

An iteration solver for the Poisson–Nernst–Planck system and its convergence analysis

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ABSTRACT

In this paper, we provide a theoretical analysis for an iteration solver to implement a finite difference numerical scheme for the Poisson–Nernst–Planck (PNP) system, based on the Energetic Variational Approach (EnVarA), in which a non-constant mobility H^{-1} gradient flow is formulated. In particular, the nonlinear and singular nature of the logarithmic energy potentials has always been the essential difficulty. In the numerical design, the mobility function is explicitly updated, for the sake of unique solvability analysis. The logarithmic and the electric potential diffusion terms, which come from the gradient of convex energy functional parts, are implicitly computed. The positivity-preserving property for all the concentrations, an unconditional energy stability, and the optimal rate error estimate have been established in a recent work. A modified Newton iteration for the nonlinear and logarithmic part, combined with a linear iteration for the electric potential part, is proposed to implement the given numerical scheme, in which a non-constant linear elliptic equation needs to be solved at each iteration stage. A theoretical analysis is presented in this article, and a linear convergence is proved for such an iteration, with an asymptotic error constant in the same order of the time step size. A numerical test is also presented in this article, which demonstrates the linear convergence rate of the proposed iteration solver.

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1. Introduction

The Poisson–Nernst–Planck (PNP) system is formulated as

$$\partial_t n = D_n \Delta n - \frac{z_0 e_0}{k_B \theta_0} \nabla \cdot (D_n n \nabla \phi), \quad (1.1)$$

$$\partial_t p = D_p \Delta p + \frac{z_0 e_0}{k_B \theta_0} \nabla \cdot (D_p p \nabla \phi), \quad (1.2)$$

$$-\varepsilon \Delta \phi = z_0 e_0 (p - n) + \rho^f, \quad (1.3)$$

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where n and p are the concentrations of negatively and positively charged ions, and ϕ is the electric potential. In this model, k_B , θ_0 , ε , z_0 , e_0 stand for the Boltzmann constant, the absolute temperature, the dielectric coefficient, valence of ions, the charge of an electron, respectively; the parameters D_n and D_p are diffusion/mobility coefficients. The periodic boundary conditions are assumed in this paper, for simplicity of presentation, and the presented analysis could be extended to more complicated, more physical boundary conditions, such as the homogeneous Neumann one. Furthermore, the source term ρ^f is assumed to vanish everywhere, i.e., $\rho^f \equiv 0$. An extension to a non-homogeneous source term is straightforward. See the related works [1–6] for more detailed descriptions of this physical model.

In particular, the Energetic Variational Approach (EnVarA) [7] for the PNP system has attracted more and more attentions, since the PDE system is formulated as a gradient flow with respect to certain free energy. This framework has provided great convenience in the structure preserving analysis, at both the PDE and numerical levels. In fact, the dimensionless dynamical equations of the PNP system could be rewritten as (see the detailed derivation in [8])

$$\partial_t n = \nabla \cdot (\nabla n - n \nabla \phi), \quad (1.4)$$

$$\partial_t p = D \nabla \cdot (\nabla p + p \nabla \phi), \quad (1.5)$$

$$-\Delta \phi = p - n. \quad (1.6)$$

In fact, the parameter D plays the role of a non-dimensional relative mobility. The corresponding dimensionless energy is given by

$$E(n, p) = \int_{\Omega} \{n \ln n + p \ln p\} d\mathbf{x} + \frac{1}{2} \|n - p\|_{H^{-1}}^2, \quad (1.7)$$

under the assumption that $n - p$ is of mean zero, and the H^{-1} norm is defined via

$$\|f\|_{H^{-1}} := \sqrt{(f, f)_{H^{-1}}}, \quad (f, g) = (f, (-\Delta)^{-1}g) = ((-\Delta)^{-1}f, g), \quad \text{for } f \text{ and } g \text{ with mean zero.}$$

In turn, the PNP system (1.4)–(1.6) could be rewritten as the following conserved H^{-1} gradient flow, with non-constant mobility:

$$\partial_t n = \nabla \cdot (n \nabla \mu_n), \quad \partial_t p = D \nabla \cdot (p \nabla \mu_p), \quad (1.8)$$

$$\mu_n := \delta_n E = \ln n + 1 + (-\Delta)^{-1}(n - p) = \ln n + 1 - \phi, \quad (1.9)$$

$$\mu_p := \delta_p E = \ln p + 1 + (-\Delta)^{-1}(p - n) = \ln p + 1 + \phi, \quad (1.10)$$

in which the electric potential is defined as $\phi = (-\Delta)^{-1}(p - n)$. A careful calculation implies that the energy dissipation law becomes $E'(t) = - \int_{\Omega} \{n |\nabla \mu_n|^2 + D p |\nabla \mu_p|^2\} d\mathbf{x} \leq 0$.

Among the existing numerical works for the PNP system, the theoretical analysis for the positivity-preserving property, energy stability and convergence analysis turns out to be very challenging, due to the nonlinear and singular nature of the logarithmic terms in the EnVarA formulation. Some progresses have been made in recent years, such as the positivity-preserving analysis reported in [4,9–16], the energy stability analysis in [17–19], the convergence analysis in [20–23], as well as a few other related works [19,24–28]. In particular, a finite difference numerical scheme was proposed in [8], so that all three theoretical features have been established in the numerical analysis. In more details, the numerical scheme is based on the variational structure of the original PNP system, so that the energy stability analysis could be formulated in an appropriate framework. The mobility concentration function is explicitly updated in the scheme, for the sake of unique solvability analysis. In the chemical potential expansion, all the terms are implicitly computed, which comes from the convexity of both the logarithmic energy functional and the electric energy potential. The positivity-preserving property has been theoretically established for both ion concentration variables, with the help of the singularity feature of the logarithmic term, combined with its convex nature. In fact, similar techniques have been successfully applied to other gradient models with singular energy potential [29–36], etc. The energy stability is a direct consequence of the convexity analysis. In addition, an optimal rate convergence analysis for the proposed numerical scheme has been reported in [8], based on an asymptotic expansion for the numerical solution, combined with rough error estimate and refined error estimate.

On the other hand, this numerical scheme is highly nonlinear and singular, due to the implicit treatment of the singular logarithmic chemical potential parts. In addition, an implicit treatment of the electric part leads to a highly coupled numerical system. These facts make the proposed numerical scheme very challenging to implement. In this article, we propose and analyze an iteration solver for this numerical scheme. A linearized Newton iteration is applied to the nonlinear and singular logarithmic parts, while a linear iteration is used for the electric potential part. In turn, a divergence-form elliptic system needs to be solved at each iteration stage, which in turn leads to a computational cost comparable to a standard Poisson solver. In addition, the positivity of both concentration variables at each iteration stage is crucial to ensure the well-posed property of the elliptic system. The convergence analysis will be provided for the proposed iteration algorithm, under the separation assumption for the exact PDE solution, i.e., a uniform distance is ensured between the exact PDE solution and the singular value of 0. With such an assumption for the exact PDE solution, a similar uniform distance could be derived for the numerical solution at each iteration stage, using an a-priori $\|\cdot\|_{\infty}$

error estimate for the iteration solution. With the help of this uniform distance, the singularity issue associated with the logarithmic term could be avoided in the iteration analysis. Moreover, the convex nature of the logarithmic energy functional will lead to a well-posed error analysis for the nonlinear part at each iteration stage. As a result of all these techniques, a linear convergence analysis is reported for the proposed iteration process, with the convergence rate in the same order of the time step size. In our knowledge, it will be the first such result for the highly nonlinear and singular PNP system.

The rest of the article is organized as follows. In Section 2 the numerical scheme is reviewed, and the main theoretical results are recalled, if the numerical solution could be exactly implemented. In turn, the iteration solver is introduced in Section 3, and a linear convergence analysis is provided in details. A numerical test is presented in Section 4, and the linear convergence rate of the proposed iteration solver is confirmed in the test. Finally, some concluding remarks are given in Section 5.

