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Convergence Analysis of a Symmetrical and Positivity-Preserving Finite Difference Scheme for 1D Poisson–Nernst–Planck System

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Abstract: The Poisson–Nernst–Planck (PNP) system is a nonlinear coupled system that describes the motion of ionic particles. As the exact solution of the system is not available, numerical investigations are essentially important, and there are quite a lot of numerical methods proposed in the existing literature. However, the theoretical analysis is usually neglected due to the complicated nature of the PNP system. In this paper, a theoretical investigation for a symmetrical finite difference method proposed in the previous literature was conducted. An L^2 error estimate of $O(\tau + h^2)$ was derived for the numerical scheme in 1D, where τ denotes the time step size and h denotes the spatial mesh size, respectively. Numerical results confirm the theoretical analysis. More importantly, a positivity-preserving condition for the scheme is provided with rigorously theoretical justification.

Keywords: Poisson–Nernst–Planck system; finite difference method; error analysis; positivity-preserving condition

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1. Introduction

W. Nernst and M. Planck first formulated the classical unsteady Poisson–Nernst–Planck (PNP) system to describe the potential difference in a galvanic cell. The PNP system can describe the evolution of positively- and negatively charged particles (or ions); it has a lot of applications in electrochemistry [1], biology [2], and semiconductors [3–5].

The classical unsteady dimensionless PNP system has the following form:

$$\begin{cases} p_t = \nabla \cdot (\nabla p + p\nabla\phi), \text{ in } \Omega_T := (0,T] \times \Omega, \\ n_t = \nabla \cdot (\nabla n - n\nabla\phi), \text{ in } \Omega_T, \\ -\Delta\phi = p - n, \text{ in } \Omega_T, \end{cases} \quad (1)$$

where p, n are positively and negatively charged particles (or ions), ϕ is the electric potential, Ω is a bounded domain, and $[0, T]$ is the time interval. In the above non-dimensional equations, the characteristic length scale is chosen as the Debye length and the characteristic time scale is chosen as the diffusive time scale.

When numerically solving PDEs, it is of great importance to keep the original physical properties. Regarding numerical simulations for the PNP system—there are many literature studies that have solved these types of equations and preserved certain physical properties. For example, Prohl and Schmuck [6] present two different nonlinear finite element methods for the PNP system with homogeneous Neumann boundary conditions, which satisfy electric potential energy dissipative and entropy decay properties, respectively. Flavell [7] and Liu and Wang [8] provide different conservative finite difference methods that satisfy the mass conservation, ion concentration positivity, and total energy dissipation numerically, where the total energy is connected with both electric potential and ion concentration. In [7], a uniform bound is assumed for the numerical first derivatives of electric potential (cf. Equation (37) in [7]) without any theoretical justification for gaining the positivity-preserving condition of the numerical scheme. In order to obtain a linear while keeping the energy- and mass-preserving numerical scheme for solving the PNP system, a linearized semi-implicit finite different scheme was proposed in [9], where the scheme was numerically shown to be the first-order convergent in the time variable and the second-order convergent in the space variable. By assuming that the numerical solutions for ion concentrations are always non-negative, the authors in [9] showed that the proposed method satisfies the electric energy decay property. However, there is no theoretical justification for the positivity-preserving and error analysis. Due to the high nonlinearity of the PNP system, it is quite difficult to carry out the theoretical error analysis and obtain the positivity-preserving condition; this is the motivation of the current work.

The novelty of this paper was to conduct a rigorous error analysis and provide a theoretical analysis for the positivity-preserving condition for the symmetrical finite difference scheme proposed in [9], where the analysis was carried out for the 1D case. The rest of the paper is organized as follows: Section 1 is the overview of the paper; Section 2 reviews the linearized scheme proposed in [9] for the 1D case; Section 3 provides the positivity-preserving condition and shows its theoretical justification for the scheme in 1D; Section 4 presents a rigorous error analysis in the L^2 norm; Section 5 presents the numerical computations. Finally, the conclusions and future work are presented in Section 6.

2. A Review of the Numerical Method in 1D

In this paper, we consider the following 1D PNP system

$$p_t = (p_x + p\phi_x)_x, \qquad \text{in } \Omega_T = (0,T] \times [a,b]\,, \tag{2}$$

$$n_t = (n_x - n\phi_x)_x, \qquad \text{in } \Omega_T = (0,T] \times [a,b]\,, \tag{3}$$

$$-\phi_{xx} = p - n, \qquad \text{in } \Omega_T = (0,T] \times [a,b] \tag{4}$$

with the following initial and homogeneous Neumann boundary conditions

$$p(x,0) = p_0(x), \quad n(x,0) = n_0(x), \qquad \text{for } x \in (a,b), \tag{5}$$

$$p_x = n_x = \phi_x = 0, \qquad \text{on } x = a,b. \tag{6}$$

Let J be a positive integer. The domain $\Omega = [a,b]$ is uniformly partitioned with $h = (b-a)/J$ and variables are stored at the midpoints of each interval as follows

