2} \| \partial_t \nabla (C_i - \tilde{C}_i) \|_{L^2}^2,
\]
\[
\leq \frac{1}{2} \| \nabla \Phi \|_{L^\infty}^2 \| \partial_t (C_i - \tilde{C}_i) \|_{L^2}^2 + \frac{1}{2} \| \partial_t \nabla (C_i - \Pi_h C_i) \|_{L^2}^2 + \frac{1}{2} \| \partial_t \nabla (C_i - \tilde{C}_i) \|_{L^2}^2.
\]

Since $\epsilon$ is arbitrary small, and $\Phi \in W^{1,\infty}(0, T; W^{k+1,\infty}(\Omega))$, we can get
\[
\| \partial_t \nabla (C_i - \tilde{C}_i) \|_{L^2} \leq M \left( \| C_i - \tilde{C}_i \|_{L^2} + \| \partial_t \nabla (C_i - \Pi_h C_i) \|_{L^2} + \| \partial_t (C_i - \tilde{C}_i) \|_{L^2} \right).
\]

Use (4.12) and the interpolation error estimate [52], we have
\[
\| \partial_t \nabla (C_i - \tilde{C}_i) \|_{L^2} \leq M \left( h^k \left( \| C_i \|_{H^{k+1}} + \| \partial_t C_i \|_{H^{k+1}} \right) + \| \partial_t (C_i - \tilde{C}_i) \|_{L^2} \right).
\]

Again, by a similar Aubin–Nitsche duality argument, we can obtain (4.13).

For the maximum norm error estimates of $C_i - \tilde{C}_i$, we give the following lemma. The proof can be done using a similar fashion as Lemma 4.4 and some classic results of the error estimate in maximum norm given in [51–53].

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Y. Sun et al. / Journal of Computational and Applied Mathematics 301 (2016) 28–43

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Theorem 4.1. Let \((C_1, C_2, \Phi)\) be the solution of (2.3)–(2.4) satisfying the regularity assumptions (4.1). Let \(\tilde{C}_{i}(\tau)\) be defined in (4.11), then for \(\tau \in (0, T]\), we have the following error estimates:

\[
\left\| \tilde{C}_{i}(\tau) - C_{i}(\tau) \right\|_{L^\infty} + \left\| \partial_t \left( \tilde{C}_{i}(\tau) - C_{i}(\tau) \right) \right\|_{L^\infty} \leq \begin{cases} \frac{Mh^{k+1}}{2} \left| \log h \right| \left( \|C_{i}(\tau)\|_{H^{k+1}} + \|\partial_t C_{i}(\tau)\|_{H^{k+1}} \right), & \text{when } k = 1, \\
\frac{Mh^{k+1}}{2} \left( \|C_{i}(\tau)\|_{H^{k+1}} + \|\partial_t C_{i}(\tau)\|_{H^{k+1}} \right), & \text{when } k > 1.
\end{cases}
\] (4.16)

Finally, we give a priori error estimate for \(C_{i} - C_{i,h}\) and \(\Phi - \Phi_h\) in \(L^\infty(L^2)\) and \(L^\infty(H^1)\) norms in the following theorem.

Theorem 4.1. Let \((C_1, C_2, \Phi)\) be the solution of (2.3) and (2.4) satisfying the regularity assumptions (4.1) and \((C_{1,h}, C_{2,h}, \Phi_h)\) be the solution of (3.1) and (3.2). Then we have the following a priori error estimates for \(\tau \in (0, T]\),

\[
\|C_{i}(\tau) - C_{i,h}(\tau)\|_{L^\infty(L^2)} + \|\nabla(C_{i}(\tau) - C_{i,h}(\tau))\|_{L^\infty(L^2)}
+ \|\Phi(\tau) - \Phi_h(\tau)\|_{L^\infty(L^2)} + \|\nabla(\Phi(\tau) - \Phi_h(\tau))\|_{L^\infty(L^2)} \leq M h^k,
\] (4.17)

where \(i = 1, 2\) and \(M\) is a constant depending only on the regularities of \(C_i\) and \(\Phi\).

Proof. Subtract (3.1) from (2.3), and use the Galerkin orthogonality (4.11), we have

\[
(\partial_t(C_i - C_{i,h}), v_h) + (\nabla(C_i - C_{i,h}), \nabla v_h) + q_i(\tilde{C}_{i} - C_{i,h}) \nabla \Phi, \nabla v_h) = 0, \quad \forall v_h \in S_h.
\]

Hence,

\[
(\partial_t(\tilde{C}_{i} - C_{i,h}), v_h) + (\nabla(\tilde{C}_{i} - C_{i,h}), \nabla v_h) = -(\partial_t(C_i - C_{i}), v_h) - q_i((C_{i} - C_{i,h}) \nabla \Phi, \nabla v_h)
+ q_i(C_{i} - C_{i,h}) \nabla(\Phi - \Phi_h), \nabla v_h) - q_i(C_{i} \nabla(\Phi - \Phi_h), \nabla v_h).
\] (4.18)

Let \(\eta_i = C_i - \tilde{C}_{i}\) and \(\xi_i = C_{i,h} - \tilde{C}_{i}\), choose \(v_h = \xi_i \in S_h\), we can write (4.18) as

\[
(\partial_t \eta_i, \eta_i) + (\nabla \xi_i, \nabla \xi_i) = \sum_{i=1}^{4} H_i, \quad (4.19)
\]

where \(H_i, \ i = 1, 2, 3, 4\), are defined as

\[
H_1 := -(\partial_t \eta_i, \xi_i),
H_2 := -q_i(\xi_i \nabla \Phi, \nabla \xi_i),
H_3 := q_i((C_i - C_{i,h}) \nabla(\Phi - \Phi_h), \nabla \xi_i),
H_4 := -q_i(C_i \nabla(\Phi - \Phi_h), \nabla \xi_i).
\]

