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Optimal Rate Convergence Analysis of a Second Order Numerical Scheme for the Poisson–Nernst–Planck System

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Abstract. In this work, we propose and analyze a second-order accurate numerical scheme, both in time and space, for the multi-dimensional Poisson-Nernst-Planck system. Linearized stability analysis is developed, so that the second order accuracy is theoretically justified for the numerical scheme, in both temporal and spatial discretization. In particularly, the discrete $W^{1,4}$ estimate for the electric potential field, which plays a crucial role in the proof, are rigorously established. In addition, various numerical tests have confirmed the anticipated numerical accuracy, and further demonstrated the effectiveness and robustness of the numerical scheme in solving problems of practical interest.

AMS subject classifications: 65M06, 82C21, 35Q92

Key words: Poisson-Nernst-Planck system, linearized stability analysis, second order accuracy, convergence analysis.

1. Introduction

The Poisson–Nernst–Planck (PNP) system has been widely used in modeling transmembrane ion channels, semiconductor, and electrochemical devices. The Poisson's equation describes the electrostatic potential stemming from the charge density that consists of mobile ions and fixed charges. The Nernst-Planck equations model the diffusion and migration of ion species in the gradient of electrostatic potential. For symmetric 1 : 1 electrolytes, the ion transport is described by the PNP system

$$n_t = D_n \Delta n - e\beta \nabla \cdot \left(D_n n \nabla \phi \right), \tag{1.1a}$$

$$p_t = D_p \Delta p + e\beta \nabla \cdot \left(D_p p \nabla \phi \right), \tag{1.1b}$$

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla \phi = e(p - n) + \rho^f, \tag{1.1c}$$

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where p and n are the concentrations of positive and negative charged species, D_p and D_n are their diffusion constants, e is the elementary charge, β is the inverse of thermal energy, ϕ is the electrostatic potential, ε_0 is the vacuum permittivity, ε_r is the relative permittivity(or dielectric coefficient), and ρ^f is the density of fixed charge.

Let L, D_0, and c_0 be the characteristic length, diffusion constant, and concentration, respectively. Denote another characteristic length $\lambda_D = \sqrt{\frac{\varepsilon_0\varepsilon_r}{2\beta e^2 c_0}}$ for an ionic solution with bulk ionic concentration c_0 and homogenous dielectric coefficient ε_r. We shall introduce the following dimensionless parameters and variables:

$$\tilde{x} = x/L, \qquad \tilde{t} = tD_0/L\lambda_D, \quad \tilde{p} = p/c_0, \quad \tilde{n} = n/c_0, \tag{1.2a}$$

$$\tilde{D}_p = D_p/D_0, \ \tilde{D}_n = D_n/D_0, \qquad \tilde{\phi} = \beta e\phi, \quad \tilde{\rho}^f = \rho^f/c_0 e. \tag{1.2b}$$

Rescaling above quantities and dropping all the tildes lead to a nondimensionalized PNP system

$$\begin{cases} \partial_t p = \dfrac{\lambda_D}{L} D_p \nabla\cdot\left(\nabla p + p\nabla\phi\right), \\ \partial_t n = \dfrac{\lambda_D}{L} D_n \nabla\cdot\left(\nabla n - n\nabla\phi\right), \\ -2\dfrac{\lambda_D^2}{L^2}\Delta\phi = p - n + \rho^f. \end{cases} \tag{1.3}$$

For ease of presentation, we choose a computational domain $\Omega = (0,1)^3$, and consider zero Neumann boundary conditions

$$\frac{\partial\phi}{\partial \boldsymbol{n}} = 0, \quad \frac{\partial p}{\partial \boldsymbol{n}} = \frac{\partial n}{\partial \boldsymbol{n}} = 0 \qquad \text{on } \partial\Omega. \tag{1.4}$$

For simplicity, we denote by $C_n = \frac{\lambda_D}{L} D_n$, $C_p = \frac{\lambda_D}{L} D_p$, and $\kappa = \frac{L^2}{2\lambda_D^2}$.

Recently, there has been growing interests in incorporating effects that are beyond the mean-field description to the PNP theory, such as the steric effect, ion-ion correlations, and inhomogeneous dielectric environment [12, 13, 16, 19, 22, 23, 27, 31]. Various versions of modified PNP theory have been developed to account for such ignored effects within the framework of the PNP theory. For instance, the steric effect of ions have been taken into account by including excess free energy of solvent entropy [13–15, 22, 33], hard-sphere interaction kernels [12, 27], or the fundamental measure theory [23]. A modified PNP model has been proposed to consider Coulombic ion-ion correlations in inhomogeneous dielectric environment [19].

Due to the nonlinear coupling of the electrostatic potential and ionic concentrations, it is not trivial to solve the PNP system analytically, even numerically. Much effort has been devoted to the development of numerical methods that possess desired properties [1–3, 5, 8–10, 17, 18, 20, 21, 24–27, 29, 32]. For instance, a hybrid numerical scheme that employs adaptive grids has been proposed to solve a two-dimensional PNP system [25]. A delicate temporal discretization scheme has been recently developed to preserve free energy dynamics [8]. Using Slotboom variables, Liu and Wang [17] have developed a free energy