2. Review of the numerical scheme

2.1. The finite difference spatial discretization

The standard centered finite difference spatial approximation is applied. We present the numerical approximation on the computational domain $\Omega = (0, 1)^3$ with a periodic boundary condition, and $\Delta x = \Delta y = \Delta z = h = \frac{1}{N}$ with $N \in \mathbb{N}$ to be the spatial mesh resolution throughout this work. In particular, $f_{i,j,k}$ stands for the numerical value of f at the cell centered mesh points $((i + \frac{1}{2})h, (j + \frac{1}{2})h, (k + \frac{1}{2})h)$, and we denote C_{per} as

$$C_{\text{per}} := \{f_{i,j,k} \mid f_{i,j,k} = f_{i+\alpha N, j+\beta N, k+\gamma N}, \forall i, j, k, \alpha, \beta, \gamma \in \mathbb{Z}\},$$

with the discrete periodic boundary condition imposed. In turn, the discrete average and difference operators are evaluated at $((i + 1)h, (j + \frac{1}{2})h, (k + \frac{1}{2})h)$, $((i + \frac{1}{2})h, (j + 1)h, (k + \frac{1}{2})h)$ and $((i + \frac{1}{2})h, (j + \frac{1}{2})h, (k + 1)h)$, respectively:

$$\begin{aligned} A_x f_{i+1/2,j,k} &:= \frac{1}{2} (f_{i+1,j,k} + f_{i,j,k}), & D_x f_{i+1/2,j,k} &:= \frac{1}{h} (f_{i+1,j,k} - f_{i,j,k}), \\ A_y f_{i,j+1/2,k} &:= \frac{1}{2} (f_{i,j+1,k} + f_{i,j,k}), & D_y f_{i,j+1/2,k} &:= \frac{1}{h} (f_{i,j+1,k} - f_{i,j,k}), \\ A_z f_{i,j,k+1/2} &:= \frac{1}{2} (f_{i,j,k+1} + f_{i,j,k}), & D_z f_{i,j,k+1/2} &:= \frac{1}{h} (f_{i,j,k+1} - f_{i,j,k}). \end{aligned}$$

Conversely, the corresponding operators at the staggered mesh points are defined as follows:

$$\begin{aligned} a_x f_{i,j,k}^x &:= \frac{1}{2} (f_{i+1/2,j,k}^x + f_{i-1/2,j,k}^x), & d_x f_{i,j,k}^x &:= \frac{1}{h} (f_{i+1/2,j,k}^x - f_{i-1/2,j,k}^x), \\ a_y f_{i,j,k}^y &:= \frac{1}{2} (f_{i,j+1/2,k}^y + f_{i,j-1/2,k}^y), & d_y f_{i,j,k}^y &:= \frac{1}{h} (f_{i,j+1/2,k}^y - f_{i,j-1/2,k}^y), \\ a_z f_{i,j,k}^z &:= \frac{1}{2} (f_{i,j,k+1/2}^z + f_{i,j,k-1/2}^z), & d_z f_{i,j,k}^z &:= \frac{1}{h} (f_{i,j,k+1/2}^z - f_{i,j,k-1/2}^z). \end{aligned}$$

In turn, for a scalar cell-centered function g and a vector function $\vec{f} = (f^x, f^y, f^z)^T$, with f^x , f^y and f^z evaluated at $((i + 1)h, (j + \frac{1}{2})h, (k + \frac{1}{2})h)$, $((i + \frac{1}{2})h, (j + 1)h, (k + \frac{1}{2})h)$, $((i + \frac{1}{2})h, (j + \frac{1}{2})h, (k + 1)h)$, respectively, the discrete divergence is defined as

$$\nabla_h \cdot (g \vec{f})_{i,j,k} = d_x (A_x g \cdot f^x)_{i,j,k} + d_y (A_y g \cdot f^y)_{i,j,k} + d_z (A_z g \cdot f^z)_{i,j,k}. \quad (2.1)$$

In particular, if $\vec{f} = \nabla_h \phi = (D_x \phi, D_y \phi, D_z \phi)^T$ for certain scalar grid function ϕ , the corresponding divergence becomes

$$\nabla_h \cdot (g \nabla_h \phi)_{i,j,k} = d_x (A_x g \cdot D_x \phi)_{i,j,k} + d_y (A_y g \cdot D_y \phi)_{i,j,k} + d_z (A_z g \cdot D_z \phi)_{i,j,k}, \quad (2.2)$$

$$(\Delta_h \phi)_{i,j,k} = \nabla_h \cdot (\nabla_h \phi)_{i,j,k} = d_x (D_x \phi)_{i,j,k} + d_y (D_y \phi)_{i,j,k} + d_z (D_z \phi)_{i,j,k}. \quad (2.3)$$

For two cell-centered grid functions f and g , its discrete L^2 inner product and the associated ℓ^2 norm are defined as

$$\langle f, g \rangle_{\Omega} := h^3 \sum_{i,j,k=1}^N f_{i,j,k} g_{i,j,k}, \quad \|f\|_2 := (\langle f, f \rangle_{\Omega})^{\frac{1}{2}}.$$

In turn, the mean zero space is introduced as $\mathring{C}_{\text{per}} := \{f \in C_{\text{per}} \mid 0 = \bar{f} := \frac{h^3}{|\Omega|} \sum_{i,j,k=1}^m f_{i,j,k}\}$. Similarly, for two vector grid functions $\vec{f} = (f^x, f^y, f^z)^T$, $\vec{g} = (g^x, g^y, g^z)^T$, with f^x (g^x), f^y (g^y), f^z (g^z) evaluated at $((i + 1)h, (j + \frac{1}{2})h, (k + \frac{1}{2})h)$, $((i + \frac{1}{2})h, (j + 1)h, (k + \frac{1}{2})h)$, $((i + \frac{1}{2})h, (j + \frac{1}{2})h, (k + 1)h)$, respectively, the corresponding discrete inner product becomes

$$\begin{aligned} [\vec{f}, \vec{g}] &:= [f^x, g^x]_x + [f^y, g^y]_y + [f^z, g^z]_z, \\ [f^x, g^x]_x &:= \langle a_x(f^x g^x), 1 \rangle, \quad [f^y, g^y]_y := \langle a_y(f^y g^y), 1 \rangle, \quad [f^z, g^z]_z := \langle a_z(f^z g^z), 1 \rangle. \end{aligned}$$

In addition to the discrete $\|\cdot\|_2$ norm, the discrete maximum norm is defined as $\|f\|_\infty := \max_{1 \leq i,j,k \leq N} |f_{i,j,k}|$. Moreover, the discrete H_h^1 and H_h^2 norms are introduced as

$$\begin{aligned}\|\nabla_h f\|_2^2 &:= [\nabla_h f, \nabla_h f] = [D_x f, D_x f]_x + [D_y f, D_y f]_y + [D_z f, D_z f]_z, \\ \|f\|_{H_h^1}^2 &:= \|f\|_2^2 + \|\nabla_h f\|_2^2, \quad \|f\|_{H_h^2}^2 := \|f\|_{H_h^1}^2 + \|\Delta_h f\|_2^2.\end{aligned}$$

The summation by parts formulas are recalled in the following lemma; the detailed proof could be found in [37–40], etc.

Lemma 2.1 ([37–40]). *For any $\psi, \phi, g \in C_{\text{per}}$, and any $\vec{f} = (f^x, f^y, f^z)^T$, with f^x, f^y, f^z evaluated at $((i+1)h, (j+\frac{1}{2})h, (k+\frac{1}{2})h)$, $((i+\frac{1}{2})h, (j+1)h, (k+\frac{1}{2})h)$, $((i+\frac{1}{2})h, (j+\frac{1}{2})h, (k+1)h)$, respectively, the following summation by parts formulas are valid:*

$$\langle \psi, \nabla_h \cdot \vec{f} \rangle_\Omega = -[\nabla_h \psi, \vec{f}], \quad \langle \psi, \nabla_h \cdot (g \nabla_h \phi) \rangle_\Omega = -[\nabla_h \psi, \mathcal{A}_h g \nabla_h \phi], \quad (2.4)$$

in which $\mathcal{A}_h$ corresponds to the average operator given by A_x, A_y and A_z .

In addition, a few notations need to be introduced, to facilitate the analysis in later sections. For any $\varphi \in \mathcal{C}_{\text{per}}$ and a positive cell centered grid function g (at a point-wise level), the weighed discrete norm is defined as

$$\|\varphi\|_{\mathcal{L}_g^{-1}} = \sqrt{\langle \varphi, \mathcal{L}_{\mathcal{M}}^{-1}(\varphi) \rangle_\Omega}, \quad (2.5)$$

in which $\psi = \mathcal{L}_g^{-1}(\varphi) \in \mathcal{C}_{\text{per}}$ is the unique solution that solves

$$\mathcal{L}_g(\psi) := -\nabla_h \cdot (g \nabla_h \psi) = \varphi. \quad (2.6)$$

In a simplified case of $g \equiv 1$, it is obvious that $\mathcal{L}_g(\psi) = -\Delta_h \psi$, and the discrete H_h^{-1} inner product and H_h^{-1} norm are introduced as $\langle \varphi_1, \varphi_2 \rangle_{-1,h} = \langle \varphi_1, (-\Delta_h)^{-1} \varphi_2 \rangle_\Omega$, and $\|\varphi\|_{-1,h} = \sqrt{\langle \varphi, (-\Delta_h)^{-1} \varphi \rangle_\Omega}$.