In the following, we shall estimate \(H_1, H_2, H_3,\) and \(H_4,\) respectively.

\[
H_1 \leq \|\partial_t \eta_i\|_{L^2} \|\xi_i\|_{L^2} \leq Mh^{k+1} \|\xi_i\|_{L^2} \leq \frac{M}{2} h^{2k+2} + \frac{1}{2} \|\xi_i\|_{L^2}^2, \quad (by \ (4.13))
\]

\[
H_2 \leq \|\nabla \Phi\|_{L^\infty} \|\eta_i\|_{L^2} \|\nabla \xi_i\|_{L^2} \leq \frac{1}{4\epsilon} \|\nabla \Phi\|_{L^\infty}^2 \|\xi_i\|_{L^2}^2 + \epsilon \|\nabla \xi_i\|_{L^2}^2,
\]

\[
H_3 \leq M \|\eta_i\|_{L^2} \|\nabla(\Phi - \Phi_h)\|_{L^\infty} + q_i(\xi_i \nabla(\Phi - \Phi_h), \nabla \xi_i)
\leq M \|\eta_i\|_{L^2} \left( \|\nabla(\Phi - \Phi_h)\|_{L^\infty} + \|\nabla(\Phi - \Phi_h)\|_{L^\infty} \right) \|\nabla \xi_i\|_{L^2}
\leq M \left( h^{2k+1} \|\xi_i\|_{L^2}^2 + h^k \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} \right) + M \left( h^{k+1} + \|\xi_i\|_{L^2} \right) \|\nabla(\Phi - \Phi_h)\|_{L^\infty} \|\nabla \xi_i\|_{L^2}, \quad (by \ (4.4), \ (4.12)).
\]

By inverse inequality and (4.5), we have

\[
\|\nabla(\Phi - \Phi_h)\|_{L^\infty} \leq M h^{-\frac{d}{2}} \|\nabla(\Phi - \Phi_h)\|_{L^2} \leq M h^{-\frac{d}{2}} \sum_{j=1}^{2} \|\zeta_j - C_{j,h}\|_{L^2} \leq M h^{-\frac{d}{2}} \sum_{j=1}^{2} (\|\xi_j\|_{L^2} + \|\eta_j\|_{L^2}).
\]
also by (4.4) and (4.12),

\[ H_3 \leq M \left( h^{2k+1} \| \nabla \xi_i \|_{L^2} + h^k \| \xi_i \|_{L^2} \| \nabla \xi_i \|_{L^2} \right) + M \left( h^{k+1-\frac{d}{2}} + h^{\frac{d}{2}} \| \xi_i \|_{L^2} \right) \sum_{j=1}^{\infty} \left( \| \xi_j \|_{L^2} + \| \eta_j \|_{L^2} \right) \| \nabla \xi_i \|_{L^2} \]

\[ \leq M \left( h^{2k+\frac{d}{2}} \| \nabla \xi_i \|_{L^2} + h^{k+1-\frac{d}{2}} \sum_{j=1}^{\infty} \| \xi_j \|_{L^2} \| \nabla \xi_i \|_{L^2} + h^{\frac{d}{2}} \| \xi_i \|_{L^2} \sum_{j=1}^{\infty} \| \xi_j \|_{L^2} \| \nabla \xi_i \|_{L^2} \right). \]

Now we conduct a mathematical induction process and propose the following induction hypothesis

\[ h^{-\frac{d}{2}} \| \xi_i(t) \|_{L^2} \leq M, \quad \forall t \in [0, T]. \quad (4.20) \]

By the initial conditions and (4.12), we have

\[ h^{-\frac{d}{2}} \| \xi_i(0) \|_{L^2} \leq h^{-\frac{d}{2}} \| C_i(0) - C_{i,h}(0) \|_{L^2} + h^{-\frac{d}{2}} \| \eta_i(0) \|_{L^2} \leq M h^{k+1-\frac{d}{2}} \| C_i(0) \|_{H^{k+1}} \leq M. \quad (4.21) \]

Assume that (4.20) holds for any \( t \in [0, T^*], T^* < T \). Use Young’s inequality, we have

\[ H_3 \leq M \left( h^{4k+1} + \sum_{j=1}^{\infty} \| \xi_j \|_{L^2}^2 + \varepsilon \| \nabla \xi_i \|_{L^2}^2 \right). \]

Hence (4.19) reads,

\[ \frac{1}{2} \partial_t \| \xi_i \|_{L^2}^2 + \| \nabla \xi_i \|_{L^2}^2 \leq M \left( h^{4k+1} + h^{2k+2} + h^{2k} + \sum_{j=1}^{\infty} \| \xi_j \|_{L^2}^2 + \varepsilon \| \nabla \xi_i \|_{L^2}^2 \right). \]

Take integral with respect to \( t \),

\[ \| \xi_i \|_{L^2}^2 + \int_0^t \| \nabla \xi_i \|_{L^2}^2 \leq M \left( h^{2k} + \sum_{j=1}^{\infty} \int_0^t \| \xi_j \|_{L^2}^2 \right), \]

therefore,

\[ \sum_{i=1}^2 \left( \| \xi_i \|_{L^2}^2 + \int_0^t \| \nabla \xi_i \|_{L^2}^2 \right) \leq M \left( h^{2k} + \sum_{j=1}^{\infty} \int_0^t \| \xi_j \|_{L^2}^2 \right), \]

then use Gronwall’s inequality, we have for \( 0 \leq t \leq T^* \),

\[ \sum_{i=1}^2 \left( \| \xi_i \|_{L^2(0^2)} + \| \nabla \xi_i \|_{L^2(0^2)} \right) \leq M h^k, \]

thus for \( i = 1, 2, \)

\[ \| \xi_i \|_{L^2(0^2)} + \| \nabla \xi_i \|_{L^2(0^2)} \leq M h^k. \]

