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Gradient Recovery-Type a Posteriori Error Estimates for Steady-State Poisson-Nernst-Planck Equations

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Abstract. In this article, we derive the a posteriori error estimators for a class of steady-state Poisson-Nernst-Planck equations. Using the gradient recovery operator, the upper and lower bounds of the a posteriori error estimators are established both for the electrostatic potential and concentrations. It is shown by theory and numerical experiments that the error estimators are reliable and the associated adaptive computation is efficient for the steady-state PNP systems.

AMS subject classifications: 65N15, 65N30

Key words: Poisson-Nernst-Planck equations, gradient recovery, a posteriori error estimate.

1 Introduction

Poisson-Nernst-Planck (PNP) equations are a coupled system of nonlinear partial differential equations consisting of the Nernst-Planck equation and the electrostatic Poisson equation. They describe the electrodiffusion of ions and are applied in many systems such as the solvated biomolecular system [1–3], the semiconductors devices [4–6], electrochemical systems [7–9] and biological membrane channel [2, 10–12]. In this paper, we

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consider the following steady-state Poisson-Nernst-Planck equations

$$\begin{cases} -\nabla\cdot\left(\nabla p^i+q^ip^i\nabla\phi\right)=F_i & \text{in } \Omega, \quad i=1,2,\\ -\Delta\phi-\sum\limits_{i=1}^{2}q^ip^i=F_3 & \text{in } \Omega, \end{cases} \tag{1.1}$$

for $x\in\Omega\subset\mathbb{R}^d$, $(d=2,3)$ with the homogeneous Dirichlet boundary conditions

$$\begin{cases} \phi=0 & \text{on } \partial\Omega,\\ p^i=0 & \text{on } \partial\Omega, \end{cases} \tag{1.2}$$

where $p^i(x)$ is the concentration of the i-th species particles carrying charge q^i, $\phi(x)$ is the electrostatic potential and F_i, $(i=1,2,3)$ are the reaction source terms.

Because of the nonlinearity and strong coupling, in general, PNP equations are almost impossible to find the analytic solutions. The numerical methods including the finite element method, the boundary element method, the finite difference method and finite volume method are widely used to solve PNP systems (cf. [2, 3, 13, 14]). In practical problems such as the ion channel [11,12,15], since there are many charges on the interface of membranes which lead to the singularity of the solution, the numerical methods such as the finite element method can not be effectively applied to the PNP equations if the discrete mesh is not good. Note that for many problems with local singularities, adaptive finite element method is one of the most effective finite element methods and plays an important role in the numerical solution of partial differential equations. The adaptive finite element method was originally proposed by Babuška et al. [16, 17], which offers a systematic approach. The adaptive calculation mainly includes the following loop:

$$Solve\rightarrow Estimate\rightarrow Mark\rightarrow Refine.$$

In the adaptive computing the "Estimate" is one of the most important steps and generally achieved by using the a posteriori error estimator. In 1987, Zienkiewicz and Zhu [18] put forward the gradient recovery type a posterior error estimator that based on the postprocessing technology. Since the calculation is simple and easy to understand, it is widely welcomed. The calculation is effective and the gradient recovery type a posteriori error estimator is asymptotically exact if the data of the underlying problem is smooth [19,20]. Latter, this method has been widely used in many finite element computations, see [21–24].

Note that the adaptive finite element method is used to solve PNP systems in application (cf. [2, 25–27]). A novel hybrid finite-difference/finite-volume method based on the adaptive Cartesian grids is presented in [25], in which the mesh refinement criteria is according to a level-set function instead of any error estimators for PNP calculations. In order to describe the electrodiffusion processes, the literature [2] proposed a hybrid of adaptive finite element and boundary element methods to solve PNP equations. The grid generation and refinement are just by a biomolecular mesh generation tool rather than indicated by a error estimator. In [26, 27], Tu and Xie et al. proposed a parallel adaptive finite element algorithm for solving PNP equations. However, the a posteriori error estimator used is not designed for the PNP equations itself, but only for Poisson equations (one of the two parts of PNP equations). Hence, the effect of another part for the NP equation is neglected in [26] and [27], which leads to somewhat inaccuracy and incompleteness of the a posteriori error estimator they used.

In this paper, we present a posteriori error analysis for steady-state PNP equations. Since PNP equations are a coupled nonlinear system, the analysis can not directly follow the related work for Poisson-Boltzmann equation (cf. [28]). By using the gradient recovery operator, the upper bounds and lower bounds of the a posteriori error estimators are presented both for the electrostatic potential and concentrations. Based on the a posteriori error estimators, the corresponding adaptive finite element method is provided for the PNP system. In contrast to the existing related work such as [26, 27], our adaptive algorithm is based on the posteriori error analysis for the PNP system and hence the estimator we applied is more accurate and complete in adaptive computing.

The rest of this paper is organized as follows. In Section 2, some notations and error estimates for the finite element approximation are introduced. The Clément interpolations and gradient recovery type operator are also presented in this section. The upper and lower bounds of the a posteriori error estimators are derived in Section 3. In Section 4, the adaptive finite element algorithm is introduced and some numerical experiments are reported to support our theory. Finally, in Section 5, some conclusions are presented.

2 Preliminaries

In this section, we shall describe some basic notations and assumptions. Let $\Omega\subset\mathbb{R}^d$ $(d=2,3)$ be a bounded domain with a Lipschitz-continuous boundary $\partial\Omega$. We shall adopt the standard notations for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms, see, e.g., [29, 30]. For $p=2$, we denote $H^s(\Omega)=W^{s,2}(\Omega)$ and $H^s_0(\Omega)=\{v|v\in H^s(\Omega): v\,|_{\partial\Omega}=0\}$, where $v\,|_{\partial\Omega}=0$ is in the sense of trace, $\|\cdot\|_{s,p,\Omega}=\|\cdot\|_{W^{s,p}(\Omega)}$ and $(\cdot,\cdot)$ is the standard L^2-inner product. Throughout this paper, C denotes a positive constant independent of h, and may denote a different value at its different places.

Let $T^h=\{\tau\}$ be a shape-regular mesh of Ω with mesh size $h=\max_{\tau\in T^h}\{h_\tau\}$, where h_τ is the diameter of the elements. Denote ∂T^h the set of all edges or surfaces of simplices, $\partial^2 T^h$ the set of all vertices of T^h and $\Lambda=\partial^2 T^h\backslash\partial\Omega$. We define the linear finite element space

$$S^h=\{v\in H^1(\Omega): v|_\tau\in\mathcal{P}^1(\tau),\ \forall\tau\in T^h\},\quad S^h_0(\Omega)=S^h(\Omega)\cap H^1_0(\Omega), \tag{2.1}$$

where $\mathcal{P}^1(\tau)$ is the space of linear polynomial on τ.

The weak formulation of (1.1)-(1.2) reads: find $p^i\in H^1_0(\Omega)$, $i=1,2$ and $\phi\in H^1_0(\Omega)$ such that

$$(\nabla p^i,\nabla v)+(q^i p^i\nabla\phi,\nabla v)=(F_i,v), \qquad \forall v\in H_0^1(\Omega), \tag{2.2a}$$

$$(\nabla\phi,\nabla w)-\sum_{i=1}^{2}q^i(p^i,w)=(F_3,w), \qquad \forall w\in H_0^1(\Omega). \tag{2.2b}$$

Assume there exists a unique solution (ϕ,p^i) $(i=1,2)$ satisfying (1.1). The corresponding standard finite element approximation to (2.2a)-(2.2b) is to find $(p_h^1,p_h^2,\phi_h)\in[S_0^h]^3$ such that

$$(\nabla p_h^i,\nabla v_h)+(q^i p_h^i\nabla\phi_h,\nabla v_h)=(F_i,v_h), \qquad \forall v_h\in S_0^h, \tag{2.3a}$$

$$(\nabla\phi_h,\nabla w_h)-\sum_{i=1}^{2}q^i(p_h^i,w_h)=(F_3,w_h), \qquad \forall w_h\in S_0^h. \tag{2.3b}$$

In order to construct a posteriori error estimator, in the following, we will describe the useful Clément interpolations and gradient recovery type operator, we must point out that they are important in our latter analysis.

Let $\{\varphi_z:z\in\partial^2\mathcal{T}^h\}\subset S^h$ be the standard nodal basis functions of S^h, namely,

$$\varphi_{z_1}(z_2)=\delta_{z_1z_2}, \quad \forall z_1,z_2\in\partial^2\mathcal{T}^h,$$

where δ is the Kronecker symbol. For given $z\in\partial^2T^h$, $l\in\partial T^h$ and $\tau\in T^h$, denote $\omega_z=\bigcup_{z\in\bar\tau}\tau$, $\omega_l=\bigcup_{l\in\bar\tau}\tau$, $\omega_\tau=\bigcup_{\bar\tau'\cap\bar\tau\neq 0}\tau'$, and introduce two Clément-type interpolation operators π_h and $\Pi_h:L^2(\Omega)\to S_0^h(\Omega)$, which are defined respectively by (cf. [21,31])

$$\pi_h v=\sum_{z\in\Lambda}v_z\varphi_z, \qquad v_z=\frac{(v,\varphi_z)}{(\varphi_z,1)}, \qquad \forall v\in L^2(\Omega),$$

$$\Pi_h v=\sum_{z\in\partial^2T^h}v^z\varphi_z, \qquad v^z=\sum_{j=1}^{J_z}\alpha_z^j v|_{\tau_z^j}(z), \qquad \forall v\in L^2(\Omega),$$

where $\bigcup_{j=1}^{J_z}=\omega_z$, $\sum_{j=1}^{J_z}\alpha_z^j=1$, and $\alpha_z^j\geq 0$. For instance, $\alpha_z^j=\frac{1}{J_z}$ or $\alpha_z^j=\frac{|\tau_z^j|}{|\omega_z|}$. It should be pointed out that here $v|_{\tau_z^j}$ is understood in the sense of trace in τ_z^j. For $v\in H_0^1(\Omega)$, there hold (see e.g., [21,32–34])

$$\|v-\pi_h v\|_{0,\tau}\leq Ch_\tau\|\nabla v\|_{0,\omega_\tau}, \qquad \forall\tau\in T^h, \tag{2.4a}$$

$$\|v-\pi_h v\|_{0,l}\leq Ch_l^{1/2}\|\nabla v\|_{0,\omega_l}, \qquad \forall l\in T^h, \tag{2.4b}$$

$$|\pi_h v|_{1,\tau}\leq C|v|_{1,\omega_\tau}, \qquad \forall\tau\in T^h. \tag{2.4c}$$

And it is seen that for $v\in W^{1,p}(\Omega)$ $(p>d)$, there holds

$$\|\Pi_h v-v\|_{0,\tau}\leq Ch_\tau\|\nabla v\|_{0,p,\omega_\tau}, \quad \forall\tau\in T^h.$$

We also need a gradient recovery type operator $G_h: S_0^h(\Omega)\to[S^h(\Omega)]^d$, which is defined by

$$G_h v=\Pi_h(\nabla v),\quad \forall v\in S_0^h(\Omega). \tag{2.5}$$

According to the definition of the operator G_h and the properties of the basis function, we have the following estimates.

Lemma 2.1.

$$\|G_h w_h\|_0\le C\|\nabla w_h\|_0,\qquad \forall w_h\in S_0^h, \tag{2.6a}$$

$$\|G_h w_h\|_{0,\infty}\le C\|\nabla w_h\|_{0,\infty},\qquad \forall w_h\in S_0^h. \tag{2.6b}$$

Proof. For

$$\|G_h w_h\|_0=\Big(\sum_{\tau\in T^h}\int_\tau\Big|\sum_{z\in\partial^2T^h}\Big(\sum_{j=1}^{J_z}\alpha_z^j(\nabla w_h)_{\tau_z^j}(z)\Big)\varphi_z\Big|^2dV\Big)^{\frac{1}{2}}.$$

Denote the number of vertice z satisfying $\varphi_z\neq 0$ on the element $\tau\in T^h$ by m_τ. From the property of the basis function φ_z, m_τ is bounded and we can suppose $m_\tau\le C_0$. Then, we have

$$\begin{aligned}\|G_h w_h\|_0&\le CC_0\Big(\sum_{\tau\in T^h}\int_\tau|\nabla w_h|^2dV\Big)^{\frac{1}{2}}\\&\le C\|\nabla w_h\|_0,\end{aligned}$$

where we have used the property of basis function $|\varphi_z|<1$ and J_z is bounded. Thus, we get (2.6a).

Similarly, by using the property of basis function, for any $x_0\in\Omega$, we have

$$\begin{aligned}|G_h w_h(x_0)|&\le\Big|\sum_{z\in\partial^2T^h}\Big(\sum_{j=1}^{J_z}\alpha_z^j(\nabla w_h)_{\tau_z^j}(z)\Big)\varphi_z(x_0)\Big|\\&\le C\|\nabla w_h\|_{0,\infty}\Big|\sum_{z\in\partial^2T^h}\varphi_z(x_0)\Big|\\&\le C\|\nabla w_h\|_{0,\infty}.\end{aligned}$$

Hence, $\|G_h w_h\|_{0,\infty}\le C\|\nabla w_h\|_{0,\infty}$. The estimate (2.6b) is established. This completes the proof. $\square$

3 A posteriori error control

In this section, we will derive the upper and lower bounds of the gradient recovery type a posteriori error estimates for PNP equations (1.1).