2.2. Review of the numerical scheme

The mobility function at the face-centered mesh points are defined as

$$\begin{aligned}(\check{\mathcal{M}}_n^m)_{i+1/2,j,k} &:= A_x(\mathcal{M}_n^m)_{i+1/2,j,k}, \\ (\check{\mathcal{M}}_n^m)_{i,j+1/2,k} &:= A_y(\mathcal{M}_n^m)_{i,j+1/2,k}, \\ (\check{\mathcal{M}}_n^m)_{i,j,k+1/2} &:= A_z(\mathcal{M}_n^m)_{i,j,k+1/2},\end{aligned} \quad (2.7)$$

in which $(\mathcal{M}_n^m)_{i,j,k} = n_{i,j,k}^m$. Similar definitions could be introduced for $\check{\mathcal{M}}_p^m$. The following finite difference scheme has been proposed in a recent work [8]: given $n^m, p^m \in C_{\text{per}}$, find $n^{m+1}, p^{m+1} \in C_{\text{per}}$ such that

$$\frac{n^{m+1} - n^m}{\Delta t} = \nabla_h \cdot (\check{\mathcal{M}}_n^m \nabla_h \mu_n^{m+1}), \quad (2.8)$$

$$\frac{p^{m+1} - p^m}{\Delta t} = \nabla_h \cdot (\check{\mathcal{M}}_p^m \nabla_h \mu_p^{m+1}), \quad (2.9)$$

$$\mu_n^{m+1} = \ln n^{m+1} + (-\Delta_h)^{-1}(n^{m+1} - p^{m+1}), \quad (2.10)$$

$$\mu_p^{m+1} = \ln p^{m+1} + (-\Delta_h)^{-1}(p^{m+1} - n^{m+1}). \quad (2.11)$$

2.3. The theoretical results for the proposed numerical scheme

It is observed that the numerical solution to (2.8)–(2.11) is mass conservative, i.e.,

$$\bar{n}^m = \bar{n}^0 := \beta_0, \quad \bar{p}^m = \bar{p}^0 := \beta_0, \quad \text{with } 0 < \beta_0, \quad \forall m \geq 1, \quad (2.12)$$

in which the average operator is given by $\bar{f} = \frac{1}{|\Omega|} \langle f, \mathbf{1} \rangle_\Omega$.

Lemma 2.2. *Assume that the mobility function $\check{\mathcal{M}}$ has uniform lower and upper bounds: $M_0 \leq \check{\mathcal{M}} \leq M_1$. For any g with $\bar{g} = 0$, we have*

$$\frac{M_0}{M_1^2} \|g\|_{-1,h}^2 \leq \|g\|_{\mathcal{L}_{\check{\mathcal{M}}}^{-1}}^2 \leq \frac{M_1}{M_0^2} \|g\|_{-1,h}^2. \quad (2.13)$$

Proof. We denote ψ as the solution to the non-constant elliptic equation, $-\nabla_h \cdot (\check{\mathcal{M}} \nabla_h \psi_g) = g$, and $\varphi_g = (-\Delta_h)^{-1} g$, i.e., $-\Delta_h \varphi_g = g$. Taking a test function φ_g with both equations $-\nabla_h \cdot (\check{\mathcal{M}} \nabla_h \psi_g) = g$, $-\Delta_h \varphi_g = g$, respectively, we get

$$\langle \check{\mathcal{M}} \nabla_h \psi_g, \nabla_h \varphi_g \rangle_\Omega = \langle g, \varphi_g \rangle_\Omega = \|\nabla_h \varphi_g\|_2^2. \quad (2.14)$$

Meanwhile, an application of Cauchy inequality implies that

$$\begin{aligned} \|\nabla_h \varphi_g\|_2^2 &= \langle \check{\mathcal{M}} \nabla_h \psi_g, \nabla_h \varphi_g \rangle_\Omega \leq M_1 \|\nabla_h \psi_g\|_2 \cdot \|\nabla_h \varphi_g\|_2, \\ \text{which in turn gives } \|\nabla_h \psi_g\|_2 &\geq \frac{1}{M_1} \|\nabla_h \varphi_g\|_2. \end{aligned} \quad (2.15)$$

Similarly, taking a test function ψ_g to both equations $-\nabla_h \cdot (\check{\mathcal{M}} \nabla_h \psi_g) = g$, $-\Delta_h \varphi_g = g$, respectively, we get

$$\langle \check{\mathcal{M}} \nabla_h \psi_g, \nabla_h \psi_g \rangle_\Omega = \langle g, \psi_g \rangle_\Omega = \langle \nabla_h \psi_g, \nabla_h \varphi_g \rangle_\Omega, \quad (2.16)$$

which in turn results in

$$\begin{aligned} M_0 \|\nabla_h \psi_g\|_2^2 &\leq \langle \check{\mathcal{M}} \nabla_h \psi_g, \nabla_h \psi_g \rangle_\Omega = \langle \nabla_h \psi_g, \nabla_h \varphi_g \rangle_\Omega \leq \|\nabla_h \psi_g\|_2 \cdot \|\nabla_h \varphi_g\|_2, \\ \text{so that } \|\nabla_h \psi_g\|_2 &\leq \frac{1}{M_0} \|\nabla_h \varphi_g\|_2. \end{aligned} \quad (2.17)$$

Therefore, we arrive at

$$\begin{aligned} \|g\|_{\mathcal{L}_{\check{\mathcal{M}}}^{-1}}^2 &= \langle \check{\mathcal{M}} \nabla_h \psi_g, \nabla_h \psi_g \rangle_\Omega \leq M_1 \|\nabla_h \varphi_g\|_2^2 \leq \frac{M_1}{M_0^2} \|g\|_{-1,h}^2, \\ \|g\|_{\mathcal{L}_{\check{\mathcal{M}}}^{-1}}^2 &= \langle \check{\mathcal{M}} \nabla_h \psi_g, \nabla_h \psi_g \rangle_\Omega \geq M_0 \|\nabla_h \varphi_g\|_2^2 \geq \frac{M_0}{M_1^2} \|g\|_{-1,h}^2, \end{aligned} \quad (2.18)$$

in which the identity that $\|\nabla_h \varphi_g\|_2^2 = \|g\|_{-1,h}^2$ has been repeatedly applied. This finishes the proof of [Lemma 2.2](#). $\square$

The positivity-preserving and unique solvability properties are established in the following theorem.

Theorem 2.1 ([8]). *Given $n^m, p^m \in C_{\text{per}}$, with $0 < n_{i,j,k}^m, p_{i,j,k}^m$, $1 \leq i, j, k \leq N$, and $n^m - p^m \in \dot{C}_{\text{per}}$, there exists a unique solution $(n^{m+1}, p^{m+1}) \in [C_{\text{per}}]^2$ to the numerical scheme (2.8)–(2.11), with $0 < n_{i,j,k}^{m+1}, p_{i,j,k}^{m+1}$, $1 \leq i, j, k \leq N$ and $n^{m+1} - p^{m+1} \in \dot{C}_{\text{per}}$.*

In terms of the energy stability analysis, the following discrete energy is introduced:

$$E_h(n, p) := \langle n \ln n + p \ln p, \mathbf{1} \rangle_\Omega + \frac{1}{2} \|n - p\|_{-1,h}^2. \quad (2.19)$$

Theorem 2.2 ([8]). *For the numerical solution (2.8)–(2.11), we have*

$$E_h(n^{m+1}, p^{m+1}) + \Delta t \left([\check{\mathcal{M}}_n^m \nabla_h \mu_n^{m+1}, \nabla_h \mu_n^{m+1}] + [\check{\mathcal{M}}_p^m \nabla_h \mu_p^{m+1}, \nabla_h \mu_p^{m+1}] \right) \leq E_h(n^m, p^m), \quad (2.20)$$

so that $E_h(n^m, p^m) \leq E_h(n^0, p^0) \leq C_0$, for all $m \in \mathbb{N}$, where $C_0 > 0$ is a constant independent of h .