$$\Omega_h = \{x_j | x_j = a + (j - \frac{1}{2})h, 1 \le j \le J\}. \tag{7}$$

Let M be another positive integer. Then, $\tau = \frac{T}{M}$ is the time step size. We define a homogeneous mean subspace $Z_h^0 = \{\{U_j\}_{j=1}^J \,|\, < U, 1 >= \frac{1}{J}\sum_{j=1}^J U_j = 0\}$. To deal with the homogeneous Neumann boundary conditions (6), we define the values at the centers of the fictitious intervals outside the boundary, as follows

$$p_0 = p_1, \quad p_{J+1} = p_J, \quad n_0 = n_1, \quad n_{J+1} = n_J, \quad \phi_0 = \phi_1, \quad \phi_{J+1} = \phi_J, \tag{8}$$

where values at the fictitious intervals are represented by the subscripts $0, J+1$.

For a given grid function $\{f_j\}_{j=1}^J, \{g_j\}_{j=1}^J$, we define the following discrete operators:

$$\delta_x^+ f_j = \frac{f_{j+1} - f_j}{h}, \quad \delta_x^- f_j = \frac{f_j - f_{j-1}}{h},$$

$$\delta_x^2 f_j = \delta_x^- \delta_x^+ f_j = \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}, \quad \delta_x^0 f_j = \frac{f_{j+1/2} - f_{j-1/2}}{\Delta x},$$

where

$$f_{j+1/2} = \frac{f_j + f_{j+1}}{2}.$$

The discrete L^2 inner product and the discrete L^2 norm are defined as

$$< f, g >= \sum_{j=1}^{J} f_j g_j h \quad \|f\|^2 =< f, f > .$$

We define

$$< \delta_x^+ f, \delta_x^+ g >= \sum_{j=1}^{J-1} \delta_x^+ f_j \, \delta_x^+ g_j \, h \,, \quad < \delta_x^- f, \delta_x^- g >= \sum_{j=2}^{J} \delta_x^- f_j \, \delta_x^- g_j \, h.$$

The maximum norm for the grid function $\{f_j\}_{j=1}^J$ is defined as

$$\|f\|_\infty = \max_j |f_j|.$$

Now we are in the position to introduce the scheme proposed in [9] for the PNP system (2)–(4). For $j = 1, \cdots, J$, $0 \le m \le M-1$, a linearized finite difference scheme is defined by

$$\frac{P_j^{m+1} - P_j^m}{\tau} = \delta_x^2 (P_j^{m+1/2}) + \frac{1}{h} (P_{j+1/2}^m \, \delta_x^+ \Phi_j^{m+1/2} - P_{j-1/2}^m \, \delta_x^- \Phi_j^{m+1/2}) \,, \tag{9}$$

$$\frac{N_j^{m+1} - N_j^m}{\tau} = \delta_x^2 (N_j^{m+1/2}) - \frac{1}{h} (N_{j+1/2}^m \, \delta_x^+ \Phi_j^{m+1/2} - N_{j-1/2}^m \, \delta_x^- \Phi_j^{m+1/2}) \,, \tag{10}$$

$$- \delta_x^2 (\Phi_j^{m+1}) = P_j^m - N_j^{m+1} \,, \tag{11}$$

where the upper index $[]^{m+1/2}$ denotes the average of $[]^m$ and $[]^{m+1}$, i.e., $P_j^{m+1/2} = (P_j^m + P_j^{m+1})/2$.

We note that all numerical solutions are in capital letters and the initial values for $\{P_j^0\}_{j=1}^J$ and $\{N_j^0\}_{j=1}^J$ can be directly obtained from (5). The detailed implementation and mass conservation and energy decay properties are provided in [9]. However, there is no error analysis in [9]. More importantly, the positivity-preserving property of the scheme is only shown numerically. As the homogeneous Neumann boundary condition is used, ϕ is unique up to a constant. We assume that the exact solution ϕ has a zero mean value. Similarly, we require $< \Phi, 1 >= 0$ to ensure a unique numerical solution.

The following Lemmas are essential for the analysis of the numerical solution. Throughout the rest part of this paper, unless otherwise indicated, C is the notation referring to a general positive constant and ϵ denotes a general small constant, which are independent of τ and h and have different values in different contexts.

Lemma 1. *Discrete Gronwall inequality [10]: Let τ, B, and a_k, b_k, c_k, γ_k, for integers $k \ge 0$, be non-negative numbers, such that*

$$a_j + \tau \sum_{k=0}^{j} b_k \le \tau \sum_{k=0}^{j} \gamma_k a_k + \tau \sum_{k=0}^{j} c_k + B \,, \quad \text{for} \quad j \ge 0 \,,$$

suppose that $\tau \gamma_k < 1$, for all k, and set $\sigma_k = (1 - \tau \gamma_k)^{-1}$. Then,

$$a_j + \tau \sum_{k=0}^{j} b_k \le \exp(\tau \sum_{k=0}^{j} \gamma_k \sigma_k)(\tau \sum_{k=0}^{j} c_k + B) \,, \quad \text{for} \quad j \ge 0 \,.$$

According to the triangular and Cauchy inequalities, we have the following Lemma.

