

## A POSTERIORI ERROR ESTIMATES OF THE WEAK GALERKIN FINITE ELEMENT METHOD FOR POISSON-NERNST-PLANCK EQUATIONS\*

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### Abstract

In this paper, we present a posteriori error estimates of the weak Galerkin finite element method for the steady-state Poisson-Nernst-Planck equations. The a posteriori error estimators for the electrostatic potential and ion concentrations are constructed. The reliability and efficiency of the estimators are verified by the upper and lower bounds of the energy norm of the error. The a posteriori error estimators are applied to the adaptive weak Galerkin algorithm for triangle, quadrilateral and polygonal meshes with hanging nodes. Finally, numerical results demonstrate the effectiveness of the adaptive algorithm guided by our constructed estimators.

*Mathematics subject classification:* 65N15, 65N30.

*Key words:* A posteriori error estimate, Weak Galerkin finite element method, Poisson-Nernst-Planck equations, Adaptive weak Galerkin algorithm, Polygonal meshes.

## 1. Introduction

The Poisson-Nernst-Planck (PNP) equations, which describe the diffusion process of ions under the action of an electric field, are well-known ion transport models and play a crucial role in the study of many physical and biological phenomena. Since the PNP equations were proposed, their mathematical analysis and numerical approximation have attracted extensive attention. The existence of solutions to the PNP equations has been presented in [21, 24]. Due to the nonlinear coupling of PNP equations, it is challenging to compute their analytical solutions mathematically. Therefore, numerical methods are usually used to find approximate solutions [13, 17, 39]. PNP equations in some practical problems, such as ion channels [6, 31], have singularity due to many charges on the membrane interface, and the accuracy of their approximate solutions largely depends on the quality of the mesh. If the discrete mesh is not good, numerical methods such as the finite element method cannot effectively solve the PNP

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equations. In this case, the adaptive algorithm driven by an a posteriori error estimator is a good choice to improve the efficiency of mesh generation.

The a posteriori error estimator is the basis of the adaptive algorithm. As a computable quantity, the a posteriori error estimator can guide adaptive mesh refinement so that the adaptive algorithm can obtain more accurate numerical solutions with fewer mesh degrees of freedom. At present, there are some works on solving PNP equations by adaptive algorithms. In [32,37], the adaptive algorithm is applied to solve the actual ion channel problem described by the PNP equations. However, in the adaptive algorithm, only the a posteriori error estimator of the Poisson equation in PNP equations is used to guide the adaptive mesh refinement, and the influence of the NP equation is not considered. The gradient recovery-type a posteriori error for a class of steady-state PNP equations is derived in [29], and its error estimator is proven to be efficient and reliable. Then, by using a local averaging operator which is an extension of the gradient recovery operator, the locally averaged a posteriori error estimate for the nonlinear PNP problem is derived in [40]. In [16], a spatial adaptive finite element method considering geometrical singularities and boundary layer effects is proposed for the steady-state PNP equations. In [46], the residual-type a posteriori error estimate for time-dependent PNP equations is studied, the error estimators are established and the computable upper and lower bounds of the error estimators are derived. These works utilizing adaptive algorithms to solve PNP equations are suitable for regular triangular or tetrahedral meshes only. To eliminate the hanging nodes created in adaptive mesh refinement, the traditional finite element method needs to refine additional elements, resulting in higher shape regularity conditions [33], which cannot be directly applied to polygonal meshes. With the improvement of computing power and numerical calculation levels, PNP equations have been applied to simulate large-scale systems, such as actual biology and physics [3,38], in recent years, but the cost of computing on traditional structured meshes is relatively expensive. Adaptive computation on polygonal meshes allows the existence of hanging points, and no postprocessing is needed to refine the meshes. If the mesh in the adaptive algorithm has great flexibility, the mesh refinement strategy can be implemented more effectively. Hence, the convenient use of more general polygonal meshes in complex simulations has become an attractive feature.

Here, we design a posteriori error estimators of the weak Galerkin finite element method for steady-state PNP equations. The weak Galerkin finite element method (WGFEM) is a new numerical method developed in recent years to solve various partial differential equations. It was first proposed by Mu, Wang and Ye [27,34,35] for solving second-order elliptic problems. The WGFEM can be seen as an extension of the standard finite element method, and its finite element discrete scheme can be derived directly from the weak form of the corresponding PDE. The scheme for WGFEM is constructed by using fully discontinuous finite element functions. Therefore, compared with other finite element methods, it has the advantages of flexible approximation functions, a simple and stable numerical scheme, and can deal with unstructured meshes [20,26]. The WGFEM has developed rapidly since it was proposed and has been applied to solve many problems [5,8,22,30,36,41,42]. Based on the WG-mixed finite element method (MFEM), a linearized locally conservative scheme for time-dependent PNP equations is established in [14], and the prior error estimates of semidiscrete and fully discrete WG-MFEM schemes are given. There are also some works about a posteriori error estimators for the WGFEM [4,43–45]. However, the adaptive computations of these works are carried out on regular triangular mesh or tetrahedral mesh. Recently, there have been some research works devoted to the a posteriori error analysis of WGFEM on general polygonal or polyhedral