In addition, an optimal rate convergence analysis has been reported in [8]. Denote (N, P, Φ) be the exact PDE solution for the non-dimensional PNP system (1.4)–(1.6). The following regularity assumption was made for the exact solution:

$$N, P \in \mathcal{R} := H^4(0, T; C_{\text{per}}(\Omega)) \cap H^3(0, T; C_{\text{per}}^2(\Omega)) \cap L^\infty(0, T; C_{\text{per}}^6(\Omega)). \quad (2.21)$$

More importantly, the following separation property is assumed for the exact solution:

$$N \geq \epsilon_0, \quad P \geq \epsilon_0, \quad \text{for some } \epsilon_0 > 0, \quad \text{at a point-wise level.} \quad (2.22)$$

Meanwhile, the (spatial) Fourier projection of the exact solution is introduced, $N_N(\cdot, t) := \mathcal{P}_N N(\cdot, t)$, $P_N(\cdot, t) := \mathcal{P}_N P(\cdot, t)$, with the projection into $\mathcal{B}^K$, the space of trigonometric polynomials of degree to and including K (with $N = 2K + 1$). Of course, the projection approximation estimate is standard:

$$\|N_N - N\|_{L^\infty(0, T; H^k)} \leq Ch^{\ell-k} \|N\|_{L^\infty(0, T; H^\ell)}, \quad \|P_N - P\|_{L^\infty(0, T; H^k)} \leq Ch^{\ell-k} \|P\|_{L^\infty(0, T; H^\ell)}, \quad (2.23)$$

for any $0 \leq k \leq \ell$, provided that $(N, P) \in L^\infty(0, T; H_{\text{per}}^\ell(\Omega))$. In addition, denote $N_N^m = N_N(\cdot, t_m)$, $P_N^m = P_N(\cdot, t_m)$, with $t_m = m \cdot \Delta t$. Since $(N_N, P_N) \in \mathcal{B}^K$, The mass conservative property has been proved for N_N and P_N at the discrete level:

$$\overline{N_N^m} = \overline{N_N^{m-1}}, \quad \overline{P_N^m} = \overline{P_N^{m-1}}, \quad \forall m \in \mathbb{N}. \quad (2.24)$$

Meanwhile, a similar property for the numerical solution of (2.8)–(2.9) is given by (2.12). In turn, the mass conservative projection for the initial data is taken: $n^0 = \mathcal{P}_h N_N(\cdot, t = 0)$, $p^0 = \mathcal{P}_h P_N(\cdot, t = 0)$:

$$(n^0)_{i,j,k} := N_N(p_i, p_j, p_k, t = 0), \quad (p^0)_{i,j,k} := P_N(p_i, p_j, p_k, t = 0). \quad (2.25)$$

Similarly, for the exact electric potential Φ , its Fourier projection is denoted as Φ_N . Subsequently, the error grid function is defined as

$$e_n^m := \mathcal{P}_h N_N^m - n^m, \quad e_p^m := \mathcal{P}_h P_N^m - p^m, \quad e_\phi^m := \mathcal{P}_h \Phi_N^m - \phi^m, \quad \forall m \in \mathbb{N}. \quad (2.26)$$

Because of the fact that $\bar{e}_n^m = \bar{e}_p^m = 0$, for any $m \geq 0$, we see that the discrete norm $\|\cdot\|_{-1,h}$ is well defined for the error grid function.

The convergence result of the proposed numerical scheme is stated in the following theorem.

Theorem 2.3 ([8]). *Given initial data $N(\cdot, t=0), P(\cdot, t=0) \in C_{\text{per}}^6(\Omega)$, suppose the exact solution for the PNP system (1.4)–(1.5) is of regularity class $\mathcal{R}$. Then, provided Δt and h are sufficiently small, and under the linear refinement requirement $C_1 h \leq \Delta t \leq C_2 h$, we have*

$$\|e_n^m\|_2 + \|e_p^m\|_2 + \left(\Delta t \sum_{k=1}^m (\|\nabla_h e_n^k\|_2^2 + \|\nabla_h e_p^k\|_2^2) \right)^{1/2} + \|e_\phi^m\|_{H_h^2} \leq C(\Delta t + h^2), \quad (2.27)$$

for all positive integers m , such that $t_m = m\Delta t \leq T$, where $C > 0$ is independent of Δt and h .

In fact, in the convergence analysis, a few supplementary fields, $N_{\Delta t,1}$, $N_{\Delta t,2}$, $P_{\Delta t,1}$, $P_{\Delta t,2}$ and $\check{N}$, $\check{P}$, have been constructed:

$$\check{N} = N_N + \mathcal{P}_N(\Delta t N_{\Delta t,1} + \Delta t^2 N_{\Delta t,2} + h^2 N_{h,1}), \quad \check{P} = P_N + \mathcal{P}_N(\Delta t P_{\Delta t,1} + \Delta t^2 P_{\Delta t,2} + h^2 P_{h,1}), \quad (2.28)$$

so that a higher $O(\Delta t^3 + h^4)$ consistency is satisfied with the given numerical scheme (2.8)–(2.11). These constructed profiles depend solely on the exact solution (N, P) .

In turn, alternate numerical error functions have been introduced:

$$\tilde{n}^m := \mathcal{P}_h \check{N}^m - n^m, \quad \tilde{p}^m := \mathcal{P}_h \check{P}^m - p^m, \quad \tilde{\phi}^m := (-\Delta_h)^{-1}(\tilde{p}^m - \tilde{n}^m), \quad \forall m \in \mathbb{N}. \quad (2.29)$$

Finally, the following convergence estimate has been derived in [8]:

$$\|\tilde{n}^{m+1}\|_2 + \|\tilde{p}^{m+1}\|_2 + \left(\Delta t \sum_{k=1}^{m+1} (\|\nabla_h \tilde{n}^k\|_2^2 + \|\nabla_h \tilde{p}^k\|_2^2) \right)^{1/2} \leq C(\Delta t^3 + h^4). \quad (2.30)$$

As a result of the convergence estimate (with higher order asymptotic expansion in $\check{N}$ and $\check{P}$), an application of an inverse inequality leads to

$$\|\tilde{n}^k\|_\infty + \|\tilde{p}^k\|_\infty \leq \frac{C\|\tilde{n}^k\|_2 + \|\tilde{p}^k\|_2}{h^{3/2}} \leq \frac{C(\Delta t^3 + h^4)}{h^{3/2}} \leq C(\Delta t^{3/2} + h^{5/2}) \leq \Delta t, \quad (2.31)$$

for any $k \geq 0$, under the linear refinement requirement $C_1 h \leq \Delta t \leq C_2 h$. Furthermore, the following $\|\cdot\|_\infty$ estimate for the discrete temporal difference of the numerical solution could be derived:

$$\begin{aligned} \|n^{m+1} - n^m\|_\infty &\leq \|\check{N}^{m+1} - \check{N}^m\|_\infty + \|\tilde{n}^{m+1} - \tilde{n}^m\|_\infty \leq C\Delta t + \Delta t = C_3\Delta t, \\ \|p^{m+1} - p^m\|_\infty &\leq C_3\Delta t, \quad (\text{similar analysis}), \end{aligned} \quad (2.32)$$

where the inequality $\|\check{N}^{m+1} - \check{N}^m\|_\infty \leq C\Delta t$ comes from the $C^1(0, T; C^0)$ regularity of $\check{N}$.

With the help of the $\|\cdot\|_\infty$ bound (2.31) of the numerical error functions, the following bounds become available

$$\frac{\epsilon_0}{2} \leq n^k, p^k \leq C_4 + 1 =: C_5, \quad \text{at a point-wise level, for any } k \geq 0, \quad (2.33)$$

provided that Δt and h are sufficiently small. In fact, such a derivation is based on the uniform-in-time $\|\cdot\|_\infty$ bound of the constructed profiles, $\|\check{N}\|_\infty, \|\check{P}\|_\infty \leq C_4$, as well as the separation properties, $\check{N}, \check{P} \geq \frac{5\epsilon_0}{8}$.