First, we define the a posteriori error estimators on element τ for ϕ and p^i respectively as follows:

$$\begin{aligned}
&\eta_{\tau,\phi}(p_h^i,\phi_h)=h_\tau\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau}, && \tau\in T^h,\\
&\eta_{\tau,p^i}(p_h^i,\phi_h)=h_\tau\big(\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}+\|R_{2h}(p_h^i,\phi_h)\|_{0,\tau}\big)\\
&\qquad\qquad +\|\widehat{D}_h(p_h^i,\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau}, && \tau\in T^h,
\end{aligned}$$

where

$$\begin{aligned}
&R_{1h}(p_h^i,\phi_h)=\sum_{i=1}^2 q^i p_h^i+F_3+\mathrm{div}(G_h\phi_h), \qquad D_h(\phi_h)=\nabla\phi_h-G_h\phi_h,\\
&R_{2h}(p_h^i,\phi_h)=F_i+\mathrm{div}(G_hp_h^i)+\mathrm{div}(q^ip_h^iG_h\phi_h),\\
&\widehat{D}_h(p_h^i,\phi_h)=q^ip_h^i(G_h\phi_h-\nabla\phi_h)+G_hp_h^i-\nabla p_h^i.
\end{aligned}$$

In the following, we will derive the global upper bounds and the local lower bounds for $\eta_{\tau,\phi}(p_h^i,\phi_h)$ and $\eta_{\tau,p_h^i}(p_h^i,\phi_h)$, respectively.

3.1 Upper bound

In this subsection, we shall derive upper bounds of the a posteriori error estimators. First we need the following estimates.

Lemma 3.1. *Let u_I be the nodal linear Lagrange interpolant of $u\in H^3(\Omega)\cap H_0^1(\Omega)$. Then we have [35]*

$$(\nabla(u-u_I),\nabla w_h)=\mathcal{O}(h^2)|u|_3\|\nabla w_h\|_0, \quad \forall w_h\in S_0^h(\Omega), \tag{3.1}$$

and the standard interpolation error estimate [30]

$$\|u-u_I\|_0+h\|u-u_I\|_1\le Ch^2\|u\|_2. \tag{3.2}$$

Lemma 3.2. *Let (p^i,ϕ) and (p_h^i,ϕ_h) be the solutions of* (2.2a)-(2.2b) *and* (2.3a)-(2.3b)*, respectively. If $\phi\in H^3(\Omega)$, and ϕ_I is the nodal linear Lagrange interpolation of ϕ, then we have*

$$\|\phi_h-\phi_I\|_{1,\Omega}\le C\Big(h^2\|\phi\|_3+\sum_{i=1}^2\|p^i-p_h^i\|_0\Big). \tag{3.3}$$

Proof. By (2.2a)-(2.2b) and (2.3a)-(2.3b), for any $w_h\in S_0^h$, we get

$$\begin{aligned}
(\nabla(\phi_h-\phi_I),\nabla w_h)&=(\nabla(\phi_h-\phi),\nabla w_h)+(\nabla(\phi-\phi_I),\nabla w_h)\\
&=\sum_{i=1}^2 q^i(p_h^i-p^i,w_h)+(\nabla(\phi-\phi_I),\nabla w_h)\\
&\le C\Big(\sum_{i=1}^2\|p_h^i-p^i\|_0\|w_h\|_0+h^2\|\phi\|_3\|\nabla w_h\|_0\Big),
\end{aligned}$$

where we have used (3.1). Taking $w_h=\phi_h-\phi_I$, so the estimate (3.3) can be easily completed. □

Lemma 3.3. *Suppose* (p^i,ϕ) *and* (p_h^i,ϕ_h) *are the solutions of* (2.2a)-(2.2b) *and* (2.3a)-(2.3b), *respectively. If* $\phi\in H^3(\Omega)\cap W^{2,\infty}(\Omega)$, *then we have*

$$\|\nabla\phi_h\|_{0,\infty}\le C\Big(\|\phi\|_3+h^{-\frac{d}{2}}\sum_{i=1}^{2}\|p^i-p_h^i\|_0+h\|\phi\|_{2,\infty}\Big)+\|\nabla\phi\|_{0,\infty},\quad d=2,3. \tag{3.4}$$

Proof. By the inverse inequality and interpolation error estimate, we have

$$\begin{aligned}\|\nabla\phi_h\|_{0,\infty}&\le\|\nabla(\phi_h-\phi_I)\|_{0,\infty}+\|\nabla(\phi_I-\phi)\|_{0,\infty}+\|\nabla\phi\|_{0,\infty}\\&\le C(h^{-\frac{d}{2}}\|\nabla(\phi_h-\phi_I)\|_{0,\Omega}+h\|\phi\|_{2,\infty})+\|\nabla\phi\|_{0,\infty}\\&\le C\Big(h^{2-\frac{d}{2}}\|\phi\|_3+h^{-\frac{d}{2}}\sum_{i=1}^{2}\|p^i-p_h^i\|_0+h\|\phi\|_{2,\infty}\Big)+\|\nabla\phi\|_{0,\infty},\end{aligned}$$

where we have used (3.3) in the last inequality. Choosing h sufficiently small such that $Ch^{2-\frac{d}{2}}<1$, we get

$$\|\nabla\phi_h\|_{0,\infty}\le C\Big(\|\phi\|_3+h^{-\frac{d}{2}}\sum_{i=1}^{2}\|p^i-p_h^i\|_0+h\|\phi\|_{2,\infty}\Big)+\|\nabla\phi\|_{0,\infty}.$$

This completes the proof. □

Now, we present the upper bounds for $\|\nabla(\phi-\phi_h)\|_{0,\Omega}$ and $\|\nabla(p^i-p_h^i)\|_{0,\Omega}$ in the following.

Theorem 3.1. *Let* (p^i,ϕ) *and* (p_h^i,ϕ_h) *be the solutions of* (2.2a)-(2.2b) *and* (2.3a)-(2.3b), *respectively. There holds*

$$\|\nabla(\phi-\phi_h)\|_0\le C\Big(\eta_\phi(p_h^i,\phi_h)+\sum_{i=1}^{2}\|p^i-p_h^i\|_0\Big), \tag{3.5}$$

where

$$\begin{aligned}&\eta_\phi(p_h^i,\phi_h)=\sum_{\tau}\big(h_\tau\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau}\big),\\&R_{1h}(p_h^i,\phi_h)=\sum_{i=1}^{2}q^ip_h^i+F_3+\mathrm{div}(G_h\phi_h),\quad D_h(\phi_h)=\nabla\phi_h-G_h\phi_h.\end{aligned}$$

Proof. For any $w\in H_0^1(\Omega)$, it follows from (2.2b) that

$$(\nabla(\phi-\phi_h),\nabla w)$$

$$
\begin{aligned}
&=\Big(\sum_{i=1}^{2}q^ip^i+F_3,w-\pi_hw\Big)+\Big(\sum_{i=1}^{2}q^ip^i+F_3,\pi_hw\Big)\\
&\qquad-(\nabla\phi_h,\nabla\pi_hw)+(\nabla\phi_h,\nabla(\pi_hw-w))\\
&=\Big(\sum_{i=1}^{2}q^ip^i+F_3,w-\pi_hw\Big)+\Big(\sum_{i=1}^{2}q^i(p^i-p_h^i),\pi_hw\Big)+\Big(\sum_{i=1}^{2}q^ip_h^i+F_3,\pi_hw\Big)\\
&\qquad-(\nabla\phi_h,\nabla\pi_hw)+(\nabla\phi_h,\nabla(\pi_hw-w)). \qquad (3.6)
\end{aligned}
$$

Further, according to (2.3b), we have

$$
\begin{aligned}
&(\nabla(\phi-\phi_h),\nabla w)\\
=&\Big(\sum_{i=1}^{2}q^ip^i+F_3,w-\pi_hw\Big)+\Big(\sum_{i=1}^{2}q^i(p^i-p_h^i),\pi_hw\Big)+(\nabla\phi_h,\nabla(\pi_hw-w))\\
=&\Big(\sum_{i=1}^{2}q^ip_h^i+F_3,w-\pi_hw\Big)+\Big(\sum_{i=1}^{2}q^i(p^i-p_h^i),w\Big)+(\nabla\phi_h,\nabla(\pi_hw-w)). \qquad (3.7)
\end{aligned}
$$

By Green's formula, we rewrite the third term on the right-hand side of (3.7) as follows

$$
\begin{aligned}
&(\nabla\phi_h,\nabla(\pi_hw-w))\\
=&(\nabla\phi_h-G_h\phi_h,\nabla(\pi_hw-w))-(G_h\phi_h,-\nabla(\pi_hw-w))\\
=&(\nabla\phi_h-G_h\phi_h,\nabla(\pi_hw-w))+\sum_\tau\Big(\int_\tau\mathrm{div}(G_h\phi_h)(w-\pi_hw)-\int_{\partial\tau}G_h\phi_h\cdot\mathbf{n}(w-\pi_hw)\Big)\\
=&(\nabla\phi_h-G_h\phi_h,\nabla(\pi_hw-w))+\sum_\tau\int_\tau\mathrm{div}(G_h\phi_h)(w-\pi_hw), \qquad (3.8)
\end{aligned}
$$

where we have used the fact that

$$\sum_\tau\int_{\partial\tau}G_h\phi_h\cdot\mathbf{n}(w-\pi_hw)=0,$$

since $G_h\phi_h\in[S^h(\Omega)]^d$ and $(w-\pi_hw)\in H_0^1(\Omega)$.

Substituting (3.8) into (3.7) and using Clément interpolation (2.4a) and (2.4c), it yields

$$
\begin{aligned}
(\nabla(\phi-\phi_h),\nabla w)\le C\sum_\tau\Big(\Big(\Big\|\sum_{i=1}^{2}q^ip_h^i+F_3+\mathrm{div}(G_h\phi_h)\Big\|_{0,\tau}h_\tau\\
+\|\nabla\phi_h-G_h\phi_h\|_{0,\tau}\Big)\|w\|_{1,w_\tau}+\sum_{i=1}^{2}\|p^i-p_h^i\|_0\|w\|_0\Big).
\end{aligned}
$$

Taking $w=\phi-\phi_h$ in the above equality, we can easily obtain the desired result (3.5). This completes the proof of Theorem 3.1. □

Now we turn to present the upper bound of $\|\nabla(p^i-p_h^i)\|_{0,\Omega}$ as follows.

Theorem 3.2. *Let (p^i,ϕ) and (p_h^i,ϕ_h) be the solutions of* (2.2a)-(2.2b) *and* (2.3a)-(2.3b), *respectively. There holds*

$$\|\nabla(p^i-p_h^i)\|_0\leq C\Big(\eta_{p^i}(p_h^i,\phi_h)+\sum_{i=1}^{2}\|p^i-p_h^i\|_0+\|p^i-p_h^i\|_0\|\nabla\phi_h\|_{0,\infty}\Big), \tag{3.9}$$

where

$$\begin{aligned}
\eta_{p^i}(p_h^i,\phi_h)=&\sum_{\tau}\Big(\big(\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}+\|R_{2h}(p_h^i,\phi_h)\|_{0,\tau}\big)h_\tau\\
&\qquad+\|\widehat{D}_h(p_h^i,\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau}\Big),\\
R_{1h}(p_h^i,\phi_h)=&\sum_{i=1}^{2}q^ip_h^i+F_3+\mathrm{div}(G_h\phi_h),\\
R_{2h}(p_h^i,\phi_h)=&F_i+\mathrm{div}(G_hp_h^i)+\mathrm{div}(q^ip_h^iG_h\phi_h),\\
\widehat{D}_h(p_h^i,\phi_h)=&q^ip_h^i(G_h\phi_h-\nabla\phi_h)+G_hp_h^i-\nabla p_h^i,\\
D_h(\phi_h)=&\nabla\phi_h-G_h\phi_h.
\end{aligned}$$

Proof. For any $v\in H_0^1(\Omega)$, from (2.2a), we get

$$\begin{aligned}
&(\nabla(p^i-p_h^i),\nabla v)\\
=&(\nabla p^i,\nabla v)-(\nabla p_h^i,\nabla v)\\
=&(F_i,v)-(q^ip^i\nabla\phi,\nabla v)-(\nabla p_h^i,\nabla v)\\
=&(F_i,v-\pi_hv)-(q^ip^i\nabla\phi-q^ip_h^i\nabla\phi_h,\nabla v)-(\nabla p_h^i,\nabla v)\\
&-(q^ip_h^i\nabla\phi_h,\nabla v)+(F_i,\pi_hv).
\end{aligned} \tag{3.10}$$

By using (2.3a), the last two terms on the right-hand side of (3.10) becomes

$$\begin{aligned}
&(F_i,\pi_hv)-(q^ip_h^i\nabla\phi_h,\nabla v)\\
=&(F_i,\pi_hv)-(q^ip_h^i\nabla\phi_h,\nabla\pi_hv)-(q^ip_h^i\nabla\phi_h,\nabla(v-\pi_hv))\\
=&(\nabla p_h^i,\nabla\pi_hv)-(q^ip_h^i\nabla\phi_h,\nabla(v-\pi_hv)).
\end{aligned} \tag{3.11}$$

Substituting (3.11) into (3.10), it yields

$$\begin{aligned}
&(\nabla(p^i-p_h^i),\nabla v)\\
=&(F_i,v-\pi_hv)-(q^ip^i\nabla\phi-q^ip_h^i\nabla\phi_h,\nabla v)\\
&-(\nabla p_h^i,\nabla(v-\pi_hv))-(q^ip_h^i\nabla\phi_h,\nabla(v-\pi_hv))\\
=&(F_i,v-\pi_hv)-(q^ip^i\nabla(\phi-\phi_h),\nabla v)-(q^i(p^i-p_h^i)\nabla\phi_h,\nabla v)\\
&-(\nabla p_h^i,\nabla(v-\pi_hv))-(q^ip_h^i\nabla\phi_h,\nabla(v-\pi_hv)).
\end{aligned} \tag{3.12}$$

Now we rewrite the last two terms on the right-hand side of (3.12) as follows.