This implies that for \( k \geq d - 1, \)

\[ h^{-\frac{d}{2}} \| \xi_i \|_{L^2} \leq M h^{-\frac{d}{2}} \leq M. \]

On the other hand, since \( h^{-\frac{d}{2}} \| \xi_i \|_{L^2} \) is a continuous function with respect to \( t \in [0, T] \), thus due to the uniform continuity with time, there exists \( \delta \) such that for any \( t \in [0, T^* + \delta] \), we have \( h^{-\frac{d}{2}} \| \xi_i \|_{L^2} \leq M \). Because \([0, T]\) is a finite interval, so the induction hypothesis (4.20) holds true for all \( t \in [0, T] \).

Therefore, for any \( t \in [0, T], \)

\[ \| C_i - C_{i,h} \|_{L^2(0^2)} + \| \nabla (C_i - C_{i,h}) \|_{L^2(0^2)} \leq M h^k. \]

Use (4.23) in (4.7) and (4.8), we can get

\[ \| \phi - \phi_h \|_{L^2(0^2)} + \| \nabla (\phi - \phi_h) \|_{L^2(0^2)} \leq M h^k. \]

Lastly, we use a similar approach as above to obtain the error estimate \( \| \nabla (C_i - C_{i,h}) \|_{L^2(0^2)} \). Choose \( v_h = \partial_t \xi_i \in S_h \) in (4.18), thus

\[ (\nabla \xi_i, \partial_t \nabla \xi_i) + (\partial_t \xi_i, \partial_t \nabla \xi_i) = \sum_{i=1}^4 \hat{H}_i \]

(4.25)
where $\hat{H}_i$, $i = 1, 2, 3, 4$, are defined as

$$
\hat{H}_1 := - (\partial_t \eta_i, \partial_t \xi_i), \\
\hat{H}_2 := - q_i((\bar{C}_i - C_{i,h}) \nabla \theta_i, \partial_t \nabla \xi_i), \\
\hat{H}_3 := q_i((C_i - C_{i,h}) \nabla (\Phi - \Phi_h), \partial_t \nabla \xi_i), \\
\hat{H}_4 := - q_i(C_i \nabla (\Phi - \Phi_h), \partial_t \nabla \xi_i).
$$

We estimate $\hat{H}_i$ respectively below:

$$
\hat{H}_1 \leq \|\partial_t \eta_i\|_{L^2} \|\partial_t \xi_i\|_{L^2} \leq M \left(h^{2k+2} + \epsilon \|\partial_t \xi_i\|_{L^2}^2 \right), \quad \text{by (4.13)}
$$

$$
\hat{H}_2 = q_i \left( \partial_t \xi_i \nabla \Phi, \nabla \left( \bar{C}_i - C_{i,h} \right) \right) + q_i \left( \left( \bar{C}_i - C_{i,h} \right) \partial_t \nabla \Phi, \nabla \xi_i \right) - q_i \partial_t \left( \xi_i \nabla \Phi, \nabla \xi_i \right)
$$

$$
\leq \|\nabla \Phi\|_{L^\infty} \|\partial_t \xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} + \|\bar{C}_i \nabla \Phi\|_{L^\infty} \|\xi_i\|_{L^2} \|\nabla \xi_i\|_{L^2} - q_i \partial_t \left( \xi_i \nabla \Phi, \nabla \xi_i \right)
$$

$$
\leq M \left(h^{2k} + \epsilon \|\partial_t \xi_i\|_{L^2}^2 + \|\nabla \xi_i\|_{L^2}^2 \right) - q_i \partial_t \left( \xi_i \nabla \Phi, \nabla \xi_i \right). \quad \text{by (4.22)}
$$

$$
\hat{H}_3 = - q_i \left( \partial_t \xi_i \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right) - q_i \left( (C_i - C_{i,h}) \partial_t \nabla (\Phi - \Phi_h), \nabla \xi_i \right)
$$

$$
+ q_i \partial_t \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right)
$$

$$
\leq \|\partial_t \xi_i\|_{L^2} \|\nabla (\Phi - \Phi_h)\|_{L^\infty} \|\nabla \xi_i\|_{L^2} + \|\bar{C}_i - C_{i,h}\|_{L^2} \|\partial_t \nabla (\Phi - \Phi_h)\|_{L^\infty} \|\nabla \xi_i\|_{L^2}
$$

$$
+ q_i \partial_t \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right)
$$

$$
\leq M \left(h^{2k} + \epsilon \|\partial_t \xi_i\|_{L^2}^2 + \|\nabla \xi_i\|_{L^2}^2 \right) + q_i \partial_t \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right). \quad \text{by (4.4), (4.6), (4.13), (4.20), (4.23)}
$$

$$
\hat{H}_4 = q_i \left( \partial_t \xi_i \nabla \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right) - q_i \left( (C_i - C_{i,h}) \partial_t \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right)
$$

$$
\leq \|\partial_t \xi_i\|_{L^2} \|\nabla (\Phi - \Phi_h)\|_{L^\infty} \|\nabla \xi_i\|_{L^2} + \|C_i - C_{i,h}\|_{L^2} \|\partial_t \nabla (\Phi - \Phi_h)\|_{L^\infty} \|\nabla \xi_i\|_{L^2}
$$

$$
- q_i \partial_t \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right). \quad \text{by (4.8), (4.10), (4.13), (4.17)}
$$