3. The iteration solver and the convergence analysis

Of course, an iteration solver is needed to implement the fully nonlinear scheme (2.8)–(2.11) at each time step. A method was proposed in [8] and is recounted here. First, the initial value for the nonlinear iteration is taken as $n^{(0)} := n^m$, $p^{(0)} := p^m$, and $\phi^{(0)} := \phi^m$. Subsequently, given the k th iterates, $n^{(k)}, p^{(k)}, \phi^{(k)}$, we obtain the $k+1$ st iterate by solving the following system:

$$\begin{aligned} \frac{n^{(k+1)} - n^m}{\Delta t} - \nabla_h \cdot \left(\check{\mathcal{M}}_n^m \nabla_h \left(\frac{n^{(k+1)} - n^{(k)}}{n^{(k)}} \right) \right) &= \nabla_h \cdot \left(\check{\mathcal{M}}_n^m \nabla_h (\ln n^{(k)} - \phi^{(k)}) \right), \\ \frac{p^{(k+1)} - p^m}{\Delta t} - \nabla_h \cdot \left(\check{\mathcal{M}}_p^m \nabla_h \left(\frac{p^{(k+1)} - p^{(k)}}{p^{(k)}} \right) \right) &= \nabla_h \cdot \left(\check{\mathcal{M}}_p^m \nabla_h (\ln p^{(k)} + \phi^{(k)}) \right), \\ -\Delta_h \phi^{(k+1)} &= p^{(k+1)} - n^{(k+1)}. \end{aligned} \quad (3.1)$$

The point-wise positivity of $\check{\mathcal{M}}_n^m$ and $\check{\mathcal{M}}_p^m$ has been justified by the positivity-preserving analysis. In fact, the unique solvability of the linear elliptic system (3.1), in the divergence form, can be theoretically ensured, provided that the point-wise positivity of the iteration solution $n^{(k)}$ and $p^{(k)}$ is available. The system (3.1) makes use of a Newton linearization

with respect to the logarithmic nonlinear parts: for any $a, b > 0$,

$$\ln(a) = \ln(b) + \frac{a-b}{b} - \frac{1}{2} \frac{(a-b)^2}{\zeta^2}, \quad (3.2)$$

for some ζ between a and b . In addition, we observe that

$$\overline{n^{(k+1)}} = \overline{n^{(k)}} = \overline{n^m}, \quad \overline{p^{(k+1)}} = \overline{p^{(k)}} = \overline{p^m}, \quad \overline{n^m} = \overline{p^m}, \quad (3.3)$$

so that $\mathcal{L}_{\check{\mathcal{M}}_n^m}(n^{(k+1)} - n^m)$, $\mathcal{L}_{\check{\mathcal{M}}_p^m}(p^{(k+1)} - p^m)$, as well as $(-\Delta_h)^{-1}(p^{(k+1)} - n^{(k+1)})$, are well defined.

Given the numerical solution (n^m, p^m) at the previous time step t^m , and we assume that the numerical scheme (2.8)–(2.11) has been exactly implemented up to time step t^m . As a result of the point-wise bound (2.33) of n^m and p^m , the following lower and upper bounds for $\check{\mathcal{M}}_n^m$ and $\check{\mathcal{M}}_p^m$ are straightforward:

$$\frac{\epsilon_0}{2} \leq \check{\mathcal{M}}_n^m \leq C_4 + 1 = C_5, \quad \frac{D\epsilon_0}{2} \leq \check{\mathcal{M}}_p^m \leq DC_5, \quad \text{at a point-wise level.} \quad (3.4)$$

We introduce the following iteration error functions:

$$\hat{e}_n^{(k)} = n^{m+1} - n^{(k)}, \quad \hat{e}_p^{(k)} = p^{m+1} - p^{(k)}, \quad \hat{e}_\phi^{(k)} = \phi^{m+1} - \phi^{(k)}. \quad (3.5)$$

By the fact that $\overline{n^{m+1}} = \overline{n^m}$, $\overline{p^{m+1}} = \overline{p^m}$, and $\overline{n^m} = \overline{p^m}$, we see that

$$\overline{\hat{e}_n^{(k)}} = \overline{\hat{e}_p^{(k)}} = 0, \quad \forall k \geq 0, \quad (3.6)$$

so that $\mathcal{L}_{\check{\mathcal{M}}_n^m}(\hat{e}_n^{(k+1)})$, $\mathcal{L}_{\check{\mathcal{M}}_p^m}(\hat{e}_p^{(k+1)})$, as well as $(-\Delta_h)^{-1}(\hat{e}_p^{(k)} - \hat{e}_n^{(k)})$, are well defined. Finally, the following weighed numerical “error energy” is defined:

$$F^{(k)} := \frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(k)}\|_{-1,h}^2 + \|\hat{e}_p^{(k)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(k)}\|_2^2 + \|\hat{e}_p^{(k)}\|_2^2). \quad (3.7)$$

The main theoretical result of this article is stated in the following theorem.

Theorem 3.1. *Given the numerical solution n^m, p^m and $\phi^m = (-\Delta_h)^{-1}(p^m - n^m)$ at the previous time step. Then, provided Δt and h are sufficiently small, and under the linear refinement requirement $C_1 h \leq \Delta t \leq C_2 h$, the following estimates hold:*

$$F^{(1)} \leq C_6 \Delta t^2 F^{(0)}, \quad (3.8)$$

$$F^{(2)} \leq C_7 \Delta t F^{(1)}, \quad (3.9)$$

$$F^{(k+1)} \leq C_8 \Delta t^2 F^{(k)}, \quad \forall k \geq 2, \quad (3.10)$$

where C_6, C_7 and $C_8 > 0$ are independent of Δt and h .

Proof. First we make an a-priori assumption:

$$\frac{\epsilon_0}{4} \leq n^{(k)}, p^{(k)} \leq C_5 + 1, \quad \text{at a point-wise level.} \quad (3.11)$$

This a-priori assumption will be recovered by the convergence analysis at the next iteration stage. With such an assumption, the iteration algorithm (3.1) is well-defined.

Subtracting the iteration algorithm (3.1) from the exact numerical solution (2.8)–(2.11) gives

$$\begin{aligned} \frac{\hat{e}_n^{(k+1)}}{\Delta t} &= \nabla_h \cdot \left(\check{\mathcal{M}}_n^m \nabla_h \left(\ln n^{m+1} - \ln n^{(k)} - \frac{n^{(k+1)} - n^{(k)}}{n^{(k)}} + (-\Delta_h)^{-1}(\hat{e}_n^{(k)} - \hat{e}_p^{(k)}) \right) \right), \\ \frac{\hat{e}_p^{(k+1)}}{\Delta t} &= \nabla_h \cdot \left(\check{\mathcal{M}}_p^m \nabla_h \left(\ln p^{m+1} - \ln p^{(k)} - \frac{p^{(k+1)} - p^{(k)}}{p^{(k)}} + (-\Delta_h)^{-1}(\hat{e}_p^{(k)} - \hat{e}_n^{(k)}) \right) \right). \end{aligned} \quad (3.12)$$

In fact, such an error system could be rewritten as

$$\begin{aligned} \frac{1}{\Delta t} \mathcal{L}_{\check{\mathcal{M}}_n^m}(\hat{e}_n^{(k+1)}) + \ln n^{m+1} - \ln n^{(k)} - \frac{n^{(k+1)} - n^{(k)}}{n^{(k)}} + (-\Delta_h)^{-1}(\hat{e}_n^{(k)} - \hat{e}_p^{(k)}) &= 0, \\ \frac{1}{\Delta t} \mathcal{L}_{\check{\mathcal{M}}_p^m}(\hat{e}_p^{(k+1)}) + \ln p^{m+1} - \ln p^{(k)} - \frac{p^{(k+1)} - p^{(k)}}{p^{(k)}} + (-\Delta_h)^{-1}(\hat{e}_p^{(k)} - \hat{e}_n^{(k)}) &= 0. \end{aligned} \quad (3.13)$$

Next we look at the first equation in (3.13), the error equation for $\hat{e}_n^{(k+1)}$. An application of Taylor’s Theorem reveals that

$$\ln n^{m+1} - \ln n^{(k)} = \frac{1}{\xi_n^{(k)}} \hat{e}_n^{(k)}, \quad (3.14)$$

for some $\xi_n^{(k)}$ between n^{m+1} and $n^{(k)}$ in a point-wise sense. Since $\xi_n^{(k)}$ is “between” n^{m+1} and $n^{(k)}$, we conclude that

$$|\xi_n^{(k)} - n^{(k)}| \leq |n^{m+1} - n^{(k)}| \leq |\hat{e}_n^{(k)}|,$$

so that

$$\|\xi_n^{(k)} - n^{(k)}\|_\infty \leq \|\hat{e}_n^{(k)}\|_\infty. \quad (3.15)$$

Because of the separation properties and upper bounds satisfied by both n^{m+1} and $n^{(k)}$ – see (2.33) and (3.11), respectively – the following estimate is valid for $\xi_n^{(k)}$:

$$\frac{\epsilon_0}{4} \leq \xi_n^{(k)} \leq C_5 + 1, \quad \text{at a point-wise level.} \quad (3.16)$$

Meanwhile, for the term $n^{(k+1)} - n^{(k)}$, we have

$$n^{(k+1)} - n^{(k)} = (n^{m+1} - \hat{e}_n^{(k+1)}) - (n^{m+1} - \hat{e}_n^{(k)}) = -(\hat{e}_n^{(k+1)} - \hat{e}_n^{(k)}). \quad (3.17)$$