In fact, by Green's formula, we get

$$
\begin{aligned}
&-(\nabla p_h^i,\nabla(v-\pi_h v))-(q^i p_h^i\nabla\phi_h,\nabla(v-\pi_h v))\\
=&-(\nabla p_h^i-G_h p_h^i,\nabla(v-\pi_h v))-(q^i p_h^i(\nabla\phi_h-G_h\phi_h),\nabla(v-\pi_h v))\\
&-(G_h p_h^i,\nabla(v-\pi_h v))-(q^i p_h^i G_h\phi_h,\nabla(v-\pi_h v))\\
=&\big(G_h p_h^i-\nabla p_h^i,\nabla(v-\pi_h v)\big)+\big(q^i p_h^i(G_h\phi_h-\nabla\phi_h),\nabla(v-\pi_h v)\big)\\
&+\sum_\tau\Big(\int_\tau \mathrm{div}(G_h p_h^i)(v-\pi_h v)-\int_{\partial\tau}G_h p_h^i\cdot\mathbf{n}(v-\pi_h v)\Big)\\
&+\sum_\tau\Big(\int_\tau \mathrm{div}(q^i p_h^i G_h\phi_h)(v-\pi_h v)-\int_{\partial\tau}q^i p_h^i G_h\phi_h\cdot\mathbf{n}(v-\pi_h v)\Big)\\
=&\big(G_h p_h^i-\nabla p_h^i,\nabla(v-\pi_h v)\big)+\big(q^i p_h^i(G_h\phi_h-\nabla\phi_h),\nabla(v-\pi_h v)\big)\\
&+\sum_\tau\int_\tau\big(\mathrm{div}(G_h p_h^i)+\mathrm{div}(q^i p_h^i G_h\phi_h)\big)(v-\pi_h v). \qquad (3.13)
\end{aligned}
$$

Inserting (3.13) into (3.12) and applying the Clément interpolation (2.4a) and (2.4c), we have

$$
\begin{aligned}
&(\nabla(p^i-p_h^i),\nabla v)\\
=&\sum_\tau\int_\tau\big(F_i+\mathrm{div}(G_h p_h^i)+\mathrm{div}(q^i p_h^i G_h\phi_h)\big)(v-\pi_h v)-(q^i p^i\nabla(\phi-\phi_h),\nabla v)\\
&-(q^i(p^i-p_h^i)\nabla\phi_h,\nabla v)+\big(q^i p_h^i(G_h\phi_h-\nabla\phi_h)+G_h p_h^i-\nabla p_h^i,\nabla(v-\pi_h v)\big)\\
\le& C\sum_\tau\big(\|F_i+\mathrm{div}(G_h p_h^i)+\mathrm{div}(q^i p_h^i G_h\phi_h)\|_{0,\tau}h_\tau+\|\nabla(\phi-\phi_h)\|_{0,\tau}\\
&+\|p^i-p_h^i\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau}+\|q^i p_h^i(G_h\phi_h-\nabla\phi_h)+G_h p_h^i-\nabla p_h^i\|_{0,\tau}\big)\|v\|_{1,\omega_\tau}. \qquad (3.14)
\end{aligned}
$$

Finally, taking $v=p^i-p_h^i$ and substituting (3.5) into (3.14), then the desired result (3.9) is completed. □

Remark 3.1. If $\phi\in H^3(\Omega)\cap W^{2,\infty}(\Omega)$, $p^i\in H^2(\Omega)$ and $\|p^i-p_h^i\|_{0,\Omega}\le Ch^2\|p^i\|_2$ holds, then from Lemma 3.3, Theorems 3.1 and 3.2, we have

$$
\begin{aligned}
&\|\nabla(\phi-\phi_h)\|_{0,\Omega}\le C\eta_\phi(p_h^i,\phi_h)+C_{p^i}h^2,\\
&\|\nabla(p^i-p_h^i)\|_{0,\Omega}\le C\eta_{p^i}(p_h^i,\phi_h)+C_{p^i,\phi}h^2,
\end{aligned}
$$

where C_{p^i} is a constant dependent on p^i and $C_{p^i,\phi}$ is related to p^i and ϕ.

Note that the assumption $\|p^i-p_h^i\|_0\le Ch^2$ is used in Remark 3.1. For time-dependent PNP equations, it is shown in [36] that this L^2 norm error estimate for p^i hold for a linearized backward Euler scheme. For the steady-state PNP equations discussed in this paper, it is difficult to derive the L^2 norm error estimate for p^i by using the traditional duality arguments. Although we can not present the theoretical proof for this assumption, many numerical examples including PNP for practical biological problems show the error in L^2 norm for p^i could achieve second order (see Fig. 3 and Fig. 5 in our work [1], where Fig. 5 is the results of a practical biological problem).

3.2 Lower bound

In this subsection, we discuss the lower bounds of the a posteriori error estimators.

Denote $[g]_l$ the jump of g across the surface $l\in\partial\mathcal{T}^h$, $l\not\subset\partial\Omega$, for example,

$$[\nabla v\cdot n_l]=\lim_{s\to 0^+}\big[\big(\nabla v\big)(x+sn_l)-\big(\nabla v\big)(x-sn_l)\big]\cdot n_l,$$

where n_l is the unit normal vector to l and $v\in H_0^1(\Omega)$.

For any $u_h\in S_0^h$, denote the jump of u_h across the edge or surface $l\in\partial T^h$, $l\not\subset\partial\Omega$ by $J_{h,l}(u_h)=[\nabla u_h\cdot n_l]$.

In order to present the lower bounds of the a posteriori error estimators, first, we need the following lemma, which was shown in [33, 34].

Lemma 3.4 (cf. [33,34]). *Let $\tau\in T^h$ and $l\in\partial T^h$. Then there exists $\mu_\tau:\mathcal{P}^1(\tau)\to H_0^1(\tau)$ such that*

$$C^{-1}\|\mu_\tau v\|_{0,\tau}^2\le\|v\|_{0,\tau}^2\le C(v,\mu_\tau v)_\tau,\qquad \forall v\in\mathcal{P}^1(\tau), \tag{3.15a}$$

$$\|\mu_\tau v\|_{1,\tau}\le Ch_\tau^{-1}\|v\|_{0,\tau},\qquad \forall v\in\mathcal{P}^1(\tau). \tag{3.15b}$$

And there exists $\nu_l:\mathcal{P}^1(l)\to H_0^1(\omega_l)$ such that $\forall v\in\mathcal{P}^1(l)$,

$$C^{-1}\|\nu_l v\|_{0,l}^2\le\|v\|_{0,l}^2\le C(v,\nu_l v)_l, \tag{3.16a}$$

$$\|\nu_l v\|_{0,\omega_l}\le Ch_{\omega_l}^{\frac{1}{2}}\|v\|_{0,l}, \tag{3.16b}$$

$$\|\nu_l v\|_{1,\omega_l}\le Ch_{\omega_l}^{-\frac{1}{2}}\|v\|_{0,l}. \tag{3.16c}$$

In addition, the following result was proved in [21], which shall be used in our analysis.

Lemma 3.5 ([21]). *For any $v_h\in S_0^h(\Omega)$, $\tau\in T^h$, $l\in T^h$,$l\not\subset\partial\Omega$, we have*

$$\|\nabla v_h-G_hv_h\|_{0,\tau}\le C\sum_{l\subset(\omega_\tau\backslash\partial\omega_\tau)}h_l^{\frac{1}{2}}\|J_{h,l}(v_h)\|_{0,l}.$$

Lemma 3.6. *For any $l\in\partial T^h$, $l\not\subset\partial\Omega$, $\forall\phi_h\in S_0^h(\Omega)$, there holds*

$$h_{\omega_l}^{\frac{1}{2}}\|J_{h,l}(\phi_h)\|_{0,l}\le C\|\phi-\phi_h\|_{1,\omega_l}+r_{\omega_l}, \tag{3.17}$$

where

$$J_{h,l}(\phi_h)=[\nabla\phi_h\cdot n_l],\quad r_{\omega_l}\le Ch_{\omega_l}^2\Big(\|F_3\|_{1,\omega_l}+\sum_{i=1}^{2}\|p^i\|_{1,\omega_l}\Big).$$

Proof. For any $w\in H_0^1(\Omega)$, by (2.2b) and Green's formula, we get

$$\begin{aligned}&(\nabla(\phi-\phi_h),\nabla w)\\=&(F_3+\sum_{i=1}^{2}q^ip^i,w)-(\nabla\phi_h,\nabla w)\\=&\sum_{\tau\in T^h}\Big(F_3+\sum_{i=1}^{2}q^ip^i,w\Big)_\tau-\sum_{l\in\partial T^h,l\not\subset\partial\Omega}\int_l[\nabla\phi_h\cdot n_l]w\\=&(M^h(\phi_h),w)-\sum_{l\in\partial T^h,l\not\subset\partial\Omega}\int_l J_{h,l}(\phi_h)w,\end{aligned}\tag{3.18}$$

where

$$M^h(\phi_h)=F_3+\sum_{i=1}^{2}q^ip^i,\quad J_{h,l}(\phi_h)=[\nabla\phi_h\cdot n_l].$$

Hence, from (3.18), for $w\in H_0^1(\omega_l)$,

$$\begin{aligned}&(J_{h,l}(\phi_h),w)_l=\int_l[\nabla\phi_h\cdot n_l]w=\sum_{\tilde{l}\in\partial\omega_l}\int_{\tilde{l}}[\nabla\phi_h\cdot n_{\tilde{l}}]w\\=&(M^h(\phi_h),w)_{\omega_l}-(\nabla(\phi-\phi_h),\nabla w)_{\omega_l}\\\le&\|M^h(\phi_h)\|_{0,\omega_l}\|w\|_{0,\omega_l}+\|\nabla(\phi-\phi_h)\|_{0,\omega_l}\|\nabla w\|_{0,\omega_l},\end{aligned}\tag{3.19}$$

where ω_l represents the set of all the elements including l and denote by $\partial\omega_l=\bigcup_{\tilde{l}\in\omega_l}\tilde{l}$.

Then, let $w=\nu_lJ_{h,l}(\phi_h)$ in (3.19), and from (3.16a)-(3.16c), we have

$$\begin{aligned}&\|J_{h,l}(\phi_h)\|_{0,l}^2\le C(J_{h,l}(\phi_h),\nu_lJ_{h,l}(\phi_h))_l\\\le&C(\|M^h(\phi_h)\|_{0,\omega_l}\|\nu_lJ_{h,l}(\phi_h)\|_{0,\omega_l}+\|\nabla(\phi-\phi_h)\|_{0,\omega_l}\|\nu_lJ_{h,l}(\phi_h)\|_{1,\omega_l}\\\le&C\Big(h_{\omega_l}^{\frac{1}{2}}\|M^h(\phi_h)\|_{0,\omega_l}\|J_{h,l}(\phi_h)\|_{0,l}+h_{\omega_l}^{-\frac{1}{2}}\|\phi-\phi_h\|_{1,\omega_l}\|J_{h,l}(\phi_h)\|_{0,l}\Big).\end{aligned}$$

From the above inequality, it easily yields

$$h_{\omega_l}^{\frac{1}{2}}\|J_{h,l}(\phi_h)\|_{0,l}\le C(\|\phi-\phi_h\|_{1,\omega_l}+h_{\omega_l}\|M^h(\phi_h)\|_{0,\omega_l}).\tag{3.20}$$

Now we turn to estimate $\|M^h(\phi_h)\|_{0,\omega_l}$. Define

$$\widetilde{M}^h(\phi_h)=\frac{1}{|\tau|}\int_\tau F_3+\frac{1}{|\tau|}\int_\tau\sum_{i=1}^{2}q^ip^i.$$

It is easy to see that $\widetilde{M}^h(\phi_h)\in\mathcal{P}^1(\tau)$ and

$$\|M^h(\phi_h)-\widetilde{M}^h(\phi_h)\|_{0,\tau}\le Ch_\tau\Big(\|F_3\|_{1,\tau}+\sum_{i=1}^{2}\|p^i\|_{1,\tau}\Big).\tag{3.21}$$

For any $w\in H_0^1(\tau)$, according to (3.18), we obtain

$$(\widetilde{M}^h(\phi_h),w)=(\nabla(\phi-\phi_h),\nabla w)-(M^h(\phi_h)-\widetilde{M}^h(\phi_h),w), \tag{3.22}$$

where we have used $(J_{h,l}(\phi_h),w)_\tau=0$, for $w\in H_0^1(\tau)$.