Lemma 2. *Let $\{U^m\}_{m=0}^M$ be a sequence of the discrete functions defined on Ω_h. Then, for any norm $\|\cdot\|$, we have*

$$\begin{aligned} \tau\|U^m\| &\le 2\tau\sum_{l=1}^{m}\|\frac{U^l+U^{l-1}}{2}\|+\tau\|U^0\| \\ &\le 2\sqrt{T}\left(\sum_{l=0}^{m-1}\tau\|U^{l+1/2}\|^2+\tau\|U^0\|^2\right)^{\frac{1}{2}} \end{aligned} \tag{12}$$

Lemma 3. *For any grid function $\{U_j\}_{j=1}^{j}$ defined on mesh Ω_h, where Ω_h is described as (7) and $< U, 1 >= 0$, we have*

$$\| U \|_\infty \le C \| \delta_x^+ U \|, \tag{13}$$

and

$$\| U \| \le C \| \delta_x^+ U \| \ . \tag{14}$$

Proof. For any $j = 1, \cdots, J$, we have

$$\begin{aligned} U_j &= h\sum_{m=k}^{j-1}\delta_x^+ U_m + U_k, && \text{for } k < j \\ U_j &= U_j, && \text{for } k = j \\ U_j &= -h\sum_{m=j}^{k-1}\delta_x^+ U_m + U_k, && \text{for } j < k \le J \end{aligned}$$

Thus, summing up the index $k = 1, \ldots, J$ and noting $< U, 1 >= 0$, we have

$$\begin{aligned} |U_j| &= \frac{1}{J}\left|\sum_{k=1}^{j-1}\left(h\sum_{m=k}^{j-1}\delta_x^+ U_m\right)+\sum_{k=j+1}^{J}\left(-h\sum_{m=j}^{k-1}\delta_x^+ U_m\right)\right| \\ &\le \sum_{m=1}^{J-1}\left|h\delta_x^+ U_m\right| \\ &\le \left(\sum_{m=1}^{J-1}h|\delta_x^+ U_m|^2\right)^{\frac{1}{2}}\left(\sum_{m=1}^{J-1}h\right)^{\frac{1}{2}} \\ &\le \sqrt{b-a}\|\delta_x^+ U\| \end{aligned}$$

In addition,

$$\|U\|^2 = \sum_{j=1}^{J}|U_j|^2 h \le \sum_{j=1}^{J}\|U\|_\infty^2 h = (b-a)\|U\|_\infty^2 \le C\|\delta_x^+ U\|^2.$$

The proof is complete. □

Lemma 4. *Discrete Sobolev inequality [11,12]: if any grid function $\{U_j\}_{j=1}^J$ with $U_J = 0$, then*

$$\|U\| \le C\|\delta_x^- U\|, \quad \|U\|_\infty \le C\|\delta_x^- U\|.$$

If the grid function $\{U_j\}_{j=1}^J$ satisfies $U_0 = 0$, then

$$\|U\| \le C\|\delta_x^+ U\|, \quad \|U\|_\infty \le C\|\delta_x^+ U\|.$$

Proof. The proof is omitted. □

3. An Unconditional Optimal Error Analysis

Denote that $C^{2,4}(t,x)$ are the set of functions with the second-order continuous differentiable in time and the fourth-order continuous differentiable in space.

Theorem 1. *Suppose the exact solutions (p,n,ϕ) of (2)–(4) under the boundary conditions (6) all belong to $C^{2,4}(t,x)$. For the numerical solutions (P,N,Φ) of (9)–(11) with homogeneous boundary conditions (8), there are two small positive constants τ_0 and h_0, such that when $\tau < \tau_0$ and $h < h_0$, the following L^2 norm error estimates hold*

$$\max_{0\le m\le M}(\|p^m - P^m\| + \|n^m - N^m\|) \le C_0(\tau + h^2), \tag{15}$$
$$\max_{0\le m\le M}\|\phi^m - \Phi^m\|_\infty \le C_0(\tau + h^2),$$

where C_0 is a positive constant, independent of h and τ.

Proof. Denote that $e_p^m = p^m - P^m$, $e_n^m = n^m - N^m$, $e_\phi^m = \phi^m - \Phi^m$. Substituting the exact solution into the scheme (9)–(11), results in

$$\frac{p_j^{m+1} - p_j^m}{\tau} = \delta_x^2(p_j^{m+1/2}) + \frac{1}{h}(p_{j+1/2}^m\,\delta_x^+\phi_j^{m+1/2} - p_{j-1/2}^m\,\delta_x^-\phi_j^{m+1/2}) + (R_p^m)_j, \tag{16}$$
$$\frac{n_j^{m+1} - n_j^m}{\tau} = \delta_x^2(n_j^{m+1/2}) - \frac{1}{h}(n_{j+1/2}^m\,\delta_x^+\phi_j^{m+1/2} - n_{j-1/2}^m\,\delta_x^-\phi_j^{m+1/2}) + (R_n^m)_j, \tag{17}$$
$$-\delta_x^2(\phi_j^{m+1}) = p_j^{m+1} - n_j^{m+1} + (R_\phi^{m+1})_j, \tag{18}$$

where the truncation terms satisfy

$$(R_p^m)_j = O(\tau + h^2), \quad (R_n^m)_j = O(\tau + h^2), \quad (R_\phi^m)_j = O(h^2). \tag{19}$$

