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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