Next, in order to estimate $\|\widetilde{M}^h(\phi_h)\|_{0,\tau}$, let $w=\mu_\tau\widetilde{M}^h(\phi_h)$ in (3.22), then by (3.15a) and (3.15b), there holds

$$\|\widetilde{M}^h(\phi_h)\|_{0,\tau}\le C(h_\tau^{-1}\|\phi-\phi_h\|_{1,\tau}+\|M^h(\phi_h)-\widetilde{M}^h(\phi_h)\|_{0,\tau}). \tag{3.23}$$

Combining (3.21) and (3.23), we get

$$\begin{aligned}\|M^h(\phi_h)\|_{0,\tau}\le&\|\widetilde{M}^h(\phi_h)\|_{0,\tau}+\|M^h(\phi_h)-\widetilde{M}^h(\phi_h)\|_{0,\tau}\\ \le& C\Big(h_\tau^{-1}\|\phi-\phi_h\|_{1,\tau}+h_\tau\Big(\|F_3\|_{1,\tau}+\sum_{i=1}^2\|p^i\|_{1,\tau}\Big)\Big).\end{aligned} \tag{3.24}$$

Substituting (3.24) into (3.20), then the desired result is obtained. □

Lemma 3.7. *For any $l\in\partial T^h$, $l\not\subset\partial\Omega$, $\forall p_h^i\in S_0^h(\Omega)$, $i=1,2$, there holds*

$$h_{\omega_l}^{\frac{1}{2}}\|J_{h,l}(p_h^i)\|_{0,l}\le C\big(\|p^i-p_h^i\|_{1,\omega_l}+\|\phi-\phi_h\|_{1,w_l}\big)+\widehat{r}_{\omega_l}, \tag{3.25}$$

where

$$\begin{aligned}&J_{h,l}(p_h^i)=[\nabla p_h^i\cdot n_l],\\ &\widehat{r}_{\omega_l}\le Ch_{\omega_l}^2\Big(\|F_3\|_{1,\omega_l}+\|F_i\|_{1,\omega_l}+\sum_{i=1}^2\|p^i\|_{1,\omega_l}+\|p^i\|_{2,\infty,\omega_l}\Big).\end{aligned}$$

Proof. In what follows, we use the similar arguments as Lemma 3.6 to derive the estimate (3.25).

First of all, for any $v\in H_0^1(\Omega)$, by Green's formula, it is from (2.2a) that

$$(\nabla(p^i-p_h^i),\nabla v)=(F_i,v)-(q^ip^i\nabla\phi,\nabla v)-\sum_{l\in\partial T^h,l\not\subset\partial\Omega}\int_l J_{h,l}(p_h^i)v, \tag{3.26}$$

where $J_{h,l}(p_h^i)=[\nabla p_h^i\cdot n_l]$.

For the second term on the right-hand side of (3.26), we have

$$\begin{aligned}(q^ip^i\nabla\phi,\nabla v)=&(q^ip^i\nabla\phi,\nabla v)-(q^ip^i\nabla\phi_h,\nabla v)+(q^ip^i\nabla\phi_h,\nabla v)\\ &-(q^ip^iG_h\phi_h)+(q^ip^iG_h\phi_h)\\ =&(q^ip^i((\nabla\phi-\nabla\phi_h)+D_h(\phi_h)),\nabla v)+(q^ip^iG_h\phi_h,\nabla v),\end{aligned} \tag{3.27}$$

where $D_h(\phi_h)=\nabla\phi_h-G_h\phi_h$.

Denote by $\overline{w}\in S_0^h$ a linear interpolation of w. It is easy to know that

$$\|w-\overline{w}\|_{0,\infty,\tau}\le Ch_\tau^2\|w\|_{2,\infty,\tau}. \tag{3.28}$$

By Green's formula, we rewrite the second term on the right-hand side of (3.27) as follows

$$\begin{aligned}(q^ip^iG_h\phi_h,\nabla v)&=(q^i(p^i-\bar{p^i})G_h\phi_h,\nabla v)+(q^i\bar{p^i}G_h\phi_h,\nabla v)\\&=(q^i(p^i-\bar{p^i})G_h\phi_h,\nabla v)-q^i\sum_\tau\Big(\int_\tau \mathrm{div}(\bar{p^i}G_h\phi_h)v+\int_{\partial\tau}\bar{p^i}G_h\phi_h\cdot\mathbf{n}\, v\Big)\\&=(q^i(p^i-\bar{p^i})G_h\phi_h,\nabla v)-(q^i\mathrm{div}(\bar{p^i}G_h\phi_h),v),\end{aligned}\tag{3.29}$$

where we have used the fact that q^i is a constant.

By the similar arguments as in (3.19), for $v\in H_0^1(\omega_l)$, inserting (3.27) and (3.29) into (3.26), we obtain

$$\begin{aligned}(J_{h,l}(p_h^i),v)_l&=\int_l[\nabla p_h^i\cdot n_l]v=\sum_{\widetilde{l}\in\partial\omega_l}\int_{\widetilde{l}}[\nabla p_h^i\cdot n_{\widetilde{l}}]v\\&=(R^h(p_h^i),v)_{\omega_l}-(q^ip^i((\nabla\phi-\nabla\phi_h)+D_h(\phi_h)),\nabla v)_{\omega_l}\\&\quad-(q^i(p^i-\bar{p^i})G_h\phi_h,\nabla v)_{\omega_l}-(\nabla(p^i-p_h^i),\nabla v)_{\omega_l},\end{aligned}\tag{3.30}$$

where

$$R^h(p_h^i)=F_i+q^i\mathrm{div}(\bar{p^i}G_h\phi_h),$$

ω_l represents the set of all the elements including l and denote by $\partial\omega_l=\bigcup_{\widetilde{l}\in\omega_l}\widetilde{l}$.

Note that by (2.6a) and (3.28), we have

$$\begin{aligned}&(q^i(p^i-\bar{p^i})G_h\phi_h,\nabla v)\\\le&C\|p^i-\bar{p^i}\|_{0,\infty}\|G_h\phi_h\|_0\|\nabla v\|_0\\\le&C\sum_\tau h_\tau^2\|p^i\|_{2,\infty,\tau}\|\nabla\phi_h\|_{0,\tau}\|v\|_{1,\tau}.\end{aligned}\tag{3.31}$$

Then, for any $v\in H_0^1(w_l)$, let $v=\nu_lJ_{h,l}(p_h^i)$, the following estimate can be obtained by (3.16a)-(3.16c) and (3.31) that

$$\begin{aligned}&\|J_{h,l}(p_h^i)\|_{0,l}^2\le C(J_{h,l}(p_h^i),\nu_lJ_{h,l}(p_h^i))_l\\\le&C\Big(\|R^h(p_h^i)\|_{0,\omega_l}\|\nu_lJ_{h,l}(p_h^i)\|_{0,\omega_l}+\big(\|\phi-\phi_h\|_{1,\omega_l}+\|D_h(\phi_h)\|_{0,\omega_l}\\&\quad+h_{\omega_l}^2\|p^i\|_{2,\infty,\omega_l}\|\nabla\phi_h\|_{0,\omega_l}+\|p^i-p_h^i\|_{1,\omega_l}\big)\|\nabla\nu_lJ_{h,l}(p_h^i)\|_{0,\omega_l}\Big)\\\le&C\Big(h_{\omega_l}^{\frac12}\|R^h(p_h^i)\|_{0,\omega_l}+h_{\omega_l}^{-\frac12}\big(\|\phi-\phi_h\|_{1,w_l}+\|D_h(\phi_h)\|_{0,w_l}\\&\quad+h_{\omega_l}^2\|p^i\|_{2,\infty,\omega_l}\|\nabla\phi_h\|_{0,\omega_l}\big)+\|p^i-p_h^i\|_{1,\omega_l}\Big)\|J_{h,l}(p_h^i)\|_{0,l}.\end{aligned}$$

Hence, from Lemma 3.5 and 3.6, we get

$$
\begin{aligned}
h_{\omega_l}^{\frac{1}{2}}\|J_{h,l}(p_h^i)\|_{0,l} \le & C\big(h_{\omega_l}\|R^h(p_h^i)\|_{0,\omega_l}+\|\phi-\phi_h\|_{1,\omega_l}+\|p^i-p_h^i\|_{1,\omega_l} \\
& +r_{\omega_l}+h_{\omega_l}^2\|p^i\|_{2,\infty,\omega_l}\|\nabla\phi_h\|_{0,\omega_l}\big).
\end{aligned} \tag{3.32}
$$

where

$$
r_{\omega_l} \le Ch_{\omega_l}^2\Big(\|F_3\|_{1,\omega_l}+\sum_{i=1}^{2}\|p^i\|_{1,\omega_l}\Big).
$$

Now, our task is to derive the error estimate of $\|R^h(p_h^i)\|_{0,\omega_l}$. In order to do this, we define

$$
\widetilde{R}^h(p_h^i)=q^i\mathrm{div}(\bar{p^i}G_h\phi_h)+\frac{1}{|\tau|}\int_\tau F_i.
$$

Since $\bar{p^i}$ is the linear interpolation of p^i, it is easy to see that $\widetilde{R}^h(p_h^i)\in\mathcal{P}^1(\tau)$ and

$$
\|R^h(p_h^i)-\widetilde{R}^h(p_h^i)\|_{0,\tau} \le Ch_\tau\|F_i\|_{1,\tau}. \tag{3.33}
$$

For any $v\in H_0^1(\tau)$, from (3.30), we get

$$
\begin{aligned}
(\widetilde{R}^h(p_h^i),v)=&(\nabla(p^i-p_h^i),\nabla v)-(R^h(p_h^i)-\widetilde{R}^h(p_h^i),v) \\
&+(q^ip^i((\nabla\phi-\nabla\phi_h)+D_h(\phi_h)),\nabla v)+(q^i(p^i-\bar{p^i})G_h\phi_h,\nabla v),
\end{aligned} \tag{3.34}
$$

where we have used $(J_{h,l}(p_h^i),v)_\tau=0$, for $v\in H_0^1(\tau)$.

Next, we turn to estimate $\|\widetilde{R}^h(p_h^i)\|_{0,\tau}$. Let $v=\mu_\tau\widetilde{R}^h(p_h^i)$ in (3.34), then we get the following estimate from(3.15a), (3.15b), (3.17) and (3.31) that

$$
\begin{aligned}
\|\widetilde{R}^h(p_h^i)\|_{0,\tau} \le & C\big(h_\tau^{-1}(\|p^i-p_h^i\|_{1,\tau}+\|\phi-\phi_h\|_{1,\tau}+\|\phi-\phi_h\|_{1,\omega_l} \\
&+r_{\omega_l}+h_\tau^2\|p^i\|_{2,\infty,\tau}(\|\nabla(\phi_h-\phi)\|_{0,\tau}+\|\nabla\phi\|_{0,\tau}) \\
&+\|R^h(p_h^i)-\widetilde{R}^h(p_h^i)\|_{0,\tau}\big).
\end{aligned} \tag{3.35}
$$

Hence, combining (3.33) and (3.35), it yields

$$
\begin{aligned}
&\|R^h(p_h^i)\|_{0,\tau} \le \|\widetilde{R}^h(p_h^i)\|_{0,\tau}+\|R^h(p_h^i)-\widetilde{R}^h(p_h^i)\|_{0,\tau} \\
\le & C\Big(h_{w_l}^{-1}(\|p^i-p_h^i\|_{1,\omega_l}+\|\phi-\phi_h\|_{1,w_l}+h_{\omega_l}^2\|p^i\|_{2,\infty,\omega_l}+r_{\omega_l})+h_{\omega_l}\|F_i\|_{1,\omega_l}\Big).
\end{aligned} \tag{3.36}
$$

Inserting (3.36) into (3.32), we obtain the desired estimate (3.25). Thus, this completes the proof. □

Apply the above results, we can prove

Theorem 3.3. *For any $\tau\in T^h$, there holds*

$$\eta_{\tau,\phi}(p_h^i,\phi_h)\le C\Big(\|\phi-\phi_h\|_{1,\omega_\tau}+h_\tau\sum_{i=1}^{2}\|p^i-p_h^i\|_{0,\tau}\Big)+r_{\omega_\tau},$$

where

$$\begin{aligned}&\eta_{\tau,\phi}(p_h^i,\phi_h)=h_\tau\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau},\\ &R_{1h}(p_h^i,\phi_h)=\mathrm{div}(G_h\phi_h)+\sum_{i=1}^{2}q^ip_h^i+F_3,\\ &D_h(\phi_h)=\nabla\phi_h-G_h\phi_h,\quad r_{\omega_\tau}\le Ch_{\omega_\tau}^2\Big(\|F_3\|_{1,\omega_\tau}+\sum_{i=1}^{2}\|p^i\|_{1,\omega_\tau}\Big).\end{aligned}$$

Proof. From Lemma 3.5 and 3.6, we have

$$\|D_h(\phi_h)\|_{0,\tau}\le Ch_{\omega_l}^{\frac{1}{2}}\|J_{h,l}(\phi_h)\|_{0,l}\le C\|\phi-\phi_h\|_{1,\omega_l}+r_{\omega_l},\tag{3.37}$$

where

$$r_{\omega_l}\le Ch_{\omega_l}^2\Big(\|F_3\|_{1,\omega_l}+\sum_{i=1}^{2}\|p^i\|_{1,\omega_l}\Big).$$