Note that it is necessary to assume that the exact solutions (p,n,ϕ) all belong to $C^{2,4}(t,x)$ so that the truncation terms R_p^m, R_n^m, R_ϕ^m satisfy the above order of magnitude estimates.

Subtracting (9)–(11) from (16)–(18), the error equations satisfy

$$\frac{(e_p^{m+1})_j - (e_p^m)_j}{\tau} = \delta_x^2(e_p^{m+1/2})_j + (H_p^m)_j + (R_p^m)_j, \tag{20}$$
$$\frac{(e_n^{m+1})_j - (e_n^m)_j}{\tau} = \delta_x^2(e_n^{m+1/2})_j + (H_n^m)_j + (R_n^m)_j, \tag{21}$$
$$-\delta_x^2(e_\phi^{m+1})_j = (e_p^{m+1})_j - (e_n^{m+1})_j + (R_\phi^{m+1})_j, \tag{22}$$

where the two nonlinear error terms

$$\begin{aligned}
(H_p^m)_j &= \frac{1}{h}(p_{j+1/2}^m\,\delta_x^+\phi_j^{m+1/2} - p_{j-1/2}^m\,\delta_x^-\phi_j^{m+1/2}) \\
&\quad - \frac{1}{h}(P_{j+1/2}^m\,\delta_x^+\Phi_j^{m+1/2} - P_{j-1/2}^m\,\delta_x^-\Phi_j^{m+1/2}) \\
&= \delta_x^0(p_j^m\delta_x^0\phi_j^{m+1/2}) - \delta_x^0(P_j^m\delta_x^0\Phi_j^{m+1/2}), \\
(H_n^m)_j &= -\frac{1}{h}(n_{j+1/2}^m\,\delta_x^+\phi_j^{m+1/2} - n_{j-1/2}^m\,\delta_x^-\phi_j^{m+1/2}) \\
&\quad + \frac{1}{h}(N_{j+1/2}^m\,\delta_x^+\Phi_j^{m+1/2} - N_{j-1/2}^m\,\delta_x^-\Phi_j^{m+1/2}) \\
&= -\delta_x^0(n_j^m\delta_x^0\phi_j^{m+1/2}) + \delta_x^0(N_j^m\delta_x^0\Phi_j^{m+1/2}).
\end{aligned}$$

To estimate the nonlinear terms, we first derive some bound for $(e_\phi^{m+1})_j$. Applying Lemma 4 to error Equation (22), we can deduce that

$$\begin{aligned}\|\delta_x^+ e_\phi^{m+1/2}\|_\infty \leq & \; C\|\delta_x^-(\delta_x^+ e_\phi^{m+1/2})\| \\ \leq & \; C\|\delta_x^2 e_\phi^{m+1/2}\| \\ \leq & \; C\|e_p^{m+1/2} - e_n^{m+1/2} + R_\phi^{m+1/2}\| \\ \leq & \; C(\|e_p^{m+1/2}\| + \|e_n^{m+1/2}\| + \|R_\phi^{m+1/2}\|).\end{aligned} \tag{23}$$

Multiplying both sides of (20) by $e_p^{m+1/2}$ and taking the inner product, we have

$$\frac{\|e_p^{m+1}\|^2 - \|e_p^m\|^2}{2\tau} = -\|\delta_x^+(e_p^{m+1/2})\|^2 + (H_p^m, e_p^{m+1/2}) + (R_p^m, e_p^{m+1/2}), \tag{24}$$

and

$$\begin{aligned}& |(H_p^m, e_p^{m+1/2})| \\ = & \; |(\delta_x^0(p_j^m \delta_x^0 \phi_j^{m+1/2}) - \delta_x^0(P_j^m \delta_x^0 \Phi_j^{m+1/2}), e_p^{m+1/2})| \\ = & \; \left|(\delta_x^0(e_p^m \delta_x^0 \phi^{m+1/2}) + \delta_x^0(p^m \delta_x^0 e_\phi^{m+1/2}) - \delta_x^0(e_p^m \delta_x^0 e_\phi^{m+1/2}), e_p^{m+1/2})\right| \\ = & \; \left|-(e_{pR}^m \delta_x^+ \phi^{m+1/2} + p_R^m \delta_x^+ e_\phi^{m+1/2} - e_{pR}^m \delta_x^+ e_\phi^{m+1/2}, \delta_x^+ e_p^{m+1/2})\right| \\ \leq & \; \|\delta_x^+ \phi^{m+1/2}\|_\infty \|e_{pR}^m\| \|\delta_x^+ e_p^{m+1/2}\| + \|p_R^m\|_\infty \|\delta_x^+ e_\phi^{m+1/2}\| \|\delta_x^+ e_p^{m+1/2}\| \\ & + \|\delta_x^+ e_\phi^{m+1/2}\|_\infty \|e_{pR}^m\| \|\delta_x^+ e_p^{m+1/2}\| \\ \leq & \; (C + C\|e_p^m\|^2)(\|e_p^m\|^2 + \|e_p^{m+1/2}\|^2 + \|e_n^{m+1/2}\|^2 + \|R_\phi^{m+1/2}\|^2) \\ & + \frac{1}{2}\|\delta_x^+ e_p^{m+1/2}\|^2\end{aligned} \tag{25}$$