Thus (4.25) becomes

$$
\frac{1}{2} \frac{d}{dt} \|\nabla \xi_i\|_{L^2}^2 + \|\partial_t \xi_i\|_{L^2}^2 \leq M \left(h^{2k} + \epsilon \|\partial_t \xi_i\|_{L^2}^2 + \|\nabla \xi_i\|_{L^2}^2 \right) - q_i \partial_t \left( \xi_i \nabla \Phi, \nabla \xi_i \right)
$$

$$
+ q_i \partial_t \left( (C_i - C_{i,h}) \nabla (\Phi - \Phi_h) \right), \nabla \xi_i \right).
$$

Since $C_i = C_{i,h}$ and $\Phi = \Phi_h$ when $t = 0$, take integral with respect to $t$, and use Gronwall’s inequality, we have

$$
\|\nabla \xi_i\|_{L^2}^2 + \int_0^t \|\partial_t \xi_i\|_{L^2}^2 \leq M h^{2k} + \|\xi_i\|_{L^2}^2 \|\nabla \Phi\|_{L^\infty} \|\nabla \xi_i\|_{L^2}^2 + \|C_i - C_{i,h}\|_{L^2} \|\nabla \Phi\|_{L^\infty} \|\nabla \xi_i\|_{L^2}^2
$$

$$
+ \|C_i - C_{i,h}\|_{L^2} \|\nabla (\Phi - \Phi_h)\|_{L^\infty} \|\nabla \xi_i\|_{L^2}.
$$

Thus by (4.22), (4.17), (4.23), and the error estimates of previous terms $H_1, H_2, H_3$ and $H_4$, we obtain

$$
\|\nabla \xi_i\|_{L^2}^2 + \int_0^t \|\partial_t \xi_i\|_{L^2}^2 \leq M \left(h^{2k} + \epsilon \|\nabla \xi_i\|_{L^2}^2 \right),
$$

that is,

$$
\|\nabla \xi_i\|_{L^\infty(L^2)} + \|\partial_t \xi_i\|_{L^2(L^2)} \leq M h^k.
$$

and

$$
\|\nabla (C_i - C_{i,h})\|_{L^\infty(L^2)} + \|\nabla (C_i - C_{i,h})\|_{L^2(L^2)} \leq M h^k. \quad \text{(4.26)}
$$

Finally, together with (4.23), we get

$$
\|C_i - C_{i,h}\|_{L^\infty(L^2)} + \|\nabla (C_i - C_{i,h})\|_{L^\infty(L^2)} \leq M h^k, \quad \text{(4.27)}
$$

then use (4.7) and (4.8), we get (4.17).

**Remark 4.1.** Theorem 4.1 requires that $k \geq d - 1$ in order for the error estimates to hold. This is due to the inverse estimate and mathematical induction technique used in (4.20). Therefore, this restriction of the order of the estimate polynomial should only apply to $C_i$, $i = 1, 2$, but not $\Phi$. In other words, when $d = 3$, it is sufficient to use second order finite element for $C_i$ and linear finite element for $\Phi$ in order to get the results proved in Theorem 4.1.
Theorem 4.1 shows that for PNP system with convection terms in divergence form defined in (2.1) and (2.2), its finite element approximation based upon the weak formulation (2.3) and (2.4) has an optimal convergence rate in both $L^\infty(H^1)$ and $L^2(H^1)$ norms but a sub-optimal convergence rate in $L^\infty(L^2)$ norm. Alternatively, if we break the convection terms in divergence form into two parts, then the first part, $q_i \nabla C_i \cdot \nabla \Phi$, turns out to be a convection term in non-divergence form, and the second part, $q_i C_i \Delta \Phi$, can be further transformed using (2.2), inducing an equivalent governing equation of concentrations with convection terms in non-divergence form and an extra nonlinear term on the right hand side as follows
\begin{equation}
\partial_t C_i - \Delta C_i - q_i \nabla C_i \cdot \nabla \Phi = F_i - q_i C_i (C_i - C - F_i) .
\end{equation}

Thereafter, following an analogous analysis given in [55] and the proof of Theorem 4.1, we are able to obtain the following convergence theorem for the above reformulated PNP.

**Theorem 4.2.** Let $(C_1, C_2, \Phi)$ be the solution of (2.4) and (4.28) and $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of the corresponding discretization equations. We define
\begin{equation}
M_h = \{ v \in H^1(\Omega) : v|_{\partial \Omega} = 0 \text{ and } v|_{K} \in P_1(K), \forall K \in T_h \}
\end{equation}
and
\begin{equation}
N_h = \{ v \in H^1(\Omega) : v|_{\partial \Omega} = 0 \text{ and } v|_{K} \in P_1(K), \forall K \in T_h \}
\end{equation}
such that, for $i = 1, 2$, $\| C_i \|_{L^\infty(H^r+1)}$, $\| \Phi \|_{L^\infty(H^r+1)}$ are bounded, also $C_{1,h} \in M_h$ and $\Phi_h \in N_h$. Then we have the following error estimates,
\begin{equation}
\| \Phi - \Phi_h \|_{L^\infty(\Omega^2)} + h \| \nabla (\Phi - \Phi_h) \|_{L^\infty(\Omega^2)} + \| C_i - C_{i,h} \|_{L^\infty(\Omega^2)} + h \| \nabla (C_i - C_{i,h}) \|_{L^\infty(\Omega^2)} \\
\leq M \left( h^{s+1} + h^{r+1} + h^{r+s-1} \right),
\end{equation}
where $M$ is a constant depending only on the regularity of $C_i$ and $\Phi$.