Next, we only need to estimate $\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}$. Define

$$\widetilde{R}_{1h}(p_h^i,\phi_h)=\mathrm{div}(G_h\phi_h)+\sum_{i=1}^{2}q^ip_h^i+\frac{1}{|\tau|}\int_\tau F_3.$$

Obviously, $\widetilde{R}_{1h}(p_h^i,\phi_h)\in\mathcal{P}^1(\tau)$ and

$$\|R_{1h}(p_h^i,\phi_h)-\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}\le Ch_\tau\|F_3\|_{1,\tau}.\tag{3.38}$$

On the other hand, according to (2.2b), for any $w\in H_0^1(\Omega)$, by using Green's formula, we get

$$\begin{aligned}(\nabla(\phi-\phi_h),\nabla w)=&\Big(\mathrm{div}(G_h\phi_h)+\sum_{i=1}^{2}q^ip_h^i+F_3,w\Big)\\ &-(\nabla\phi_h-G_h\phi_h,\nabla w)+\sum_{i=1}^{2}q^i(p^i-p_h^i,w).\end{aligned}$$

Thus

$$(R_{1h}(p_h^i,\phi_h),w)=(\nabla(\phi-\phi_h),\nabla w)+(D_h(\phi_h),\nabla w)-\sum_{i=1}^{2}q^i(p^i-p_h^i,w),\tag{3.39}$$

where

$$R_{1h}(p_h^i,\phi_h)=\mathrm{div}(G_h\phi_h)+\sum_{i=1}^{2}q^ip_h^i+F_3,$$
$$D_h(\phi_h)=\nabla\phi_h-G_h\phi_h.$$

Let $w=\mu_\tau\widetilde{R}_{1h}(\phi_h,p_h^i)$ in (3.39), by using (3.15a) and (3.15b), we obtain

$$\begin{aligned}
&(R_{1h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h))\\
\le&(\|\nabla(\phi-\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau})\|\nabla\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}\\
&+C\sum_{i=1}^{2}\|p^i-p_h^i\|_{0,\tau}\|\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}\\
\le&C\Big(h_\tau^{-1}(\|\nabla(\phi-\phi_h)\|_{0,\tau}+\|D_h(\phi_h)\|_{0,\tau})+\sum_{i=1}^{2}\|p^i-p_h^i\|_{0,\tau}\Big)\|\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}.
\end{aligned}\tag{3.40}$$

According to (3.15a), we have the following estimate

$$\begin{aligned}
&\|\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}^2\le C(\widetilde{R}_{1h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h))\\
\le&C\big((R_{1h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h))+(\widetilde{R}_{1h}(p_h^i,\phi_h)-R_{1h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h))\big)\\
\le&C\Big(|(R_{1h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{1h}(p_h^i,\phi_h))|+\|\widetilde{R}_{1h}(p_h^i,\phi_h)-R_{1h}(p_h^i,\phi_h)\|_{0,\tau}\|\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}\Big).
\end{aligned}\tag{3.41}$$

Substituting (3.40) into (3.41), it follows that

$$\begin{aligned}
\|\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}\le&C\Big(h_\tau^{-1}(\|\phi-\phi_h\|_{1,\tau}+\|D_h(\phi_h)\|_{0,\tau})+\sum_{i=1}^{2}\|p^i-p_h^i\|_{0,\tau}\\
&+\|\widetilde{R}_{1h}(p_h^i,\phi_h)-R_{1h}(p_h^i,\phi_h)\|_{0,\tau}\Big).
\end{aligned}\tag{3.42}$$

Therefore, by (3.37), (3.38) and (3.42), we get

$$\begin{aligned}
\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}\le&\|\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}+\|R_{1h}(p_h^i,\phi_h)-\widetilde{R}_{1h}(p_h^i,\phi_h)\|_{0,\tau}\\
\le&C\Big(h_\tau^{-1}\|\phi-\phi_h\|_{1,\tau}+\sum_{i=1}^{2}\|p^i-p_h^i\|_{0,\tau}+h_\tau^{-1}r_{\omega_\tau}+h_\tau\|F_3\|_{1,\tau}\Big),
\end{aligned}$$

which leads to

$$h_\tau\|R_{1h}(p_h^i,\phi_h)\|_{0,\tau}\le C\Big(\|\phi-\phi_h\|_{1,\tau}+h_\tau\sum_{i=1}^{2}\|p^i-p_h^i\|_{0,\tau}\Big)+r_{\omega_\tau}.\tag{3.43}$$

Combining (3.37) and (3.43), we obtain the desired result. □

Theorem 3.4. *For any $\tau\in T^h$, there holds*

$$\begin{aligned}\eta_{\tau,p^i}(p_h^i,\phi_h)\le C(&\|p^i-p_h^i\|_{1,\omega_\tau}+\|\phi-\phi_h\|_{1,\omega_\tau}+h^{-\frac{d}{2}}\|\phi-\phi_h\|_{1,\omega_\tau}\|p^i-p_h^i\|_{0,\omega_\tau}\\&+\|p^i-p_h^i\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau})+r'_{\omega_\tau},\quad d=2,3,\end{aligned}$$

where

$$\begin{aligned}&\eta_{\tau,p^i}(p_h^i,\phi_h)=h_\tau\|R_{2h}(p_h^i,\phi_h)\|_{0,\tau}+\|\hat{D}_h(p_h^i,\phi_h)\|_{o,\tau},\\&R_{2h}(p_h^i,\phi_h)=F_i+\mathrm{div}(G_hp_h^i)+\mathrm{div}(q^ip_h^iG_h\phi_h),\\&\hat{D}_h(p_h^i,\phi_h)=q^ip_h^i(G_h\phi_h-\nabla\phi_h)+G_hp_h^i-\nabla p_h^i,\\&r'_{\omega_\tau}\le Ch_{w_\tau}^2\left(|F_3|_{1,w_\tau}+|F_i|_{1,w_\tau}+\|p^i\|_{2,\infty,w_\tau}+h^{-\frac{d}{2}}\|p^i-p_h^i\|_{0,\tau}|F_3|_{1,w_\tau}\right).\end{aligned}$$

Proof. First, according to Lemma 3.5 and 3.7, it is known that

$$\begin{aligned}\|G_hp_h^i-\nabla p_h^i\|_{0,\tau}&\le Ch_{\omega_l}^{\frac{1}{2}}\|J_{h,l}(p_h^i)\|_{0,l}\\&\le C\left(\|p^i-p_h^i\|_{1,\omega_l}+\|\phi-\phi_h\|_{1,w_l}\right)+\hat{r}_{\omega_l},\end{aligned}\tag{3.44}$$

where

$$\hat{r}_{\omega_l}\le Ch_{\omega_l}^2\Big(\|F_3\|_{1,\omega_l}+\|F_i\|_{1,w_l}+\sum_{i=1}^{2}\|p^i\|_{1,\omega_l}+\|p^i\|_{2,\infty,\omega_l}\Big).$$

On the other hand, we rewrite $\hat{D}_h(p_h^i,\phi_h)$ as

$$\begin{aligned}\hat{D}_h(p_h^i,\phi_h)&=-q^ip_h^i(\nabla\phi_h-G_h\phi_h)+G_hp_h^i-\nabla p_h^i\\&=-q^i(p_h^i-p^i)(\nabla\phi_h-G_h\phi_h)-q^ip^i(\nabla\phi_h-G_h\phi_h)+G_hp_h^i-\nabla p_h^i.\end{aligned}$$

Therefore, from (3.37), (3.44), we get

$$\begin{aligned}&\|\hat{D}_h(p_h^i,\phi_h)\|_{0,\tau}\le C(\|p_h^i-p^i\|_{0,\infty,\tau}+\|p^i\|_{0,\infty})\|D_h(\phi_h)\|_{0,\tau}+\|G_hp_h^i-\nabla p_h^i\|_{0,\tau}\\&\le C(\|p^i-p_I^i\|_{0,\infty,\tau}+\|p_I^i-p_h^i\|_{0,\infty,\tau}+\|p^i\|_{0,\infty,\tau})\|D_h(\phi_h)\|_{0,\tau}+\|G_hp_h^i-\nabla p_h^i\|_{0,\tau}\\&\le C(h_\tau^2\|p^i\|_{2,\infty,\tau}+h_\tau^{-\frac{d}{2}}\|p_I^i-p_h^i\|_{0,\tau}+\|p^i\|_{0,\infty,\tau})\|D_h(\phi_h)\|_{0,\tau}+\|G_hp_h^i-\nabla p_h^i\|_{0,\tau}\\&\le C(\|\phi-\phi_h\|_{1,\omega_\tau}+\|p^i-p_h^i\|_{1,\omega_\tau}+h_\tau^{-\frac{d}{2}}\|p^i-p_h^i\|_{0,\tau}\|\phi-\phi_h\|_{1,\omega_\tau})+r'_{\omega_\tau},\end{aligned}\tag{3.45}$$

where

$$r'_{\omega_l}\le Ch_{\omega_\tau}^2(\|F_3\|_{1,\omega_\tau}+\|F_i\|_{1,\omega_\tau}+\|p^i\|_{2,\infty,\omega_\tau}+h_\tau^{-\frac{d}{2}}\|p^i-p_h^i\|_{0,\tau}\|F_3\|_{1,\omega_\tau}).$$

Now, we turn to estimate $\|R_{2h}(p_h^i,\phi_h)\|_{0,\tau}$. Define

$$\widetilde{R}_{2h}(p_h^i,\phi_h)=\mathrm{div}(G_hp_h^i)+\mathrm{div}(q^ip_h^iG_h\phi_h)+\frac{1}{|\tau|}\int_\tau F_i.$$

It is easy to see that $\widetilde{R}_{2h}(p_h^i,\phi_h)\in\mathcal{P}^1(\tau)$ and

$$\|\widetilde{R}_{2h}(p_h^i,\phi_h)-R_{2h}(p_h^i,\phi_h)\|_{0,\tau}\le Ch_\tau\|F_i\|_{1,\tau}. \tag{3.46}$$

On the other hand, for any $v\in H_0^1(\Omega)$, we have

$$\begin{aligned}
&(\nabla(p^i-p_h^i),\nabla v)=(\nabla p^i,\nabla v)-(\nabla p_h^i,\nabla v)\\
=&(F_i,v)-(q^ip^i\nabla\phi,\nabla v)-(\nabla p_h^i,\nabla v)+(q^ip_h^i\nabla\phi_h,\nabla v)-(q^ip_h^i\nabla\phi_h,\nabla v)\\
&+(G_hp_h^i,\nabla v)-(G_hp_h^i,\nabla v)\\
=&(F_i,v)-(q^ip^i\nabla\phi-q^ip_h^i\nabla\phi_h,\nabla v)-(\nabla p_h^i,\nabla v)-(q^ip_h^i\nabla\phi_h,\nabla v)\\
&+(q^ip_h^iG_h\phi_h,\nabla v)-(q^ip_h^iG_h\phi_h,\nabla v)+(G_hp_h^i,\nabla v)-(G_hp_h^i,\nabla v).
\end{aligned}$$

Then, the Green's formula is applied to the sixth and eighth terms on the right-hand side in the above equation, we get

$$\begin{aligned}
(\nabla(p^i-p_h^i),\nabla v)=&(F_i+\mathrm{div}(G_hp_h^i)+\mathrm{div}(q^ip_h^iG_h\phi_h),v)-(q^ip^i\nabla(\phi-\phi_h),\nabla v)\\
&-(q^i(p^i-p_h^i)\nabla\phi_h,\nabla v)-(q^ip_h^i(\nabla\phi_h-G_h\phi_h)+\nabla p_h^i-G_hp_h^i,\nabla v)\\
=&(R_{2h}(p_h^i,\phi_h),v)-(q^ip^i\nabla(\phi-\phi_h),\nabla v)-(q^i(p^i-p_h^i)\nabla\phi_h,\nabla v)\\
&-(q^ip_h^iD_h(\phi_h)+D_h(p_h^i),\nabla v),
\end{aligned}$$

where $D_h(p_h^i)=\nabla p_h^i-G_hp_h^i$. Thus

$$\begin{aligned}
(R_{2h}(p_h^i,\phi_h),v)=&(\nabla(p^i-p_h^i),\nabla v)+(q^ip^i\nabla(\phi-\phi_h),\nabla v)+(q^i(p^i-p_h^i)\nabla\phi_h,\nabla v)\\
&+(q^ip_h^iD_h(\phi_h)+D_h(p_h^i),\nabla v).
\end{aligned}$$

Let $v=\mu_\tau\widetilde{R}_{2h}(p_h^i,\phi_h)$ in the above equality and using (3.15b), we obtain

$$\begin{aligned}
&(R_{2h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{2h}(p_h^i,\phi_h))\\
\le& Ch_\tau^{-1}(\|p^i-p_h^i\|_{1,\tau}+\|q^ip^i\nabla(\phi-\phi_h)\|_{0,\tau}+\|q^i(p^i-p_h^i)\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau}\\
&+\|\hat{D}_h(p_h^i,\phi_h)\|_{0,\tau})\|\widetilde{R}_{2h}(p_h^i,\phi_h)\|_{0,\tau}.
\end{aligned} \tag{3.47}$$