where we use the regularity assumption for the exact solutions (23) and Young's inequality,

$$(e_{pR}^m)_j = \frac{(e_p^m)_j + (e_p^m)_{j+1}}{2}, \quad (p_R^m)_j = \frac{p_j^m + p_{j+1}^m}{2}.$$

The truncation term can be bounded by

$$|(R_p^m, e_p^{m+1/2})| \leq \|R_p^m\| \|e_p^{m+1/2}\| \leq \|e_p^{m+1/2}\|^2 + C(\tau + h^2)^2. \tag{26}$$

Substituting estimates (25) and (26) into (24) yields

$$\frac{\|e_p^{m+1}\|^2 - \|e_p^m\|^2}{2\tau} + \frac{1}{2}\|\delta_x^+ e_p^{m+1/2}\|^2 \tag{27}$$

$$\leq (C + C\|e_p^m\|^2)(\|e_p^m\|^2 + \|e_p^{m+1/2}\|^2 + \|e_n^{m+1/2}\|^2) + C(\tau + h^2)^2. \tag{28}$$

By a similar analysis for the error Equation (21) for e_n, we can deduce that

$$\begin{aligned}& \frac{\|e_n^{m+1}\|^2 - \|e_n^m\|^2}{2\tau} + \frac{1}{2}\|\delta_x^+ e_n^{m+1/2}\|^2 \\ \leq & \; (C + C\|e_n^m\|^2)(\|e_n^m\|^2 + \|e_p^{m+1/2}\|^2 + \|e_n^{m+1/2}\|^2) + C(\tau + h^2)^2.\end{aligned} \tag{29}$$

Finally, combining (28) and (29), we arrive at

$$\begin{aligned}& \frac{\|e_p^{m+1}\|^2 + \|e_n^{m+1}\|^2 - \|e_p^m\|^2 - \|e_n^m\|^2}{2\tau} + \frac{1}{2}(\|\delta_x^+ e_p^{m+1/2}\|^2 + \|\delta_x^+ e_n^{m+1/2}\|^2) \\ \leq & \; (C + C(\|e_p^m\|^2 + \|e_n^m\|^2))(\|e_p^{m+1}\|^2 + \|e_n^{m+1}\|^2 + \|e_p^m\|^2 + \|e_n^m\|^2) \\ & + C(\tau + h^2)^2.\end{aligned} \tag{30}$$

Now, we are ready to prove (15). We shall prove slightly stronger error estimates for $m = 0, \ldots, J$

$$\|e_p^m\|^2 + \|e_n^m\|^2 + \tau \sum_{l=0}^{m-1} (\|\delta_x^+ e_p^{l+1/2}\|^2 + \|\delta_x^+ e_n^{l+1/2}\|^2) \le C_0(\tau + h^2)^2, \tag{31}$$

by mathematical induction. Obviously, $\|e_p^0\| = 0, \|e_n^0\| = 0$. Now suppose that (31) holds for $0 \le m \le k$, we shall find a constant C_0, independent of m, h, τ, such that (31) is valid for $0 \le m \le k+1$. By this induction assumption, we have

$$\|e_p^m\|^2 + \|e_n^m\|^2 \le C_0(\tau + h^2)^2 \le 1\,, \quad \text{for } m \le k \tag{32}$$

where we require that $C_0(\tau + h^2)^2 \le 1$.

By noting (32) and summing up (30) for index m, we have

$$\begin{aligned} &\|e_p^m\|^2 + \|e_n^m\|^2 + \tau \sum_{l=0}^{m-1} (\|\delta_x^+ e_p^{l+1/2}\|^2 + \|\delta_x^+ e_n^{l+1/2}\|^2) \\ &\le C\tau \sum_{l=1}^{m} (\|e_p^l\|^2 + \|e_n^l\|^2) + C(\tau + h^2)^2, \quad \text{for } m \le k+1. \end{aligned} \tag{33}$$

With the help of the Gronwall inequality in Lemma 1, we can derive that when $\tau < \tau_0$ for a certain small number τ_0

$$\|e_p^m\|^2 + \|e_n^m\|^2 + \tau \sum_{l=0}^{m-1} (\|\delta_x^+ e_p^{l+1/2}\|^2 + \|\delta_x^+ e_n^{l+1/2}\|^2) \le C \exp(\frac{2CT}{1 - 2C\tau})(\tau + h^2)^2. \tag{34}$$

Thus, (31) is valid for $m \le k+1$ if we choose $C_0 \ge C \exp(4CT)$. Then C_0 is fixed and the induction is complete. Equation (15) is proved.

