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ERROR ANALYSIS OF VIRTUAL ELEMENT METHODS FOR THE TIME-DEPENDENT POISSON-NERNST-PLANCK EQUATIONS*

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Abstract

We discuss and analyze the virtual element method on general polygonal meshes for the time-dependent Poisson-Nernst-Planck (PNP) equations, which are a nonlinear coupled system widely used in semiconductors and ion channels. After presenting the semi-discrete scheme, the optimal H^1 norm error estimates are presented for the time-dependent PNP equations, which are based on some error estimates of a virtual element energy projection. The Gummel iteration is used to decouple and linearize the PNP equations and the error analysis is also given for the iteration of fully discrete virtual element approximation. The numerical experiment on different polygonal meshes verifies the theoretical convergence results and shows the efficiency of the virtual element method.

Mathematics subject classification: 65N15, 65N30, 35K61.
Key words: Virtual element method, Error estimate, Poisson-Nernst-Planck equations, Polygonal meshes, Energy projection, Gummel iteration.

1. Introduction

The virtual element method (VEM) could be seen as a deformation of the classical mimetic finite difference method, which was originally proposed in [5] as a generalization of the finite element method (FEM). This method is applicable to general polygon/polyhedral grids even including the multiply-connected or non-convex polygon grids, and hence has low requirements on grid quality. The VEM, in comparison to the traditional FEM, does not require an explicit expression of the discrete basis functions. In addition to that, it only needs to define the appropriate degrees of freedom to convert the discrete formulation into the matrix form. Thanks to its applicability and simplicity, the VEM has been applied to many equations, for instance, the second-order elliptic equation [8], the parabolic equations [1, 46], hyperbolic equation [45], the Stokes equations [4,11,17], the elasticity problems [6,24] and the plate bending problem [16], etc.

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Here, we consider the time-dependent Poisson-Nernst-Planck (PNP) equations. The classic PNP equations are a coupled nonlinear system of partial differential equations, which consist of the electrostatic Poisson equation and the Nernst-Planck equation. The coupled nonlinear system was originally derived by Nernst [37] and Planck [38] and has been widely applied in semiconductors [36, 47], biological ion channels [22, 43] and electrochemical systems [35, 39, 48].

Because of the high nonlinearity and strong coupling, it is difficult to find the analytic solution for PNP equations. Many numerical methods were developed to find the approximate solutions, for instance, finite volume methods [12, 18], finite difference methods [23, 30] and FEMs [33, 49], etc. The FEM has been applied to PNP equations for many years and it is popular because of its flexibility and adaptability in dealing with the irregular interface. In recent years, some work on convergence analysis of FEM has emerged. We presented some error bounds in [51] for a piecewise finite element approximation to the steady-state PNP equations describing the electrodiffusion of ions in a solvated biomolecular system. In [44], the authors discussed a priori error estimates of FEM for the time-dependent PNP equations, where the optimal error estimates are obtained in $L^\infty(H^1)$ and $L^2(H^1)$ norms and the suboptimal error estimate is obtained in the $L^\infty(L^2)$ norm. An optimal L^2 norm error estimate of the FEM to a linearized backward Euler scheme for the time-dependent PNP equations has been obtained in [26]. Recently, we presented a decoupling two-grid FEM for the time-dependent PNP equations in [42]. This method costs less computational time and remains the same order of accuracy compared with the FEM combined with the Gummel iteration. The optimal L^2 error estimate for the classic nonlinear backward Euler scheme was also presented in [42] with a generic regularity assumption of the solution. In [52], we studied the superconvergent gradient recovery based on the finite element approximation for the strong nonlinear PNP equations. The superconvergence results are successfully applied to improve the efficiency of the external iteration in the computation of a practical ion channel problem. The a posteriori error estimates and adaptive FEM for the steady-state PNP equations are studied in [29, 41].

In this paper, the main purpose is to provide the a priori error analysis for the virtual element discretization of the time-dependent PNP equations. First, we design a suitable virtual element discretization scheme for the equations. Compared with the finite element discretization for PNP equations, it can be used on very general polygonal meshes, so the requirements for mesh quality are lower. It could be more suitable for PNP practical problems with extremely irregular interfaces, for example ion channel problems. Then, we present the a priori error analysis for the VEM. We focus mainly on the error estimates for the semi-discrete system. The suboptimal L^2 norm and the optimal H^1 norm error estimates with k-th ($k \geq 1$) order virtual element are presented for semi-discrete virtual element approximations. After that, a fully discrete virtual element scheme is given for the PNP equations. Considering the coupling and nonlinearity of the fully discrete system, the Gummel iteration is applied to decouple and linearize it. This iteration is a commonly used decoupling method for solving PNP equations, see e.g. [13, 28, 34]. Here we introduce the Gummel iteration of the fully discrete virtual element approximation and present the error analysis for it. The suboptimal L^2 norm error estimates are obtained for the Gummel iteration of the VEM for PNP equations.

From a mathematical point of view, the PNP equations consist of a linear elliptic (Poisson) equation and two nonlinear parabolic (NP) equations. We follow the frame of convergence analysis in [32] to present the error estimate for the elliptic equation. Some arguments in [44] are used in the analysis of the nonlinear parabolic equation. Compared with these relevant work, we have some own characteristics in the analysis. For example, although our scheme was