According to (3.15a) we have the following estimate

$$\begin{aligned}
&\|\widetilde{R}_{2h}(p_h^i,\phi_h)\|_{0,\tau}^2\le C(\widetilde{R}_{2h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{2h}(p_h^i,\phi_h))\\
\le& C\big((R_{2h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{2h}(p_h^i,\phi_h))+(\widetilde{R}_{2h}(p_h^i,\phi_h)-R_{2h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{2h}(p_h^i,\phi_h))\big)\\
\le& C\big(|(R_{2h}(p_h^i,\phi_h),\mu_\tau\widetilde{R}_{2h}(p_h^i,\phi_h))|+\|\widetilde{R}_{2h}(p_h^i,\phi_h)-R_{2h}(p_h^i,\phi_h)\|_{0,\tau}\|\widetilde{R}_{2h}(p_h^i,\phi_h)\|_{0,\tau}\big).
\end{aligned} \tag{3.48}$$

Substituting (3.47) into (3.48), it follows that

$$\begin{aligned}
&\|\widetilde{R}_{2h}(p_h^i,\phi_h)\|_{0,\tau}\\
\le& C\big(h_\tau^{-1}(\|p^i-p_h^i\|_{1,\tau}+\|q^ip^i\nabla(\phi-\phi_h)\|_{0,\tau}+\|q^i(p^i-p_h^i)\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau}\\
&+\|\hat{D}_h(p_h^i,\phi_h)\|_{0,\tau})+\|\widetilde{R}_{2h}(p_h^i,\phi_h)-R_{2h}(p_h^i,\phi_h)\|_{0,\tau}\big).
\end{aligned} \tag{3.49}$$

Combining (3.46) and (3.49), we have

$$\begin{aligned}\|R_{2h}(p_h^i,\phi_h)\|_{0,\tau} \le& \|\widetilde{R}_{2h}(p_h^i,\phi_h)\|_{0,\tau}+\|R_{2h}(p_h^i,\phi_h)-\widetilde{R}_{2h}(p_h^i,\phi_h)\|_{0,\tau}\\ \le& C\big(h_\tau^{-1}(\|p^i-p_h^i\|_{1,\tau}+\|\phi-\phi_h\|_{1,\tau}+\|p^i-p_h^i\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau}\\ &+\|\hat{D}_h(p_h^i,\phi_h)\|_{0,\tau})+h_\tau\|F_i\|_{1,\tau}\big)\\ \le& C\big(h_\tau^{-1}(\|p^i-p_h^i\|_{1,\omega_\tau}+\|\phi-\phi_h\|_{1,\omega_\tau}+h_\tau^{-\frac{d}{2}}\|p^i-p_h^i\|_{0,\omega_\tau}\|\phi-\phi_h\|_{1,\omega_\tau}+r'_{\omega_\tau}\\ &+\|p^i-p_h^i\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau}+h_{\omega_\tau}\|F_i\|_{1,\omega_\tau}\big),\end{aligned}$$

where we have used (3.4) and (3.45). Hence

$$\begin{aligned}h_\tau\|R_{2h}(p_h^i,\phi_h)\|_{0,\omega_\tau}\le& C(\|p^i-p_h^i\|_{1,\omega_\tau}+\|\phi-\phi_h\|_{1,\omega_\tau}+h_\tau^{-\frac{d}{2}}\|p^i-p_h^i\|_{0,\omega_\tau}\|\phi-\phi_h\|_{1,\omega_\tau}\\ &+\|p^i-p_h^i\|_{0,\tau}\|\nabla\phi_h\|_{0,\infty,\tau})+r'_{\omega_\tau}. \end{aligned} \tag{3.50}$$

Combing (3.45) and (3.50), we obtain the desired result. The proof is completed. □

Similar as Remark 3.1, we have the following results.

Remark 3.2. If $\phi\in H^3(\Omega)\cap W^{2,\infty}(\Omega)$, $p^i\in W^{2,\infty}(\omega_\tau)$ and $\|p^i-p_h^i\|_{0,\tau}\le Ch_\tau^2\|p^i\|_{2,\tau}$ hold, for any $\tau\in T^h$, then from Lemma 3.3, Theorems 3.3 and 3.4, we have

$$\begin{aligned}&\eta_{\tau,\phi}(\phi_h,p_h^i)\le C\|\phi-\phi_h\|_{1,\omega_\tau}+\widetilde{C}_{p^i}h_{\omega_\tau}^2,\\ &\eta_{\tau,p^i}(p_h^i,\phi_h)\le C\big(\|p^i-p_h^i\|_{1,\omega_\tau}+\|\phi-\phi_h\|_{1,\omega_\tau}\big)+\widetilde{C}_{p^i,\phi}h_{\omega_\tau}^2,\end{aligned}$$

where $\widetilde{C}_{p^i}$ is a constant dependent on p^i and $\widetilde{C}_{p^i,\phi}$ is related to p^i and ϕ.

4 Numerical results

In this section, we will apply the standard refinement strategies for automatic mesh refinement based on the a posteriori error estimates derived above and report the numerical results to verify our theoretical analysis. Let $T^h=\{\tau\}$ be a shape-regular mesh of Ω with mesh size $h_\tau>0$ and the element τ. To implement the numerical experiment, the code is written in Fortran 90 and all the computations are carried out on a microcomputer.

4.1 Refinement strategies

In this subsection, we shall describe a typical adaptive algorithm based on the a posteriori error indicators derived above.

For $\tau \in T^h$, define

$$\eta_{\tau,\phi} = h_\tau \Big\| \sum_{i=1}^{2} q^i p_h^i + F_3 + \mathrm{div}(G_h\phi_h) \Big\|_{0,\tau} + \|\nabla\phi_h - G_h\phi_h\|_{0,\tau}, \tag{4.1a}$$

$$\begin{aligned}\eta_{\tau,p^i} = & h_\tau \Big(\|F_i + \mathrm{div}(G_h p_h^i) + \mathrm{div}(q^i p_h^i G_h\phi_h)\|_{0,\tau} + \Big\| \sum_{i=1}^{2} q^i p_h^i + F_3 + \mathrm{div}(G_h\phi_h) \Big\|_{0,\tau} \Big) \\ & + \|\nabla\phi_h - G_h\phi_h\|_{0,\tau} + \|q^i p_h^i (G_h\phi_h - \nabla\phi_h) + G_h p_h^i - \nabla p_h^i\|_{0,\tau}. \end{aligned} \tag{4.1b}$$

Given an initial conforming mesh T^h, an associated finite element space $S_0^h(\Omega)$ and a tolerance TOL, the typical adaptive algorithm is then designed as follows:

Algorithm 4.1 Adaptive Computing for Steady-state PNP.

- Step 1: Finite element solution computing
  Find the finite element solution $(p_h^i, \phi_h) \in [S_0^h]^3$.
- Step 2: Error estimation
  Compute the error indicators $\eta_{\tau,\phi}$, η_{τ,p^i} by (4.1a) and (4.1b) for all $\tau \in T^h$.
- Step 3: Local refinement
  If
  $$\Big(\sum_{\tau\in T^h} \eta^2_{\tau,\phi}\Big)^{\frac{1}{2}} > TOL \quad \text{or} \quad \Big(\sum_{\tau\in T^h} \eta^2_{\tau,p^i}\Big)^{\frac{1}{2}} > TOL,$$
  then refine those elements which satisfy $\eta_\tau(\eta_{\tau,\phi_h}$ or
  $$\eta_{(\tau,p_h^i)} \geq \theta \max_{\tau\in T^h} \eta_\tau$$
  with a given refinement parameter $\theta \in (0,1)$ and generate a new mesh T^h, a space $S_0^h(\Omega)$ and return to Step 1. Otherwise, the computation is terminated.

In our computations, we follow the refining strategies in [37] to obtain a new conforming mesh and choose the refinement parameter $\theta = 0.5$.

4.2 Example

In this subsection, we denote η_ϕ and η_{p^i} the a posteriori error estimator to ϕ, p^i respectively, where ϕ is the electrostatic potential and p^i $(i=1,2)$ is the concentration of positive ion or negative ion. In order to verify the validity and efficiency of the a posteriori error estimators obtained in this paper, we first consider a steady-state PNP system with a smooth solution, and then a example with a singular solution.

Example 4.1. Consider the steady-state PNP equations with a smooth solution as follows:

$$\begin{cases} -\nabla\cdot\left(\nabla p^i + q^i p^i \nabla\phi\right) = f_i & \text{in } \Omega, \quad i=1,2, \\ -\Delta\phi - \sum\limits_{i=1}^{2} q^i p^i = f_3 & \text{in } \Omega. \end{cases} \tag{4.2}$$

Here the computational domain $\Omega=[0,1]^2\subset\mathbb{R}^2$ and $q^1=1$, $q^2=-1$. The boundary condition and the right-hand side functions are chosen such that the exact solution (ϕ,p^1,p^2) is given by

$$\begin{cases} \phi = \sin\pi x \sin\pi y, \\ p^1 = \sin 2\pi x \sin 2\pi y, \\ p^2 = \sin 3\pi x \sin 3\pi y. \end{cases}$$

This example is mainly used to verify the validity of our error estimators. The a posteriori error estimators and true error $\|u-u_h\|_1$ of the electrostatic potential ϕ and concentrations p^1, p^2 under the uniform meshes and adaptive meshes are presented in Figs. 1, 2 and 3, respectively. It is apparent from Fig. 1 that the a posterior error estimator of the electrostatic potential ϕ approximates the true error as the increase of the degrees of freedom. It is also shown that the error curves keep the optimal convergence order (the slope of the right triangle is 0.5) both for the true error and error estimator, which verifies the theoretical analysis presented in Theorem 3.1. Compared the error estimator $\eta_{\phi,a}$ (symbol "$-\square$") with the error $e_{\phi,a}$ (symbol "$-\triangle$") obtained on the adaptive meshes, it is also shown that the curves of $\eta_{\phi,a}$ close to that of $e_{\phi,a}$, which suggests the a posteriori error estimator for ϕ is almost exact not only on the uniform meshes but also on the adaptive meshes.

Similarly, it is observed from Figs. 2 and 3 that the error curves of the error estimators are close to the true errors for concentrations for positive and negative ions under both the uniform meshes and the adaptive meshes (e.g., the error estimator $\eta_{p^1,u}$ (symbol "- -$\diamond$") asymptotically close to the true error $e_{p^1,u}$ (symbol "- -$*$") on uniform meshes and $\eta_{p^1,a}$ (symbol "$-\diamond$") asymptotically close to the true error $e_{p^1,a}$ (symbol "$-*$")), which suggests the error estimators η_{ϕ_h} and $\eta_{p^i_h}$ defined by (4.1a) and (4.1b) are almost exact on the uniform meshes as well as the adaptive meshes.

Figs. 1, 2 and 3 show that the numerical results coincide with the theoretical results shown in Theorems 3.1 and 3.2 respectively.

In the above, we have presented the example with a smooth solution to show the validity of the a posteriori error estimators derived in the paper. However, because of the smoothness of the solution in Example 4.1, the advantages of the adaptive computing are not obvious. In order to show the efficiency of the adaptive finite element algorithm, we consider another example in which the exact solution has a strong singularity at the point $(0,0)$.

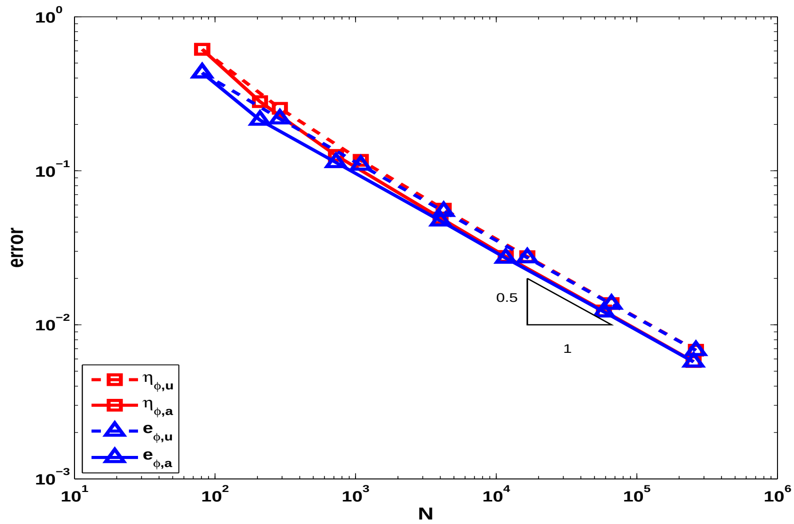

Figure 1: The error estimator $\eta_{\phi,u}$ (symbol "- -□") and the error $e_{\phi,u}$ (symbol "- -△") obtained on the uniform meshes. The error estimator $\eta_{\phi,a}$ (symbol "−□") and the error $e_{\phi,a}$ (symbol "−△") are obtained on the adaptive meshes for the electrostatic potential. N is the number of degrees of freedom.