**Remark 4.2.** Theorem 4.2 shows that, the optimal convergence rate for $C_i - C_{i,h}$ in both $L^2$ and $H^1$ norms could be reached if $s = 2$ and $r = 1$, or $s + r \geq 4$. The optimal convergence rate for $\Phi - \Phi_h$ in both $L^2$ and $H^1$ norms could be reached if $s = 1$ and $r = 2$, or $s + r \geq 4$.

**Remark 4.3.** (4.28) shows that, to achieve a fully optimal a priori error estimates given in Theorem 4.2, one has to force an extra nonlinear term into the right hand side of concentration equation, which is, however, not natural for PNP system from the physical background perspective, moreover, the original concentration equation is changed to be a more strongly nonlinear PDE, and may need an advanced linearization scheme and more nonlinear iterations in order to reach a convergent result, which is a tradeoff of such approach.

**5. Error analysis for the full discretization**

In this section we give the error estimate of the Galerkin procedure (3.3) and (3.4) in $L^\infty(H^1)$, $L^2(H^1)$ and $L^\infty(L^2)$ norms. First we give regularity assumptions for $C_i$, $i = 1, 2$, and $\Phi$ in the full discretization analysis:
\begin{equation}
C_i \in W^{1,\infty}(0, T; H^{k+1} \cap W^{1,\infty}(\Omega)) \text{ and } \Phi \in W^{2,\infty}(0, T; W^{k+1,\infty}(\Omega)).
\end{equation}
We also assume that for $i = 1, 2$,
\begin{equation}
F_i \in W^{2,\infty}(0, T; L^2(\Omega)).
\end{equation}
Next, using the similar analysis for Lemmas 4.3 and 4.4, we can prove the following results.

**Lemma 5.1.** Let $(C_1, C_2, \Phi)$ be the solution of (2.3) and (2.4) satisfying the regularity assumptions (5.1), let $(C_{1,h}, C_{2,h}, \Phi_h)$ be the solution of (3.1) and (3.2) and let $\tilde{C}_i$ be defined in (4.11). For any $n = 0, 1, \ldots, N$, we have the following error estimates:
\begin{equation}
\| \Phi^n - \Phi^n_h \|_{L^2} \leq M h^{k+1} + M \sum_{i=1}^{2} \| C^n_i - C^n_{i,h} \|_{L^2},
\end{equation}
\begin{equation}
\| \nabla (\Phi^n - \Phi^n_h) \|_{L^2} \leq M h^k + M \sum_{i=1}^{2} \| C^n_i - C^n_{i,h} \|_{L^2},
\end{equation}
and
\begin{equation}
\| \partial_t^n (C^n_i - \tilde{C}^n_i) \|_{L^2} + h \| \partial_t^n \nabla (C^n_i - \tilde{C}^n_i) \|_{L^2} \leq M h^{k+1},
\end{equation}
where $\alpha = 0, 1, 2, 3$. 
Theorem 5.1. Let \((C_1, C_2, \Phi)\) be the solution of (2.3) and (2.4) satisfying the regularity assumptions (5.1), and \((C_{1,h}, C_{2,h}, \Phi_h)\) be the solution of (3.1) and (3.2). Then there exists a constant \(M\) depending only on the regularity of \(C_i\) and \(\Phi\), such that for \(i = 1, 2\),
\[
\| C_i^N - C_{i,h}^N \|_{l^2} + \| \nabla (C_i^N - C_{i,h}^N) \|_{l^2} \leq M \left( (\Delta t)^2 + h^k \right),
\]
and
\[
\| \Phi^N - \Phi_h^N \|_{l^2} + \| \nabla (\Phi^N - \Phi_h^N) \|_{l^2} \leq M \left( (\Delta t)^2 + h^k \right).
\]

Proof. Let (2.3) and (4.11) take values at \(t^{n+1/2}, 0 \leq n \leq N - 1\). For any \(v \in H_0^1\), we get
\[
\left( \partial_t C_i \left( t^{n+\frac{1}{2}} \right), v \right) + \left( \nabla \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla v \right) + q_i \left( \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla \Phi \left( t^{n+\frac{1}{2}} \right), \nabla v \right) = \left( F_i \left( t^{n+\frac{1}{2}} \right), v \right).
\]

Subtract (3.3) from (5.7), let \(\xi_i^n = \tilde{C}_i^n - C_{i,h}^n\) and \(\eta^n_i = C_i^n - \tilde{C}_i^n\), and choose \(v_h = \xi_i^{n+\frac{1}{2}} \in S_h\), we have
\[
\left( \partial_t C_i \left( t^{n+\frac{1}{2}} \right) - d_i \xi_i^n, \xi_i^{n+\frac{1}{2}} \right) + \left( \nabla \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \gamma \nabla \xi_i^{n+\frac{1}{2}} \right) + q_i \left( \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla \Phi \left( t^{n+\frac{1}{2}} \right) - C_{i,h} \nabla \Phi_h^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}} \right) = \left( F_i \left( t^{n+\frac{1}{2}} \right) - F_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}} \right).
\]