In addition, the following estimate follows directly from (23) and Lemma 3

$$\|e_\phi^m\|_\infty \le C(\tau + h^2), \quad \text{for } m = 0, \cdots, M. \tag{35}$$

The proof of Theorem 1 is complete. □

Corollary 1. *Under the same hypothesis in Theorem 1, the following estimates for the numerical solution (P, N, Φ) hold*

$$\begin{aligned} &\max_{0 \le m \le M} (\|P^m\|_\infty + \|N^m\|_\infty) \le C_1, \\ &\max_{0 \le m \le M} (\|\delta_x^+ \Phi^m\|_\infty + \|\delta_x^- \Phi^m\|_\infty) \le C_2, \end{aligned} \tag{36}$$

where C_0 is a positive constant, independent of j, m, h, τ.

Proof. We shall first prove (36). To this end, it suffices to show $\|e_p\|_\infty + \|e_n\|_\infty \le \epsilon$. We shall consider two different cases. For the case $\tau \le h^2$, (15) gives that

$$\max_{0 \le m \le M} (\|p^m - P^m\| + \|n^m - N^m\|) \le C_0 h^2,$$

Applying inverse inequality for finite difference methods gives further

$$\begin{aligned} &\max_{0 \le m \le M} (\|p^m - P^m\|_\infty + \|n^m - N^m\|_\infty) \\ &\le \max_{0 \le m \le M} C h^{-1/2} (\|p^m - P^m\| + \|n^m - N^m\|) \\ &\le C C_0 h^{3/2} \le \epsilon \end{aligned} \tag{37}$$

For the case $\tau > h^2$, from (31) we have

$$\tau \sum_{m=0}^{J-1} (\|\delta_x^+ e_p^{m+1/2}\|^2 + \|\delta_x^+ e_n^{m+1/2}\|^2) \le C_0 \tau^2,$$

With Lemma 2, we can derive that

$$\max_{0 \le m \le J} (\|\delta_x^+ e_p^m\|^2 + \|\delta_x^+ e_n^m\|^2) \le CC_0 \tau.$$

Applying the Sobolev inequality, we can derive that

$$\max_{0 \le m \le M} (\|e_p^m\|_\infty + \|e_n^m\|_\infty) \le \max_{0 \le m \le M} C(\|\delta_x^+ e_p^m\|^2 + \|\delta_x^+ e_n^m\|^2) \le CC_0 \tau \le \epsilon, \quad (38)$$

where τ satisfies that $\tau < \tau_0$ for a small τ_0. □

For both the cases $\tau \le h^2$ and $\tau > h^2$, we have $\|e_p\|_\infty + \|e_n\|_\infty \le \epsilon$. The uniform bound (36) follows directly.

Now, using (11) and Lemma 4, we have

$$\|\delta_x^+ \Phi^m\|_\infty \le C\|\delta_x^2 \Phi^m\| \le C(\|P^m\| + \|N^m\|) \le C(\|P^m\|_\infty + \|N^m\|_\infty) \le C_2$$

$$\|\delta_x^- \Phi^m\|_\infty \le C\|\delta_x^2 \Phi^m\| \le C(\|P^m\| + \|N^m\|) \le C(\|P^m\|_\infty + \|N^m\|_\infty) \le C_2$$

□

4. Positivity-Preserving Condition

In addition to the mass conservation and energy decay properties shown in [9], positivity-preserving is another fundamental law for the system (2)–(4). The following theorem provides a sufficient condition for the positivity-preserving of the proposed numerical scheme (9)–(11).

Theorem 2. *For given initial non-negative conditions: $p_0 \ge 0$, $n_0 \ge 0$, if τ and h satisfy the following conditions:*

$$h \le \min\{\frac{1}{C_2}, h_0\}, \quad \tau \le \min\{\frac{h^2}{4 + 2C_1 h^2}, \tau_0\} \quad (39)$$

where C_1, C_2, τ_0, and h_0 refer to constants, then the numerical solutions $\{P_j^m, N_j^m, \Phi_j^m\}$ satisfy the positivity-preserving property

$$P_j^m \ge 0, \quad N_j^m \ge 0, \quad \text{for } j = 1, \cdots, J, m = 0, \cdots, M. \quad (40)$$