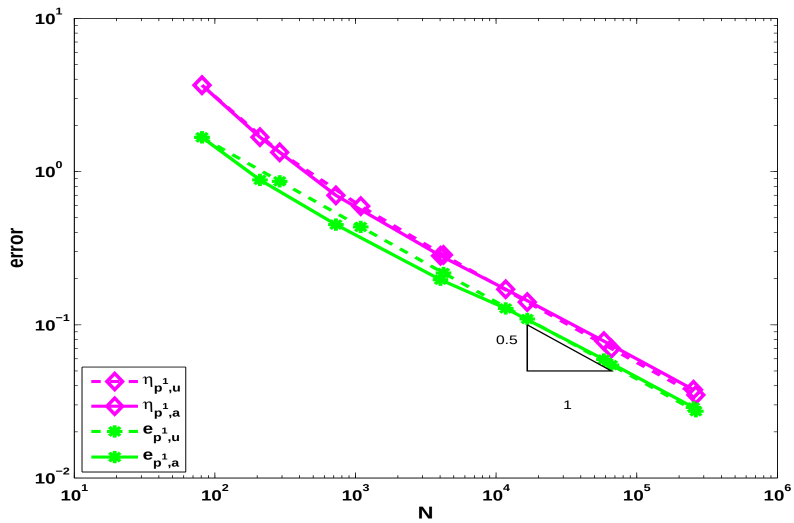

Figure 2: The error estimator $\eta_{p^1,u}$ (symbol "- -⋄") and the error $e_{p^1,u}$ (symbol "- -∗") obtained on the uniform meshes. The error estimator $\eta_{p^1,a}$ (symbol "−⋄") and the error $e_{p^1,a}$ (symbol "−∗") obtained on the adaptive meshes. N is the number of degrees of freedom.

Example 4.2. In this example, we consider the following PNP equation

$$\begin{cases} -\nabla\cdot\left(\nabla p^i+q^ip^i\nabla\phi\right)=f_i & \text{in } \Omega, \quad i=1,2, \\ -\Delta\phi-\sum\limits_{i=1}^{2}q^ip^i=f_3 & \text{in } \Omega, \end{cases} \tag{4.3}$$

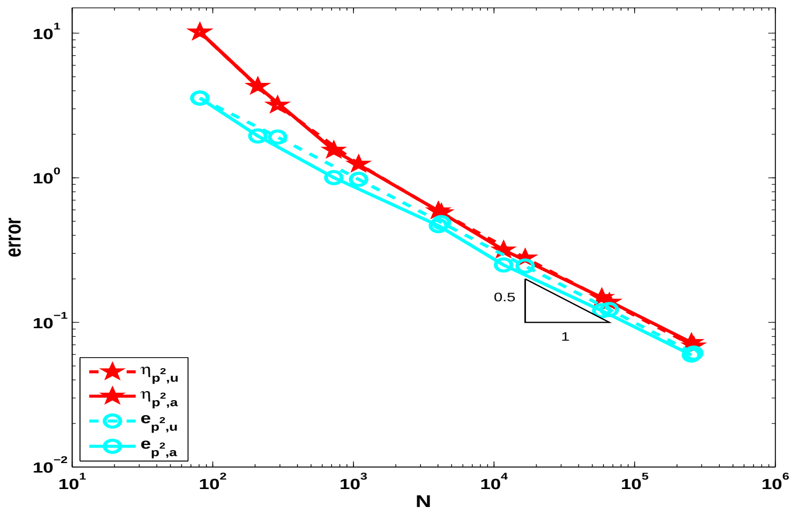

Figure 3: The error estimator $\eta_{p^2,u}$ (symbol "- -★") and the error $e_{p^2,u}$ (symbol "- -○") obtained on the uniform meshes. The error estimator $\eta_{p^2,a}$ (symbol "—★") and the error $e_{p^2,a}$ (symbol "—○") obtained on the adaptive meshes. N is the number of degrees of freedom.

where the computational domain is $\Omega=[0,1]^2\subset\mathbb{R}^2$ and $q^1=1$, $q^2=-1$. The boundary condition and the right-hand side functions are chosen such that the exact solution (ϕ,p^1,p^2) satisfy the classical Boltzmann distributions which is given by

$$\begin{cases} \phi=(x^2+y^2)^{0.1}, \\ p^1=0.5e^{-\phi}, \\ p^2=0.5e^{\phi}. \end{cases} \tag{4.4}$$

In the following, we first compute the finite element solution on uniform meshes and then solve this singular problem by Algorithm 4.1 on adaptive meshes by using error indicators (4.1a)-(4.1b). A uniform initial mesh and an adaptively refined mesh with 2733 degrees of freedom generated by the error estimators η_ϕ, η_{p^i} are shown in Fig. 4. It is observed from Figs. 5, 6 and 7 that the convergence orders of the error curves (solid line) for both true errors and error estimators of the electrostatic potential and concentrations on the adaptive meshes are optimal. Compared the true errors and error estimators on adaptive meshes (solid line) with the true errors and error estimators on the uniform meshes (dashed line), one can easily observe that the errors on the adaptive meshes are much less than that on uniform meshes. For example, for the electrostatic potential ϕ, it is shown in Fig. 5 the error value $e_\phi\leq 0.08605$ achieved with about 150 degrees of freedom on the adaptive mesh in comparison of about 260,000 degrees of freedom on a uniform mesh. The ratio of degrees of freedom is about $1:1700$. Similar results are displayed in Figs. 6 and 7 which indicates that the adaptive finite element method based on the

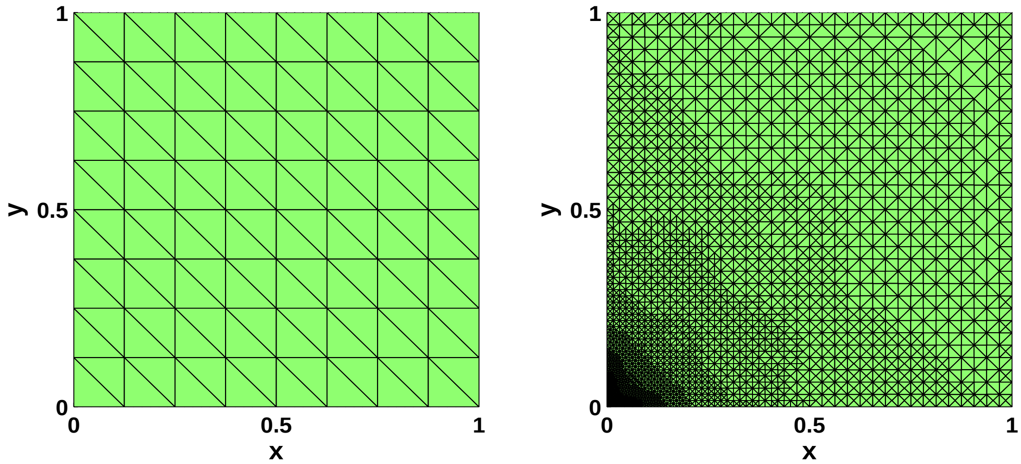

Figure 4: The left figure is the initial mesh with 81 degrees of freedom and the right one is an adaptive mesh with 2733 degrees of freedom generated by error estimators η_ϕ, η_{p^i} for Example 4.2.

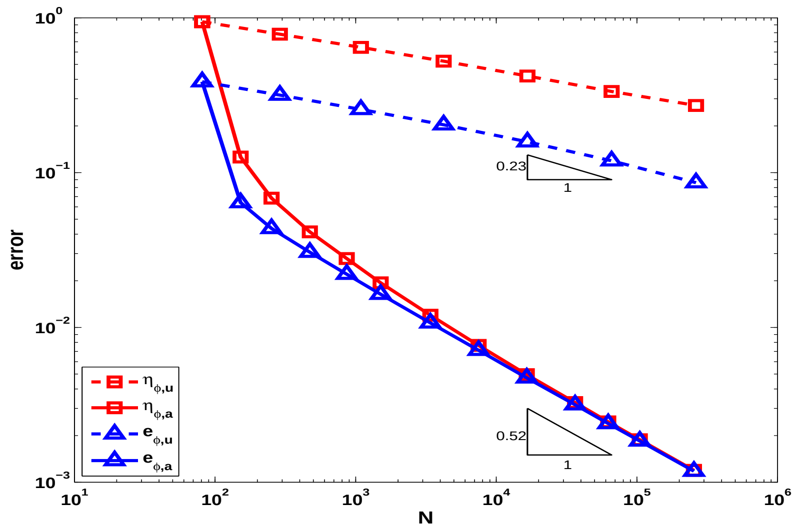

Figure 5: The error estimator $\eta_{\phi,u}$ (symbol "- -□") and the error $e_{\phi,u}$ (symbol "- -△") obtained on the uniform meshes. The error estimator $\eta_{\phi,a}$ (symbol "−□") and the error $e_{\phi,a}$ (symbol "−△") are obtained on the adaptive meshes for the electrostatic potential. N is the number of degrees of freedom.

a posteriori error estimators derived in this paper is efficient for the steady-state PNP system with a singular solution.

Note that the traditional gradient recovery type error indicators for ϕ and p^i on element $\tau \in T^h$ can be expressed respectively as follows:

$$\eta_{D,\tau,\phi} = \|\nabla \phi_h - G_h \phi_h\|_{0,\tau}, \tag{4.5a}$$

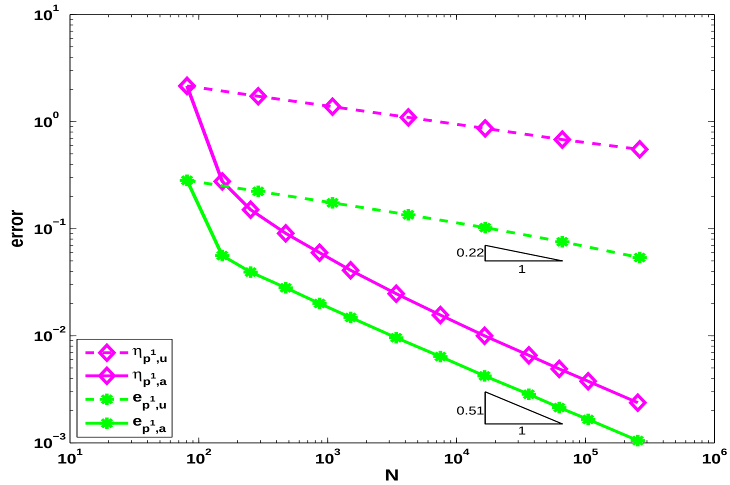

Figure 6: The error estimator $\eta_{p^1,u}$ (symbol "- -◇") and the error $e_{p^1,u}$ (symbol "- -∗") obtained on the uniform meshes. The error estimator $\eta_{p^1,a}$ (symbol "−◇") and the error $e_{p^1,a}$ (symbol "−∗") obtained on the adaptive meshes constructed by the error indicators. N is the number of degrees of freedom.

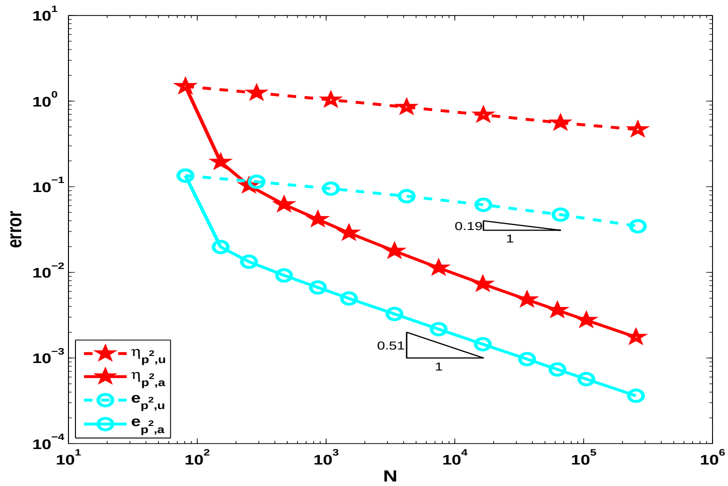

Figure 7: The error estimator $\eta_{p^2,u}$ (symbol "- -★") and the error $e_{p^2,u}$ (symbol "- -○") obtained on the uniform meshes. The error estimator $\eta_{p^2,a}$ (symbol "−★") and the error $e_{p^2,a}$ (symbol "−○") obtained on the adaptive meshes. N is the number of degrees of freedom.

$$\eta_{D,\tau,p^i} = \|\nabla p_h^i - G_h p_h^i\|_{0,\tau}, \quad i=1,2. \tag{4.5b}$$

Compared (4.5a) and (4.5b) with (4.1a) and (4.1b), respectively, the traditional gradient recovery type error indicators are a part of the indicators presented in this paper. In the following, we will study the performance of the traditional error indicators $\eta_{D,\tau,\phi}$ and

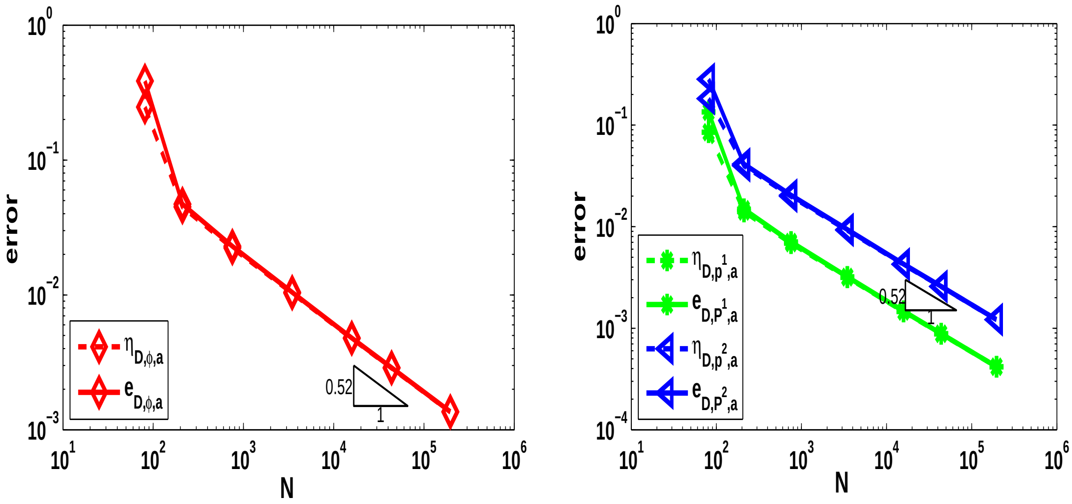

Figure 8: The left figure is the error estimator $\eta_{D,\phi,a}$ (symbol "- -◇") and the true error $e_{D,\phi,a}$ (symbol "−◇") for Example 4.2. The right figure is the error estimators $\eta_{D,p^1,a}$ (symbol "- -∗"), $\eta_{D,p^2,a}$ (symbol "- -◁") and the true errors $e_{D,p^1,a}$ (symbol "−∗"), $e_{D,p^2,a}$ (symbol "−◁") for Example 4.2. N is the number of degrees of freedom.