that is
\[
\left( \partial_t \xi_i^n, \xi_i^{n+\frac{1}{2}} \right) + \left( \nabla \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla \xi_i^{n+\frac{1}{2}} \right) = \sum_{k=1}^7 G_k^n
\]
where
\[
G_1^n := - \left( \partial_t C_i \left( t^{n+\frac{1}{2}} \right) - d_i \xi_i^n, \xi_i^{n+\frac{1}{2}} \right)
\]
\[
G_2^n := - \left( \partial_t C_i - d_i \xi_i^n, \xi_i^{n+\frac{1}{2}} \right)
\]
\[
G_3^n := - \left( \nabla \tilde{C}_i \left( t^{n+\frac{1}{2}} \right) - \tilde{C}_i^n, \nabla \xi_i^{n+\frac{1}{2}} \right)
\]
\[
G_4^n := - \left( \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla \Phi \left( t^{n+\frac{1}{2}} \right) - \Phi_h^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}} \right)
\]
\[
G_5^n := - \left( \tilde{C}_i \left( t^{n+\frac{1}{2}} \right) - \tilde{C}_i^n, \nabla \Phi_h^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}} \right)
\]
\[
G_6^n := - \left( \xi_i^{n+\frac{1}{2}}, \nabla \Phi_h^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}} \right)
\]
\[
G_7^n := \left( F_i \left( t^{n+\frac{1}{2}} \right) - F_i^{n+\frac{1}{2}}, \xi_i^{n+\frac{1}{2}} \right).
\]

Use Taylor’s expansion, Young’s inequality and (5.3), we determine the estimates for \(G_1^n\) to \(G_7^n\) as follows,
\[
|G_1^n| \leq (\Delta t)^2 \| \partial_t C_i \|_{L^\infty(t^2)} \| \xi_i^{n+\frac{1}{2}} \|_{l^2} \leq \frac{1}{2} (\Delta t)^4 \| \partial_t C_i \|_{L^\infty(t^2)}^2 + \frac{1}{2} \| \xi_i^{n+\frac{1}{2}} \|_{l^2}^2,
\]
\[
|G_2^n| = \left( d_i \eta_i^n, \xi_i^{n+\frac{1}{2}} \right) \leq (\Delta t)^2 \| \partial_t \eta_i \|_{L^\infty(t^2)} \| \xi_i^{n+\frac{1}{2}} \|_{l^2} + \| \partial_t \eta_i \|_{L^\infty(t^2)} \| \xi_i^{n+\frac{1}{2}} \|_{l^2} \leq \frac{1}{2} (\Delta t)^4 \| \partial_t \eta_i \|_{L^\infty(t^2)}^2 + \frac{1}{2} \| \partial_t \eta_i \|_{L^\infty(t^2)}^2 + \frac{1}{2} \| \xi_i^{n+\frac{1}{2}} \|_{l^2}^2,
\]
\[
|G_3^n| \leq (\Delta t)^2 \| \nabla \tilde{C}_i \|_{L^\infty(t^2)} \| \xi_i^{n+\frac{1}{2}} \|_{l^2} \leq \frac{1}{2} (\Delta t)^4 \| \partial_t \nabla \tilde{C}_i \|_{L^\infty(t^2)}^2 + \frac{1}{2} \| \xi_i^{n+\frac{1}{2}} \|_{l^2}^2,
\]
\[
|G_4^n| \leq \left| \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla \Phi \left( t^{n+\frac{1}{2}} \right) - \Phi_h^{n+\frac{1}{2}}, \nabla \xi_i^{n+\frac{1}{2}} \right| + \left| \tilde{C}_i \left( t^{n+\frac{1}{2}} \right), \nabla \left( \Phi_h^{n+\frac{1}{2}} - \Phi_h^{n+\frac{1}{2}} \right), \nabla \xi_i^{n+\frac{1}{2}} \right|.
\]
\[
\begin{align*}
&\leq (\Delta t)^2 \left\| \partial_t \nabla \Phi \right\|_{L^\infty(L^2)} \left\| \tilde{C}_i \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} + Mh^k \left\| \tilde{C}_i \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \\
&+ M \sum_{j=1}^2 \left\| \xi_j^{n+\frac{1}{2}} \right\|_{L^2} \left\| C_i \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} + Mh^{k+1} \left\| \tilde{C}_i \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \\
&\leq \frac{M}{4\varepsilon} \left\| \tilde{C}_i \right\|_{L^\infty(L^\infty)}^2 \left( (\Delta t)^4 \left\| \partial_t \nabla \Phi \right\|_{L^\infty(L^2)}^2 + \sum_{j=1}^2 \left\| \xi_j^{n+\frac{1}{2}} \right\|_{L^2}^2 + h^{2k} \right) + 2\varepsilon \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2}^2.
\end{align*}
\]

In $G_2^0$ and $G_6^0$, we shall use mathematical induction again. Since
\[
\begin{align*}
\left\| G_2^0 \right\| &\leq (\Delta t)^2 \left\| \partial_t \tilde{C}_i \right\|_{L^\infty(L^2)} \left\| \nabla \left( \Phi^{n+\frac{1}{2}} - \Phi^h \right) \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \\
&\quad + (\Delta t)^2 \left\| \partial_t \tilde{C}_i \right\|_{L^\infty(L^\infty)} \left\| \nabla \tilde{\Phi} \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \\
\left\| G_6^0 \right\| &\leq \left\| \nabla \left( \tilde{\Phi}^{n+\frac{1}{2}} - \Phi^h \right) \right\|_{L^\infty(L^\infty)} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} + \left\| \nabla \tilde{\Phi} \right\|_{L^\infty(L^\infty)} \left\| \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2},
\end{align*}
\]
and by inverse estimate and (4.12),
\[
\begin{align*}
\left\| \nabla \left( \tilde{\Phi}^{n+\frac{1}{2}} - \Phi^h \right) \right\|_{L^\infty(L^\infty)} &\leq h^{-\frac{d}{2}} \left\| \nabla \left( \tilde{\Phi}^{n+\frac{1}{2}} - \Phi^h \right) \right\|_{L^2} \\
&\leq h^{-\frac{d}{2}} \sum_{i=1}^2 \left( \left\| \xi_i^{n+\frac{1}{2}} \right\|_{L^2} + \left\| \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \right) \leq Mh^k + h^{-\frac{d}{2}} \sum_{i=1}^2 \left\| \xi_i^{n+\frac{1}{2}} \right\|_{L^2},
\end{align*}
\]
we give the following mathematical induction hypothesis to estimate $G_2^0$ and $G_6^0$, for any $n = 0, 1, \ldots, N$,
\[
h^{-\frac{d}{2}} \left\| \xi_i^n \right\|_{L^2} \leq M.
\]
(5.10)