Proof. For time level m, (9) and (10) can be rewritten using the matrix–vector form given by,

$$\left(\mathsf{I} - \frac{\tau}{2}\mathsf{K}\right) P^{m+1} = \left(\mathsf{I} + \frac{\tau}{2}\mathsf{K} + \tau \mathsf{H}(\Phi^{s+\frac{1}{2}})\right) P^m \triangleq P_{rhs}, \quad (41)$$

$$\left(\mathsf{I} - \frac{\tau}{2}\mathsf{K}\right) N^{m+1} = \left(\mathsf{I} + \frac{\tau}{2}\mathsf{K} - \tau \mathsf{H}(\Phi^{s+\frac{1}{2}})\right) N^m \triangleq N_{rhs}, \quad (42)$$

where I means the $J \times J$ identity matrix, K is the discrete matrix of the Laplace operator subjected to homogeneous Neumann boundary conditions in 1D

$$\mathsf{K} = \frac{1}{h^2}\begin{bmatrix} -1 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -1 \end{bmatrix}_{J\times J} \tag{43}$$

and

$$\mathsf{H}(\Phi^{m+\frac{1}{2}}) = \begin{bmatrix} \delta_x^2\Phi_1^{m+1/2} & \frac{1}{h}\delta_x^+\Phi_1^{m+1/2} & & & \\ \frac{1}{h}\delta_x^-\Phi_2^{m+1/2} & \delta_x^2\Phi_2^{m+1/2} & \frac{1}{h}\delta_x^+\Phi_2^{m+1/2} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{h}\delta_x^-\Phi_{J-1}^{m+1/2} & \delta_x^2\Phi_{J-1}^{m+1/2} & \frac{1}{h}\delta_x^+\Phi_{J-1}^{m+1/2} \\ & & & \frac{1}{h}\delta_x^-\Phi_J^{m+1/2} & \delta_x^2\Phi_J^{m+1/2} \end{bmatrix} \tag{44}$$

stands for the nonlinear convection matrix, respectively.

From the above matrix form, it is easy to see that K and H have the same sparse pattern. More importantly, the coefficient matrix $\mathsf{I} - \frac{\tau}{2}\mathsf{K}$ is an M-matrix [13]. Therefore, to prove the non-negative property (40), it suffices to show $P_{rhs}, N_{rhs} \geq 0$. We shall verify that under the condition on τ and h in such that the matrices

$$\mathsf{I} + \frac{\tau}{2}\mathsf{K} + \tau\mathsf{H}(\Phi^{m+\frac{1}{2}}), \quad \mathsf{I} + \frac{\tau}{2}\mathsf{K} - \tau\mathsf{H}(\Phi^{m+\frac{1}{2}})$$

are non-negative. As the boundary nodes are not essential in our analysis, we shall focus on the interior nodes. First, for the j-th diagonal entry of $\mathsf{I} + \frac{\tau}{2}\mathsf{K} + \tau\mathsf{H}(\Phi^{m+\frac{1}{2}})$, we have

$$\begin{aligned} 1 - \frac{2\tau}{h^2} + \tau\delta_x^2\Phi_j^{m+1/2} &= 1 - \frac{2\tau}{h^2} + \tau\left(N_j^{m+1/2} - P_j^{m+1/2}\right) \\ &\geq 1 - \frac{2\tau}{h^2} - \tau\left(\left\|N_j^{m+1/2}\right\|_\infty + \left\|P_j^{m+1/2}\right\|_\infty\right) \\ &\geq 1 - \frac{2\tau}{h^2} - \tau C_1 \\ &\geq \frac{1}{2} \geq 0 \end{aligned} \tag{45}$$

if we require that $\tau \leq \frac{h^2}{4+2C_1h^2}$. Second, on the jth row, for its $(j-1)$-th entry, we have

$$\frac{\tau}{h^2} + \tau\frac{1}{h}\delta_x^-\Phi_j^{m+1/2} \geq \frac{\tau}{h}(h^{-1} - \|\delta_x^-\Phi_j^{m+1/2}\|_\infty) \geq \frac{\tau}{h}(h^{-1} - C_2) \geq 0. \tag{46}$$

where we require $h \leq 1/C_2$ Third, on the jth row, for its $(j+1)$-th entry, we have

$$\frac{\tau}{h^2} + \tau\frac{1}{h}\delta_x^+\Phi_j^{m+1/2} \geq \frac{\tau}{h}(h^{-1} - \|\delta_x^+\Phi_j^{m+1/2}\|_\infty) \geq \frac{\tau}{h}(h^{-1} - C_2) \geq 0. \tag{47}$$

where we require $h \leq 1/C_2$ Now combining all of the requirements for τ and h, we verify that $\mathsf{I} + \frac{\tau}{2}\mathsf{K} + \tau\mathsf{H}(\Phi^{m+\frac{1}{2}})$ is a non-negative matrix. By a similar analysis, the matrix $\mathsf{I} + \frac{\tau}{2}\mathsf{K} - \tau\mathsf{H}(\Phi^{m+\frac{1}{2}})$ can also be shown to be non-negative. The proof of Theorem 2 is complete. □

5. Numerical Results

To numerically verify the convergence order that is analyzed in this paper, we consider the following argument equations with the exact solutions as the test problem:

$$p_t = (p_x + p\phi_x)_x + f_1, \qquad \text{in } \Omega_T = (0,T] \times [a,b]\,, \tag{48}$$
$$n_t = (n_x - n\phi_x)_x + f_2, \qquad \text{in } \Omega_T = (0,T] \times [a,b]\,, \tag{49}$$
$$-\phi_{xx} = p - n + c, \qquad \text{in } \Omega_T = (0,T] \times [a,b] \tag{50}$$

where

$$p = (3x^2 - 2x^3)e^{-t}, \quad n = x^2(1-x)^2 e^{-t}, \quad \phi = x^2(1-x)^2 e^{-t}$$

are the exact solutions of (48)–(50), satisfying the zero Neumann boundary conditions (6). Moreover, f_1, f_2, c are known functions that are given according to these exact solutions.