Therefore, the error equation for $\hat{e}_n^{(k+1)}$ could be reformulated as

$$\frac{1}{\Delta t} \mathcal{L}_{\mathcal{M}_n^m}(\hat{e}_n^{(k+1)}) + \frac{1}{\xi_n^{(k)}} \hat{e}_n^{(k)} + \frac{\hat{e}_n^{(k+1)} - \hat{e}_n^{(k)}}{n^{(k)}} + (-\Delta_h)^{-1}(\hat{e}_n^{(k)} - \hat{e}_p^{(k)}) = 0. \quad (3.18)$$

The two nonlinear iteration error terms can be rewritten as

$$\frac{1}{\xi_n^{(k)}} \hat{e}_n^{(k)} + \frac{\hat{e}_n^{(k+1)} - \hat{e}_n^{(k)}}{n^{(k)}} = \frac{n^{(k)} - \xi_n^{(k)}}{\xi_n^{(k)} n^{(k)}} \hat{e}_n^{(k)} + \frac{\hat{e}_n^{(k+1)}}{n^{(k)}}. \quad (3.19)$$

Next, define

$$\zeta_n^{(k)} := \frac{n^{(k)} - \xi_n^{(k)}}{\xi_n^{(k)}}.$$

Then, the point-wise inequality (3.15) implies that

$$|\zeta_n^{(k)}| = \frac{|n^{(k)} - \xi_n^{(k)}|}{\xi_n^{(k)}} \leq \frac{|\hat{e}_n^{(k)}|}{\xi_n^{(k)}} \leq 4\epsilon_0^{-1} |\hat{e}_n^{(k)}|, \quad (3.20)$$

in which the bound (3.16) has been applied in the last step. Going back (3.18), we get

$$\frac{1}{\Delta t} \mathcal{L}_{\mathcal{M}_n^m}(\hat{e}_n^{(k+1)}) + \frac{\hat{e}_n^{(k+1)}}{n^{(k)}} = -\frac{\zeta_n^{(k)}}{n^{(k)}} \hat{e}_n^{(k)} + (-\Delta_h)^{-1}(\hat{e}_n^{(k)} - \hat{e}_p^{(k)}). \quad (3.21)$$

Next, taking a discrete inner product of (3.21) with $\hat{e}_n^{(k+1)}$ gives

$$\frac{1}{\Delta t} \|\hat{e}_n^{(k+1)}\|_{\mathcal{L}_{\mathcal{M}_n^m}^{-1}}^2 + \left\langle \frac{1}{n^{(k)}}, (\hat{e}_n^{(k+1)})^2 \right\rangle_\Omega = - \left\langle \frac{\zeta_n^{(k)}}{n^{(k)}}, \hat{e}_n^{(k)} \hat{e}_n^{(k+1)} \right\rangle_\Omega + \langle \hat{e}_n^{(k+1)}, \hat{e}_n^{(k)} - \hat{e}_p^{(k)} \rangle_{-1,h}. \quad (3.22)$$

For the first term on the left hand side, an application of Lemma 2.2 reveals that

$$\|\hat{e}_n^{(k+1)}\|_{\mathcal{L}_{\mathcal{M}_n^m}^{-1}}^2 \geq \frac{\epsilon_0}{2C_5^2} \|\hat{e}_n^{(k+1)}\|_{-1,h}^2, \quad (3.23)$$

with the estimate (2.33) applied. The lower bound of the nonlinear inner product on the left hand side could be obtained with the help of the a-priori assumption (3.11):

$$\left\langle \frac{1}{n^{(k)}}, (\hat{e}_n^{(k+1)})^2 \right\rangle_\Omega \geq \frac{1}{C_5 + 1} \|\hat{e}_n^{(k+1)}\|_{-1,h}^2. \quad (3.24)$$

For the term associated with the electric potential, a direct application of the Cauchy–Schwarz and Young inequalities gives

$$\begin{aligned} \langle \hat{e}_n^{(k+1)}, \hat{e}_n^{(k)} - \hat{e}_p^{(k)} \rangle_{-1,h} &\leq \|\hat{e}_n^{(k+1)}\|_{-1,h} \cdot \|\hat{e}_n^{(k)} - \hat{e}_p^{(k)}\|_{-1,h} \\ &\leq \frac{\epsilon_0}{4C_5^2 \Delta t} \|\hat{e}_n^{(k+1)}\|_{-1,h}^2 + C_5^2 \epsilon_0^{-1} \Delta t \|\hat{e}_n^{(k)} - \hat{e}_p^{(k)}\|_{-1,h}^2. \end{aligned} \quad (3.25)$$

For the nonlinear error inner product on the right hand side of (3.22), a more careful calculation reveals that

$$\begin{aligned} -\left\langle \frac{\zeta_n^{(k)}}{n^{(k)}}, \hat{e}_n^{(k)} \hat{e}_n^{(k+1)} \right\rangle_{\Omega} &\leq \frac{1}{2} \left\langle \frac{1}{n^{(k)}}, (\hat{e}_n^{(k+1)})^2 \right\rangle_{\Omega} + \frac{1}{2} \left\langle \frac{1}{n^{(k)}}, (\zeta_n^{(k)})^2 (\hat{e}_n^{(k)})^2 \right\rangle_{\Omega} \\ &\leq \frac{1}{2} \left\langle \frac{1}{n^{(k)}}, (\hat{e}_n^{(k+1)})^2 \right\rangle_{\Omega} + \frac{1}{2} \cdot 4\epsilon_0^{-1} \cdot 16\epsilon_0^{-2} \|\hat{e}_n^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_n^{(k)}\|_2^2 \\ &\leq \frac{1}{2} \left\langle \frac{1}{n^{(k)}}, (\hat{e}_n^{(k+1)})^2 \right\rangle_{\Omega} + 32\epsilon_0^{-3} \|\hat{e}_n^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_n^{(k)}\|_2^2. \end{aligned} \quad (3.26)$$

Therefore, a substitution of (3.23)–(3.26) into (3.22) leads to

$$\begin{aligned} \frac{\epsilon_0}{4C_5^2 \Delta t} \|\hat{e}_n^{(k+1)}\|_{-1,h}^2 + \frac{1}{2(C_5 + 1)} \|\hat{e}_n^{(k+1)}\|_2^2 \\ \leq C_5^2 \epsilon_0^{-1} \Delta t \|\hat{e}_n^{(k)} - \hat{e}_p^{(k)}\|_{-1,h}^2 + 32\epsilon_0^{-3} \|\hat{e}_n^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_n^{(k)}\|_2^2. \end{aligned} \quad (3.27)$$

Similarly, the second equation in (3.13), the error equation for $\hat{e}_p^{(k+1)}$, could be reformulated as

$$\frac{1}{\Delta t} \mathcal{L}_{\mathcal{M}_p^m}(\hat{e}_p^{(k+1)}) + \frac{1}{\xi_p^{(k)}} \hat{e}_p^{(k)} + \frac{\hat{e}_p^{(k+1)} - \hat{e}_p^{(k)}}{p^{(k)}} + (-\Delta_h)^{-1}(\hat{e}_p^{(k)} - \hat{e}_n^{(k)}) = 0, \quad (3.28)$$

where $\xi_p^{(k)}$ is between p^{m+1} and $p^{(k)}$ and satisfies

$$|\zeta_p^{(k)}| \leq 4\epsilon_0^{-1} |\hat{e}_p^{(k)}|.$$

The error equation for p can be further rewritten as

$$\frac{1}{\Delta t} \mathcal{L}_{\mathcal{M}_p^m}(\hat{e}_p^{(k+1)}) + \frac{\hat{e}_p^{(k+1)}}{p^{(k)}} = -\frac{\zeta_p^{(k)}}{p^{(k)}} \hat{e}_p^{(k)} + (-\Delta_h)^{-1}(\hat{e}_p^{(k)} - \hat{e}_n^{(k)}). \quad (3.29)$$

In addition, taking a discrete inner product of (3.21) with $\hat{e}_p^{(k+1)}$, we are able to derive the following iteration error estimate

$$\begin{aligned} \frac{\epsilon_0}{4C_5^2 \Delta t} \|\hat{e}_p^{(k+1)}\|_{-1,h}^2 + \frac{1}{2(C_5 + 1)} \|\hat{e}_p^{(k+1)}\|_2^2 \\ \leq C_5^2 \epsilon_0^{-1} \Delta t \|\hat{e}_n^{(k)} - \hat{e}_p^{(k)}\|_{-1,h}^2 + 32\epsilon_0^{-3} \|\hat{e}_p^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_p^{(k)}\|_2^2. \end{aligned} \quad (3.30)$$