η_{D,τ,p^i}.

For simplicity, we take Example 4.2 as an example. Fig. 8 indicates the error estimators for ϕ and p^i generated by (4.5a) and (4.5b) are asymptotically exact in the adaptive computation. Note that Fig. 5 shows the error estimator for ϕ obtained from (4.1a) is also asymptotically exact in the adaptive computation, although it contains more terms than the error indicator defined in (4.5a).

In order to explain this phenomenon, we first decompose the error indicator $\eta_{\tau,\phi}$ shown in (4.1a) into two parts as follows

$$\eta_{\tau,\phi} = \eta_{D,\tau,\phi} + \eta_{R,\tau,\phi}, \tag{4.6}$$

where $\eta_{D,\tau,\phi}$ is given by (4.5a) and the element residual is defined by

$$\eta_{R,\tau,\phi} = h_\tau \Big\| \sum_{i=1}^{2} q^i p_h^i + F_3 + \mathrm{div}(G_h \phi_h) \Big\|_{0,\tau}. \tag{4.7}$$

Fig. 9 displays the residual generated by (4.7) and two error estimators obtained respectively from (4.5a) and (4.6). It is observed that the curve of the error estimators generated by (4.6) is very close to the estimators generated by (4.5a), when the degrees of freedom is large. Fig. 9 also shows that the residual induced by (4.7) is much less than that by (4.5a), which indicates the element residual $\eta_{\tau,R}$ plays a very small role in the error indicator $\eta_{\tau,\phi}$ defined in (4.6) for Example 4.2. Therefore, the error estimator for

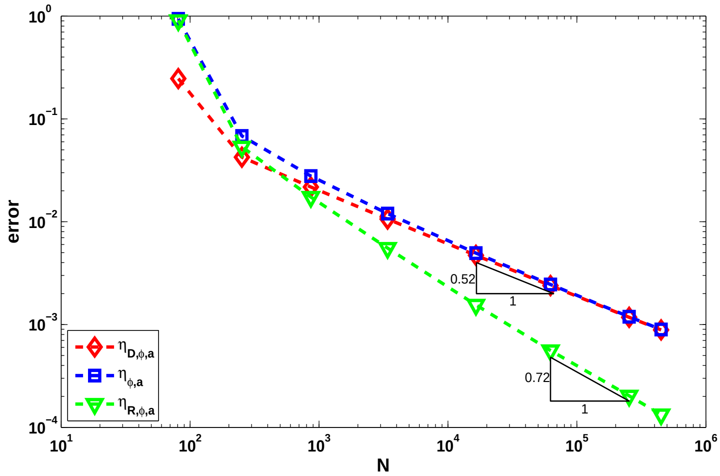

Figure 9: The error estimators $\eta_{D,\phi,a}$ (symbol "- -◇"), $\eta_{\phi,a}$ (symbol "- -□") and the residual $\eta_{R,\phi,a}$ (symbol "- -▽") on the adaptive meshes for Example 4.2. N is the number of degrees of freedom.

ϕ presented in this paper has the similar effect as the traditional error estimator in the adaptive computation for Example 4.2.

Although the numerical experiment shows that the influence of the residual is small in the error indicator presented in this paper, it is necessary to present the analysis of the upper and lower bound for the PNP equations in this paper. Furthermore, the problem tested here is a model problem. For some complex practical biological problems, the source term F_3 and $\sum_{i=1}^{2} q^i p_h^i$ in $\eta_{R,\tau,\phi}$ probably have an impact for the adaptive computation of PNP equations, which needs further study.

5 Conclusions

In this paper, we constructed a gradient recovery type a posteriori error estimator for a class of steady-state Poisson-Nernst-Planck equations. The upper bounds and lower bounds of the a posteriori error estimators are derived both for the electrostatic potential and concentrations. Theoretical analysis and numerical experiments verify the validity and efficiency of the a posteriori error estimators. The corresponding adaptive finite element computation is presented for PNP systems. Compared with the existing work on the adaptive finite element computations for PNP equations, the adaptive finite element algorithm constructed here is based on the a posteriori error analysis for PNP itself. Particularly, we discussed only a special class of Poisson-Nernst-Planck equations in the paper. In fact, this type of a posteriori error estimator is also efficient and reliable for more general and complex nonlinear PNP equations, for example, the modified nonlinear PNP equations (MNPNPE), which will be addressed in our next work.

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References

[1] Y. Yang and B. Z. Lu, *An error analysis for the finite element approximation to the steady-state Poisson-Nernst-Planck equations,* Adv. Appl. Math. Mech., 5 (2013), pp. 113–130.

[2] B. Lu, Y. Zhou, G. A. Huber, S. D. Bond, M. J. Holst and J. A. McCammon, *Electrodiffusion: a continuum modeling framework for biomolecular systems with realistic spatiotemporal resolution,* J. Chem. Phys., 127 (2007), 135102.

[3] B. Z. Lu, M. J. Holst, J. A. McCammond and Y. C. Zhou, *Poisson-Nernst-Planck equations for simulating biomolecular diffusion-reaction processes I: finite element solutions,* J. Chem. Phys., 229(2010), pp. 6979–6994.

[4] J. Jerome, Analysis of Charge Transport: A Mathematical Theory and Approximation of Semiconductor Models, Springer-Verlag, New York, 1996.

[5] S. Selberherr, Analysis and Simulation of Semiconductor Devices, Springer-Verlag/Wien, New York, 1984.

[6] P. A. Markowich, The Stationary Semiconductor Device Equation, Springer-Verlag/Wien, New York, 1986.

[7] M. Z. Bazant, M. S. Kilic, B. D. Storey and A. Ajdari, *Towards an understanding of inducedcharge electrokinetics at large applied voltages in concentrated solutions,* Advances in Colloid and Interface Science, 152 (2009), pp. 48–88.

[8] F. Ciucci and W. Lai, *Derivation of micro/macro lithium battery models from homogenization,* Transp. Porous Med., 88 (2011), pp. 249–270.

[9] J. Marcicki, A. T. Conlisk and G. Rizzoni, *Comparison of limiting descriptions of the electrical double layer using a simplified lithium-ion battery model,* ECS Transactions, 41 (2012), pp. 9–21.

[10] A. E. Cardenas, R. D. Coalson and M. G. Kurnikova, *Three-dimensional Poisson-Nernst-Planck theory studies: influence of membrane electrostatics on gramicidin a channel conductancethe,* Biophys. J., 79 (2000), pp. 80–93.

[11] R. D. Coalson sand M. G. Kurnikova, *Poisson-Nernst-Planck theory approach to the calculation of current through biological ion channels,* IEEE Transactions on Nanobioscience, 4(2005), pp. 81–93.

[12] A. Singer and J. Norbury, *A Poisson-Nernst-Planck model for biological ion channels–an asymptotic analysis in a three-dimensional narrow funnel,* SIAM J. Appl. Math., 70 (2009), pp. 949–968.

[13] Y. H. SONG, Y. J. ZHANG, C. L. BAJAJ AND N. A. BAKER, *Continuum diffusion reaction rate calculations of wild-type and mutant mouse acetylcholinesterase: adaptive finite element analysis,* Biophys. J, 87 (2004), pp. 1558–1566.

[14] D. HE, K. PAN, *An energy preserving finite difference scheme for the Poisson-Nernst-Planck system,* Appl. Math. Comput., 287-288 (2016), pp. 214–223.

[15] S. XU, M. CHEN, S. MAJD, X. YUE AND C. LIU, *Modeling and simulating asymmetrical conductance changes in gramicidin pores,* Mol. Based Math. Biol., 2 (2014), pp. 34–55.

[16] I. BABUŠKA, W. C. RHEINBOLDT, *A posteriori error estimates for the finite element method,* Int J Numer. Meth. Eng., 11 (1978), pp. 1592–1615.

[17] I. BABUŠKA, W. C. RHEINBOLDT, *Adaptive approaches and reliability estimates in finite element analysis,* Comput. Meth. Appl. Mech. Eng., 17/18 (1979), pp. 519–540.

[18] O. C. ZIENKIEWICZ AND J. Z. ZHU, *A simple error estimator and adaptive procedure for practical engineering analysis,* Int. J Numer. Meth. Eng., 24 (1987), pp. 337–357.

[19] D. MAO, L. SHEN AND A. ZHOU, *Adaptive finite element algorithms for eigenvalue problrms based on local averaging type a posteriori error estimates,* Adv. Comput. Math., 25 (2006), pp. 135–160.

[20] C. CARSTENSEN, S. BARTELS AND R. KLOSE, *An experiment survet of a posteriori Courant finite element error control for the Poisson equation,* Adv. comput. Math., 15 (2001), pp. 79–106.

[21] N. YAN AND A. ZHOU, *Gradient recovery type a posteriori error estimates for finite element approximations on irregular meshes,* Comput. Methods Appl. Mech. Eng., 190 (2001), pp. 4289–4299.

[22] Z. ZHANG AND N. YAN, *Recovery type a posteriori error estimates in finite element methods,* J Comput. Appl. Math., 8 (2001), pp. 235–251.

[23] E. CREUSÉ AND S. NICAISE, *A posteriori error estimator based on gradient recovery by averaging for discontinuous Galerkin methods,* J. Comput. Appl. Math., 234 (2010), pp. 2903–2915.

[24] E. CREUSÉ AND S. NICAISE, *A posteriori error estimator based on gradient recovery by averaging for convection-diffusion-reaction problems approximated by discontinuous Galerkin methods,* IMA J Numer. Anal., 33 (2013), pp. 212–241.

[25] M. MIRZADEH, AND F. GIBOU, *A conservative discretization of the Poisson-Nernst-Planck equations on adaptive Cartesian grids,* J. Comput. Phys., 274 (2014), pp. 633–653.

[26] B. TU, M. CHEN AND Y. XIE ET AL., *A parallel finite element simulator for ion transport through three-dimensional ion channel systems,* J. Comput. Chem., 34 (2013), pp. 2065–2078.

[27] Y. XIE, J. CHENG AND B. LU ET AL., *Parallel adaptive finite element algorithms for solving the coupled electro-diffusion equations,* Mol. Based Math. Biol., 1 (2013), pp. 90–108.

[28] Y. YANG AND A. ZHOU, *Local averaging based a posteriori finite element error control for quasi-linear elliptic problems with application to electrical potential computation,* Comput. Methods Appl. Mech. Engrg., 196 (2006), pp. 452–465.

[29] R. A. ADAMS, Sobolev Spaces, Academic Press, New York, 1975.

[30] S. C. BRENNER AND L. R. SCOTT, The Mathematical Theory of Finite Element Methods, Springer-Verlag, New York, 1994.

[31] P. CLÉMENT, *Approximation by finite element functions using local regularization,* RAIRO Anal. Numér, 9 (1975), pp. 77–84.

[32] C. CARSTENSEN, *Quasi-interpolation and a posteriori analysis in finite element methods,* M2AN Math. Model. Numer. Anal., 33 (1999), pp. 1187–1202.

[33] M. AINSWORTH AND J. T. ODEN, A Posteriori Error Estimation in Finite Element Analysis, Wiley, 2000.

[34] R. VERFÜRTH, *A posteriori error estimators for convection–diffusion equations,* Numer. Math.,

80 (1998), pp. 641–663.

[35] J. BRANDTS AND M. KŘÍŽEK, *Gradient superconvergence on uniform simplicial partitions of polytopes,* IMA J. Numer. Anal., 23 (2003), pp. 489–505.

[36] H. D. GAO AND D. D. HE, *Linearized conservative finite element methods for the Nernst-Planck-Poisson equations,* J. Sci. Comput., 72 (2017), pp. 1269–1289.

[37] R. VERFÜRTH, A Review of a Posteriori Error Estimates and Adaptive Mesh-refinement Techniques, Wiley-Teubner, New York, 1996.