The numerical schemes for the above system are given by

$$\frac{P_j^{m+1} - P_j^m}{\tau} = \delta_x^2(P_j^{m+1/2}) + \frac{1}{h}(P_{j+1/2}^m \,\delta_x^+ \Phi_j^{m+1/2} - P_{j-1/2}^m \,\delta_x^- \Phi_j^{m+1/2}) + (f_1)_{j,k}^{m+1/2}\,, \tag{51}$$
$$\frac{N_j^{m+1} - N_j^m}{\tau} = \delta_x^2(N_j^{m+1/2}) - \frac{1}{h}(N_{j+1/2}^m \,\delta_x^+ \Phi_j^{m+1/2} - N_{j-1/2}^m \,\delta_x^- \Phi_j^{m+1/2}) + (f_2)_{j,k}^{m+1/2}\,, \tag{52}$$
$$-\delta_x^2(\Phi_j^{m+1}) = P_j^{m+1} - N_j^{m+1} + c_{j,k}^{m+1}. \tag{53}$$

We carry out the numerical convergence study for both space and time variables for the above scheme (51)–(53). For the spatial convergence analysis, we set $\Delta t = 0.00001$, and use four different spatial meshes $h = \frac{1}{10\times 2^n} \triangleq h$, $n = 0, \cdots, 3$, the final time is set to be $T = 1.0$. Table 1 lists the spatial convergence results; it can be seen that all variables p, n, ϕ converge with second-order in the L^2 norm. For temporal convergence analysis, we set $h = 0.001$, and use four different time step sizes $\tau = \frac{1}{40\times 2^n} \triangleq h$, $n = 0, \cdots, 3$, the final time is also set to be $T = 1.0$. Table 2 lists the temporal convergence results, it can be seen that all variables p, n, ϕ converge with first-order in the L^2 norm. These results confirm the theoretical analysis in Section 3.

Table 1. Spatial mesh refinement analysis ($e_p = p_h - p_{exact}, e_n = n_h - n_{exact}, e_\phi = \phi_h - \phi_{exact}$, $\Delta t = 0.00001$).

h	$\lVert e_p \rVert$	Order	$\lVert e_n \rVert$	Order	$\lVert e_\phi \rVert$	Order
1/10	2.24×10^{-3}	-	6.35×10^{-3}	-	1.99×10^{-4}	-
1/20	5.69×10^{-4}	1.99	1.58×10^{-3}	2.00	5.80×10^{-5}	1.78
1/40	1.45×10^{-4}	1.97	3.96×10^{-4}	2.00	1.59×10^{-5}	1.87
1/80	3.88×10^{-5}	1.90	9.90×10^{-5}	2.00	4.48×10^{-6}	1.82

Table 2. Temporal mesh refinement analysis ($\tau = 0.001$).

τ	$\lVert e_p \rVert$	Order	$\lVert e_n \rVert$	Order	$\lVert e_\phi \rVert$	Order
1/40	8.46×10^{-3}	-	5.56×10^{-4}	-	1.14×10^{-3}	-
1/80	4.25×10^{-3}	0.99	2.79×10^{-4}	0.99	7.07×10^{-4}	0.69
1/160	2.13×10^{-3}	1.00	1.40×10^{-4}	0.99	4.05×10^{-4}	0.80
1/320	1.06×10^{-3}	1.00	7.04×10^{-5}	0.99	2.22×10^{-4}	0.87

6. Conclusions and Future Work

In this paper, we carried out a theoretical analysis for a previously proposed numerical scheme for the PNP system; the analysis was conducted for the 1D problem. Firstly, the error analysis was carried out to show that the scheme is first-order convergent in the time variable and second-order convergent in the space variable under the L^2 norm. Secondly, the numerical first derivatives of electric potential are shown to be pointwise uniformly bounded. A positivity-preserving condition for the difference scheme is provided with a rigorous theoretical justification. Finally, we should point out that the current analysis was conducted only for 1D since the essential analysis to obtain a pointwise uniform bound for the numerical first derivatives of electric potential relies on the discrete Sobolev inequality (see Equation (23)).

For higher dimensions, Equation (23) is not valid since the discrete Sobolev inequality involves a higher order of derivatives. Thus, a rigorous convergence analysis for 2D and 3D will be presented in future work.

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