The technical details are left to interested readers. Finally, a combination of (3.27) and (3.30) yields

$$\begin{aligned} \frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(k+1)}\|_{-1,h}^2 + \|\hat{e}_p^{(k+1)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(k+1)}\|_2^2 + \|\hat{e}_p^{(k+1)}\|_2^2) \\ \leq 2C_5^2 \epsilon_0^{-1} \Delta t \|\hat{e}_n^{(k)} - \hat{e}_p^{(k)}\|_{-1,h}^2 + 32\epsilon_0^{-3} (\|\hat{e}_n^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_n^{(k)}\|_2^2 + \|\hat{e}_p^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_p^{(k)}\|_2^2) \\ \leq 4C_5^2 \epsilon_0^{-1} \Delta t (\|\hat{e}_n^{(k)}\|_{-1,h}^2 + \|\hat{e}_p^{(k)}\|_{-1,h}^2) + 32\epsilon_0^{-3} (\|\hat{e}_n^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_n^{(k)}\|_2^2 + \|\hat{e}_p^{(k)}\|_{\infty}^2 \cdot \|\hat{e}_p^{(k)}\|_2^2). \end{aligned} \quad (3.31)$$

3.1. Iteration stage 1: $k = 0$

At $k = 0$, we see that the preliminary error estimate (2.32) (for the exact solution of (2.8)–(2.11)) implies that

$$\|\hat{e}_n^{(0)}\|_{\infty} = \|n^{m+1} - n^m\|_{\infty} \leq C_3 \Delta t, \quad \|\hat{e}_p^{(0)}\|_{\infty} = \|p^{m+1} - p^m\|_{\infty} \leq C_3 \Delta t, \quad (3.32)$$

due to initializations $n^{m+1,(0)} = n^m$, $p^{m+1,(0)} = p^m$. A substitution of the last inequality into (3.31) leads to the following iteration error estimate for $k = 0$:

$$\begin{aligned} \frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(1)}\|_{-1,h}^2 + \|\hat{e}_p^{(1)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(1)}\|_2^2 + \|\hat{e}_p^{(1)}\|_2^2) \\ \leq 4C_5^2 \epsilon_0^{-1} \Delta t (\|\hat{e}_n^{(0)}\|_{-1,h}^2 + \|\hat{e}_p^{(0)}\|_{-1,h}^2) + 32C_3^2 \epsilon_0^{-3} \Delta t^2 (\|\hat{e}_n^{(0)}\|_2^2 + \|\hat{e}_p^{(0)}\|_2^2). \end{aligned} \quad (3.33)$$

Consequently, we get inequality (3.8), by taking

$$C_6 = \max(16C_5^4 \epsilon_0^{-2}, 64C_3^2(C_5 + 1)\epsilon_0^{-3}).$$

3.2. Iteration stage 2: $k = 1$

The iteration error estimate (3.8) for $k = 0$ indicates that

$$\begin{aligned} F^{(1)} &= \frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(1)}\|_{-1,h}^2 + \|\hat{e}_p^{(1)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(1)}\|_2^2 + \|\hat{e}_p^{(1)}\|_2^2) \\ &\leq C_6 \Delta t^2 F^{(0)} \\ &\leq C_9 C_6 \Delta t^4, \end{aligned} \quad (3.34)$$

since $F^{(0)} \leq C_9 \Delta t^2$, which comes from the preliminary error estimate (3.32). Therefore,

$$\|\hat{e}_n^{(1)}\|_2, \|\hat{e}_p^{(1)}\|_2 \leq C_{10} \Delta t^2, \quad C_{10} := (2C_9 C_6 (C_5 + 1))^{1/2}. \quad (3.35)$$

Subsequently, an application of an inverse inequality gives

$$\|\hat{e}_n^{(1)}\|_\infty \leq \frac{C \|\hat{e}_n^{(1)}\|_2}{h^{3/2}} \leq \frac{CC_{10} \Delta t^2}{h^{3/2}} \leq C_{11} \Delta t^{1/2}, \quad \|\hat{e}_p^{(1)}\|_\infty \leq C_{11} \Delta t^{1/2}, \quad (\text{similarly}), \quad (3.36)$$

with $C_{11} = CC_{10}$, where the linear refinement constraint, $C_1 h \leq \Delta t \leq C_2 h$, has been applied. A substitution of the last inequalities into (3.31) leads to the following iteration error estimate for $k = 1$:

$$\begin{aligned} &\frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(2)}\|_{-1,h}^2 + \|\hat{e}_p^{(2)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(2)}\|_2^2 + \|\hat{e}_p^{(2)}\|_2^2) \\ &\leq 4C_5^2 \epsilon_0^{-1} \Delta t (\|\hat{e}_n^{(1)}\|_{-1,h}^2 + \|\hat{e}_p^{(1)}\|_{-1,h}^2) + 32C_{11}^2 \epsilon_0^{-3} \Delta t (\|\hat{e}_n^{(1)}\|_2^2 + \|\hat{e}_p^{(1)}\|_2^2), \end{aligned} \quad (3.37)$$

so that inequality (3.9) is valid, by taking

$$C_7 = \max(16C_5^4 \epsilon_0^{-2}, 64C_{11}^2 (C_5 + 1) \epsilon_0^{-3}).$$

3.3. Iteration stage 3: $k = 2$

The iteration error estimate (3.9) for $k = 1$ indicates that

$$\begin{aligned} F^{(2)} &= \frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(2)}\|_{-1,h}^2 + \|\hat{e}_p^{(2)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(2)}\|_2^2 + \|\hat{e}_p^{(2)}\|_2^2) \\ &\leq C_7 \Delta t F^{(1)} \\ &\leq C_9 C_6 C_7 \Delta t^5. \end{aligned} \quad (3.38)$$

Therefore,

$$\|\hat{e}_n^{(2)}\|_2, \|\hat{e}_p^{(2)}\|_2 \leq C_{12} \Delta t^{5/2}, \quad C_{12} = (2(C_5 + 1)C_9 C_6 C_7)^{1/2}. \quad (3.39)$$

In turn, an application of an inverse inequality leads to

$$\|\hat{e}_n^{(2)}\|_\infty \leq \frac{C \|\hat{e}_n^{(2)}\|_2}{h^{3/2}} \leq \frac{CC_{12} \Delta t^{5/2}}{h^{3/2}} \leq C_{13} \Delta t, \quad \|\hat{e}_p^{(2)}\|_\infty \leq C_{13} \Delta t, \quad (\text{similar argument}), \quad (3.40)$$

with $C_{13} = CC_{12}$. A substitution of the last inequalities into (3.31) leads to the following iteration error estimate for $k = 2$:

$$\begin{aligned} &\frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(3)}\|_{-1,h}^2 + \|\hat{e}_p^{(3)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(3)}\|_2^2 + \|\hat{e}_p^{(3)}\|_2^2) \\ &\leq 4C_5^2 \epsilon_0^{-1} \Delta t (\|\hat{e}_n^{(2)}\|_{-1,h}^2 + \|\hat{e}_p^{(2)}\|_{-1,h}^2) + 32C_{13}^2 \epsilon_0^{-3} \Delta t^2 (\|\hat{e}_n^{(2)}\|_2^2 + \|\hat{e}_p^{(2)}\|_2^2), \end{aligned} \quad (3.41)$$

so that inequality (3.10) is valid, by taking

$$C_8 = \max(16C_5^4 \epsilon_0^{-2}, 64C_{13}^2 (C_5 + 1) \epsilon_0^{-3}).$$

3.4. Higher iteration stages: $k \geq 3$

Assume that inequality (3.10) is valid up to the $k - 1$ st stage. Then we get

$$\begin{aligned} F^{(k)} &= \frac{\epsilon_0}{4C_5^2 \Delta t} (\|\hat{e}_n^{(k)}\|_{-1,h}^2 + \|\hat{e}_p^{(k)}\|_{-1,h}^2) + \frac{1}{2(C_5 + 1)} (\|\hat{e}_n^{(k)}\|_2^2 + \|\hat{e}_p^{(k)}\|_2^2) \\ &\leq C_8 \Delta t^2 F^{(k-1)} \\ &\leq \tilde{C} C_6 C_7 C_8 \Delta t^7 \\ &\leq \Delta t^6. \end{aligned} \quad (3.42)$$

Therefore,

$$\|\hat{e}_n^{(k)}\|_2, \|\hat{e}_p^{(k)}\|_2 \leq \Delta t^3. \quad (3.43)$$

provided that Δt is sufficiently small. In turn, an application of an inverse inequality leads to

$$\|\hat{e}_n^{(k)}\|_\infty \leq \frac{C\|\hat{e}_n^{(k)}\|_2}{h^{3/2}} \quad \|\hat{e}_p^{(k)}\|_\infty \leq \Delta t, \quad (\text{similar argument}). \quad (3.44)$$