When $h$ is sufficiently small, by the given initial conditions, we have
\[
h^{-\frac{d}{2}} \left\| \xi_i^0 \right\|_{L^2} \leq h^{-\frac{d}{2}} \left( \left\| \eta_i^0 \right\|_{L^2} + \left\| C_i^0 - C_{i,0} \right\|_{L^2} \right) \leq Mh^{k+1-\frac{d}{2}} \leq M.
\]
Assume (5.10) holds for any $n = 0, 1, \ldots, J, 0 \leq J \leq N - 2$, then
\[
\begin{align*}
\left\| G_2^0 \right\| &\leq M(\Delta t)^4 \left\| \partial_t \tilde{C}_i \right\|_{L^\infty(L^2)} \left( 1 + \left\| \nabla \tilde{\Phi} \right\|_{L^\infty(L^\infty)} \right) \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2}, \\
\left\| G_6^0 \right\| &\leq \frac{1}{4\varepsilon} \left( 1 + \left\| \nabla \tilde{\Phi} \right\|_{L^\infty(L^\infty)} \right) \left\| \xi_i^{n+\frac{1}{2}} \right\|_{L^2}^2 + \varepsilon \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2}^2.
\end{align*}
\]
Note the fact that $\left\| \nabla \tilde{\Phi} \right\|_{L^\infty(L^2)}$, $\left\| \nabla \tilde{\Phi} \right\|_{L^\infty(L^\infty)}$, $\left\| \tilde{C}_i \right\|_{L^\infty(L^\infty)}$, $\left\| \partial_t \nabla \tilde{C}_i \right\|_{L^\infty(L^2)}$ and $\left\| \partial_t \tilde{C}_i \right\|_{L^\infty(L^2)}$ are bounded following (4.3), (4.4), (4.16) and (5.4), respectively. Use the regularity of $C_i$ and $\Phi$ given in (5.1), and apply a summation of time step $n$ from 0 to $J$ on both side of (5.9), where $0 \leq J \leq N - 1$, we are then able to obtain the following inequality by means of the telescoping technique
\[
\frac{1}{2\Delta t} \left( \left\| \xi_i^{J+1} \right\|_{L^2}^2 - \left\| \xi_i^0 \right\|_{L^2}^2 \right) + \sum_{n=0}^J \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2}^2 \leq M \sum_{n=0}^J \left( (\Delta t)^4 + h^{2k} + \sum_{j=1}^2 \left\| \xi_j^{n+\frac{1}{2}} \right\|_{L^2}^2 + \varepsilon \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2}^2 \right),
\]
then apply Gronwall’s inequality,
\[
\left\| \xi_i^{J+1} \right\|_{L^2}^2 + \Delta t \sum_{n=0}^J \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2}^2 \leq M \left( (\Delta t)^4 + h^{2k} + \left\| \xi_0^0 \right\|_{L^2}^2 \right).
\]
Since
\[
\left\| \sum_{n=0}^J \nabla \xi_i^n \right\|_{L^2} \leq \left\| \sum_{n=0}^{J-1} \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} + \frac{1}{2} \left\| \nabla \xi_0^0 \right\|_{L^2} + \frac{1}{2} \left\| \nabla \xi_i^J \right\|_{L^2} \leq \sum_{n=0}^J \left\| \nabla \xi_i^{n+\frac{1}{2}} \right\|_{L^2} + \frac{1}{2} \left\| \nabla \xi_0^0 \right\|_{L^2},
\]
we have
\[ \left\| \xi_{i+1}^j \right\|_{L^2} + \left( \Delta t \right) \left\| \sum_{n=0}^j \nabla \xi^n \right\|_{L^2} \frac{1}{2} \leq M \left( (\Delta t)^2 + h^k + \left\| \nabla \xi_0^0 \right\|_{L^2} + \left\| \xi_0^0 \right\|_{L^2} \right). \]

Because \( \bar{C}_i^0 \) and \( C_{i,h}^0 \) are both defined in their approximation forms, appropriately, one can pick up an appropriate initial values for both such that \( \left\| \nabla \xi_0^0 \right\|_{L^2} + \left\| \xi_0^0 \right\|_{L^2} \leq M((\Delta t)^2 + h^k) \). Thus
\[ \left\| \xi_{i+1}^j \right\|_{L^2} + \left( \Delta t \right) \left\| \sum_{n=0}^j \nabla \xi^n \right\|_{L^2} \frac{1}{2} \leq M \left( (\Delta t)^2 + h^k \right). \]

This implies that when \( h \) and \( \Delta t \) are sufficiently small, for \( k \geq d - 1 \),
\[ h^{\frac{d}{2}} \left\| \xi_{i+1}^j \right\|_{L^2} \leq M, \]

which proves the mathematical induction hypothesis (5.10) holds uniformly for any \( n = 1, 2, \ldots, N - 1 \).