Again, a substitution of the last inequalities into (3.31) leads to the following iteration error estimate for $k \geq 3$:

$$\begin{aligned} & \frac{\epsilon_0}{4C_5^2\Delta t}(\|\hat{e}_n^{(k+1)}\|_{-1,h}^2 + \|\hat{e}_p^{(k+1)}\|_{-1,h}^2) + \frac{1}{2(C_5+1)}(\|\hat{e}_n^{(k+1)}\|_2^2 + \|\hat{e}_p^{(k+1)}\|_2^2) \\ & \leq 4C_5^2\epsilon_0^{-1}\Delta t(\|\hat{e}_n^{(k)}\|_{-1,h}^2 + \|\hat{e}_p^{(k)}\|_{-1,h}^2) + 32\epsilon_0^{-3}\Delta t^2(\|\hat{e}_n^{(k)}\|_2^2 + \|\hat{e}_p^{(k)}\|_2^2), \end{aligned} \quad (3.45)$$

so that inequality (3.10) is valid for $k \geq 3$, by taking

$$C_8 = \max(16C_5^4\epsilon_0^{-2}, 64(C_5+1)\epsilon_0^{-3}).$$

Finally, we observe that the a-priori assumption (3.11) can be recovered at the next iteration stage, by applying the $\|\cdot\|_\infty$ iteration error estimate (3.36), (3.40) and (3.44):

$$\begin{aligned} n^{(k+1)} & \geq n^{m+1} - |\hat{e}_n^{(k+1)}| \geq \frac{\epsilon_0}{2} - \frac{\epsilon_0}{4} = \frac{\epsilon_0}{4}, \\ n^{(k+1)} & \leq n^{m+1} + |\hat{e}_n^{(k+1)}| \leq C_5 + 1, \\ \frac{\epsilon_0}{4} & \leq p^{(k+1)} \leq C_5 + 1, \quad (\text{similar argument}), \end{aligned} \quad (3.46)$$

for $k = 0, k = 1$ and $k \geq 2$, provided that Δt and h are sufficiently small. This finishes the proof of Theorem 3.1. $\square$

Remark 3.1. From the above iteration convergence analysis, we see that

$$\|\hat{e}_n^{(0)}\|_2 = O(\Delta t), \quad \|\hat{e}_n^{(1)}\|_2 = O(\Delta t^2), \quad \|\hat{e}_n^{(2)}\|_2 = O(\Delta t^{5/2}), \quad \|\hat{e}_n^{(k)}\|_2 = O(\Delta t^{k+1/2}), \quad (k \geq 3), \quad (3.47)$$

so that the convergence is at least linear, with convergence rate in the order of $O(\Delta t)$. Extensive numerical experiments have demonstrated that, only four to five iteration stages are needed to achieve a near-machine error precision at each time step. In addition, each iteration stage corresponds to a non-constant coefficient elliptic solver, with the computational cost comparable to the standard Poisson solver. Therefore, the proposed iteration algorithm turns out to be a very efficient solver to implement the numerical scheme (2.8)–(2.11).

Remark 3.2. In the iteration algorithm (3.1), we treat the electric potential part explicitly in the iteration, to avoid a coupling. This approach leads to a linear convergence, with convergence rate of order $O(\Delta t)$, as stated in Theorem 3.1. Meanwhile, if such a term is treated implicitly in the iteration (which leads to a coupled system), the iteration convergence order could be further improved. In fact, a careful analysis reveals the following estimate, if the electric potential part is treated implicitly:

$$\frac{1}{2(C_5+1)}(\|\hat{e}_n^{(k+1)}\|_2^2 + \|\hat{e}_p^{(k+1)}\|_2^2) \leq 32\epsilon_0^{-3}(\|\hat{e}_n^{(k)}\|_\infty^2 \cdot \|\hat{e}_n^{(k)}\|_2^2 + \|\hat{e}_p^{(k)}\|_\infty^2 \cdot \|\hat{e}_p^{(k)}\|_2^2).$$

This estimate corresponds to a quadratic convergence order in the standard Newton iteration, i.e. $\hat{e}^{(k+1)} \approx C(\hat{e}^k)^2$, a faster convergence order than the one given by (3.10). However, a coupled system has to be solved in this approach, and the numerical experiments have demonstrated great efficiency advantages of the proposed iteration algorithm (3.1) over this approach.

4. Numerical test for the iteration solver

We perform a 2-D numerical test to demonstrate the convergence rate of the iteration algorithm (3.1). The computational box, taken as $\Omega = (0, 1)^2$, is covered by a uniform mesh with $h = 0.02$, and the time step size is chosen as $\Delta t = h$. We consider the following exact solution

$$\begin{cases} n = e^{-t} \sin(2\pi x) \cos(2\pi y) + 2, \\ p = e^{-t} \cos(2\pi x) \sin(2\pi y) + 2, \\ \psi = e^{-t} \sin(2\pi x) \sin(2\pi y), \end{cases} \quad (4.1)$$

to the PNP system (1.4)–(1.6) with additional source terms in the NP equations. The source terms and the initial conditions are determined by the known exact solution. In fact, such a test function has been used in the existing work [8] to verify the accuracy of the numerical scheme (2.8)–(2.11), and the expected numerical accuracy in both temporal and spatial

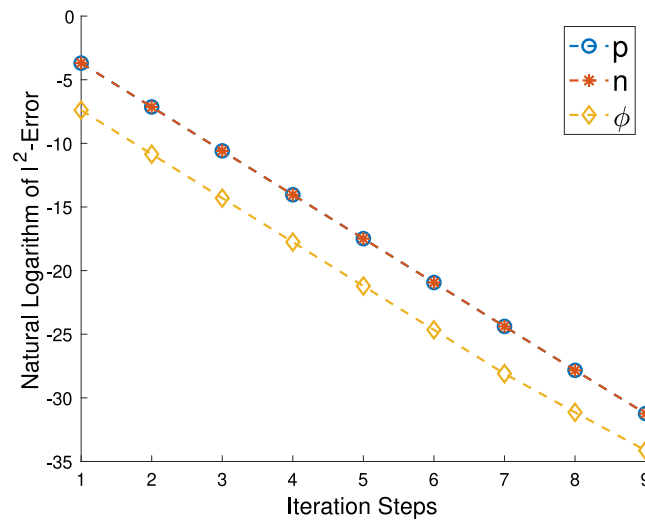


Fig. 1. Logarithmic plot of ℓ^2 -errors of p , n , and ϕ vs. iteration stages.

discretization has been reported. In this section, we focus on the convergence rate of the iteration solver (3.1) for the nonlinear discretization scheme (2.8)–(2.11).

In this test, we only focus on solving the nonlinear discretization scheme for a single time step, i.e., the first time step, and take the converged numerical solution as the reference solution. For each iteration stage, the iteration solution is compared with the reference solution. Fig. 1 displays the logarithmic plot of the ℓ^2 -error for p , n , and ϕ vs. the iteration stages. It is obvious that the natural logarithm of the ℓ^2 -error decreases linearly against the iteration stages, which demonstrates a linear convergence rate of the iteration algorithm (3.1) (as stated in Theorem 3.1). Therefore, this numerical test has verified the theoretical result of the linear convergence rate for the proposed iteration solver.

5. Concluding remarks

An iteration solver is proposed and analyzed for a finite difference scheme for the Poisson–Nernst–Planck (PNP) system, formulated in the Energetic Variational Approach (EnVarA). In the given numerical scheme, the mobility concentration function is explicitly treated to ensure the unique solvability, while both the logarithmic and the electric potential diffusion terms are treated implicitly, because of their convex natures. The positivity-preserving property for both concentrations, an unconditional energy stability, and the optimal rate error estimate have been established in a recent work. In this article, an iteration solver is proposed to implement the numerical scheme, which includes a modified Newton iteration for the nonlinear and logarithmic part, combined with a linear iteration for the electric potential part. In turn, a linear elliptic equation, in the divergence form, needs to be solved at each iteration stage. A linear convergence analysis is provided for the proposed iteration algorithm, under the separation assumption for the exact PDE solution and the numerical solution at each iteration stage. The positivity of both concentration variables at each iteration stage is crucial to ensure the well-posed property of the elliptic system. With the help of the uniform distance between the numerical solutions and the singular limit value, the singularity issue associated with the logarithmic term could be avoided in the iteration analysis, and the convex nature of the logarithmic energy functional will lead to a well-posed nonlinear error at each iteration stage. Finally, a linear convergence analysis is reported for the proposed iteration process, with convergence rate in the same order of the time step size. It will be the first such result for the highly nonlinear and singular PNP system. In addition, a numerical test has also demonstrated the linear convergence rate of the proposed iteration solver.

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