Finally, we have
\[ \left\| C_{i+1}^j - C_{i,h}^j \right\|_{L^2} + \left( \Delta t \right) \left\| \sum_{n=0}^j \nabla \left( C_i^n - C_{i,h}^n \right) \right\|_{L^2} \frac{1}{2} \leq M \left( (\Delta t)^2 + h^k \right) + \left\| \eta_{i+1}^j \right\|_{L^2} + \left( \Delta t \right) \left\| \sum_{n=0}^j \nabla \eta^n \right\|_{L^2} \frac{1}{2} \leq M \left( (\Delta t)^2 + h^k + (\Delta t)^{\frac{1}{2}} h^k \right). \]

Since \( \Delta t < 1 \), we can get
\[ \left\| C_{i+1}^j - C_{i,h}^j \right\|_{L^2} + \left( \Delta t \right) \left\| \sum_{n=0}^j \nabla \left( C_i^n - C_{i,h}^n \right) \right\|_{L^2} \frac{1}{2} \leq M \left( (\Delta t)^2 + h^k \right). \]

Let \( J = N - 1 \), we get
\[ \left\| C_i^N - C_{i,h}^N \right\|_{L^2} \leq M \left( (\Delta t)^2 + h^k \right). \tag{5.11} \]

Choosing \( v_h = \delta_i \xi_i^{n+\frac{1}{2}} \) in (5.8) instead of \( \xi_i^{n+\frac{1}{2}} \) and follow an analogous proof for \( \left\| \nabla (C_i - C_{i,h}) \right\|_{L^\infty(L^2)} \) in Theorem 4.1, we can prove the error estimate in \( L^\infty(H^1) \) norm, i.e.,
\[ \left\| \nabla (C_i^n - C_{i,h}^n) \right\|_{L^2} \leq M \left( (\Delta t)^2 + h^k \right). \tag{5.12} \]

Finally, (5.5) follows from (5.11) and (5.12), and (5.6) follows from (5.2), (5.3) and (5.5).

Having Theorem 5.1, the following corollary can be easily obtained.

**Corollary 5.1.** Let \( (C_1, C_2, \Phi) \) be the solution of (2.3) and (2.4) satisfying the regularity assumptions (5.1), and \( (C_{1,h}, C_{2,h}, \Phi_h) \) be the solution of (3.1) and (3.2). Then there exists a constant \( M \) depending only on the regularity of \( C_i \) and \( \Phi \), such that for \( i = 1, 2 \),
\[ \left( \Delta t \sum_{n=0}^{N-1} \left\| \nabla \left( C_i^n - C_{i,h}^n \right) \right\|_{L^2} \right)^{\frac{1}{2}} + \left( \Delta t \sum_{n=0}^{N-1} \left\| \nabla \left( \Phi^n - \Phi_h^n \right) \right\|_{L^2} \right)^{\frac{1}{2}} \leq M \left( (\Delta t)^2 + h^k \right). \tag{5.13} \]

### 6. Numerical experiments

Let \( \Omega = [0, 1] \times [0, 1] \) and choose the right hand side functions such that the exact solutions of (2.1) and (2.2) are given by
\[
\begin{align*}
\Phi(x_1, x_2, t) &= \sin(\pi x_1) \sin(\pi x_2)(1 - e^{-t}), \\
C_1(x_1, x_2, t) &= \sin(2\pi x_1) \sin(2\pi x_2) \sin(t), \\
C_2(x_1, x_2, t) &= \sin(3\pi x_1) \sin(3\pi x_2) \sin(2t).
\end{align*}
\tag{6.1}
\]

The boundary conditions and initial conditions are homogeneous.
In the following, we use Algorithm 1 to find the approximate solution and compute the error in $L^\infty(L^2)$, $L^\infty(H^1)$, and $L^2(H^1)$ norm using both bilinear elements and biquadratic elements. We choose the nonlinear iteration tolerance $\varepsilon = 10^{-8}$ in Algorithm 1.

We first use bilinear elements on a uniform rectangular mesh, and choose $\Delta t = h$ and $T = 0.5$. From Tables 6.1–6.3, we can see that the convergence order in $L^2(H^1)$ norm and $L^\infty(H^1)$ norm for both $C_i$ and $\Phi$ coincides with the convergence theory shown in Theorem 5.1 and Corollary 5.1. The errors in $L^\infty(L^2)$ norms are second order, which indicates our theoretical estimate is suboptimal, however, the numerical solution presents an optimal convergence phenomenon in $L^\infty(L^2)$ norm.

Next we use biquadratic elements on the same rectangular mesh and choose $\Delta t = h^2$ and $T = 0.125$. Tables 6.4–6.6 show that the convergence order is optimal in $L^\infty(L^2)$ norm which also coincide with the error estimates shown in Theorem 5.1. The convergence order in $L^\infty(H^1)$ norm and $L^2(H^1)$ norm for both $C_i$ and $\Phi$ are third order, presenting a superconvergence phenomenon. Same to the case of bilinear element which produces a numerically optimal but theoretically suboptimal order convergence rate, such a superconvergence for biquadratic element may be caused by the use of uniform meshes and tensor product elements which requires further investigation.

7. Conclusions

In this paper, we give a priori error estimates of both semi- and fully discrete finite element approximation schemes for the time-dependent Poisson–Nernst–Planck equations. The optimal convergence order in $L^\infty(H^1)$ and $L^2(H^1)$ norms and sub-optimal convergence order in $L^\infty(L^2)$ norm with linear element, and optimal order in $L^\infty(L^2)$ norm with quadratic or higher-order element, for both the ion concentration and the electrostatic potential are achieved. To the best of the authors' knowledge, it is the first time a complete a priori error analysis is given for the finite element discretization of the
time-dependent PNP equations with convection terms written in the divergence form. The theoretical results are verified by numerical experiments. Furthermore, our numerical results show certain superconvergence phenomena which will be analyzed in our future work.

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