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Efficient Time-Stepping/Spectral Methods for the Navier-Stokes-Nernst-Planck-Poisson Equations

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Abstract. This paper is concerned with numerical methods for the Navier-Stokes-Nernst-Planck-Poisson equation system. The main goal is to construct and analyze some stable time stepping schemes for the time discretization and use a spectral method for the spatial discretization. The main contribution of the paper includes: 1) an useful stability inequality for the weak solution is derived; 2) a first order time stepping scheme is constructed, and the non-negativity of the concentration components of the discrete solution is proved. This is an important property since the exact solution shares the same property. Moreover, the stability of the scheme is established, together with a stability condition on the time step size; 3) a modified first order scheme is proposed in order to decouple the calculation of the velocity and pressure in the fluid field. This new scheme equally preserves the non-negativity of the discrete concentration solution, and is stable under a similar stability condition; 4) a stabilization technique is introduced to make the above mentioned schemes stable without restriction condition on the time step size; 5) finally we construct a second order finite difference scheme in time and spectral discretization in space. The numerical tests carried out in the paper show that all the proposed schemes possess some desirable properties, such as conditionally/unconditionally stability, first/second order convergence, non-negativity of the discrete concentrations, and so on.

AMS subject classifications: 76M10, 76M22, 65M12

Key words: Navier-Stokes-Nernst-Planck-Poisson equations, stabilized finite difference schemes, spectral method.

1 Introduction

The Navier-Stokes-Nernst-Planck-Poisson (NSNPP) equations play role in both physical chemical modelling and electrohydrodynamic model. It has been frequently used to

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model the interactive behavior of charged colloidal particles, electro-hydro, and micro-/nano-fluidic dynamics. In collochemistry, precise description of the aggregation, separation, and sedimentation of charged colloidal particles is needed. In some application fields, there is need to design micro-/nano-fluidic devices to control the separation, mixing and pumping of some specific substances. Suitable computational models can be useful in a better understanding of the electrokinetic phenomena occurring in such applications, and thus helpful to improve the design of related devices.

Electrokinetic phenomena are a family of several different effects that occur in heterogeneous fluids, or in porous bodies filled with fluid, or in a fast flow over a flat surface. These phenomena were first observed by Reuss [12] in 1809, which is now known as electroosmosis or electrophoresis, depending on different generation mechanism of electrokinetic flows. The electric double layer (EDL) is the common source of the two phenomena. For the detail of the phenomena, one can refer to [8,9]. Applying the electrokinetic effect, the movement of fluid and dispersed particles can be controlled by electric field without other moving parts. The results of these theories have many applications in industry, such as dehydration and purification of certain materials, isolation and identification of enzyme, protein and virus, drug delivery, desalination, and membrane filtration. In addition, it can also be used to improve the performance and service life of lithium cell and other fuel cell.

Several models describing the electrokinetic flows have been used in the past. Poisson-Boltzmann equation describes the EDL system for the net charge distribution. Applying the thin double layer limit by asymptotic analysis, the EDL can also be modelled by the Nernst-Planck-Poisson equation [1]. As compared to the above two models, the incompressible Navier-Stokes-Nernst-Planck-Poisson equation set (NSNPP) is a more general model to describe the electrokinetic flows [9, 14]. It combines three parts: (1) Navier-Stokes equations modelling the movement of the fluid field under the action of the internal and external electric fields; (2) Nernst-Planck equations for the positive and negative ionic-densities; (3) Poisson equation for the internal potential. Schmuck [13] analyzed the well-posedness of the NSNPP system, and proved the existence and uniqueness of the solution when the domain is open bounded and convex in $\mathbb{R}^d$ for $d=2,3$. Deng et al. [3] established the well-posedness of the NSNPP system in spatio-temporal unbounded domain. In recent years, several numerical methods have been proposed to solve this couple system. Yang et al. [18] applied artificial compressibility method and approximated the system by a finite difference/alternative direction method. Tsai et al. [16] employed this method in capillary electrophoresis microchips, and tested some injection systems with different configurations. Valencia et al. [17] combined the operator-splitting and finite element method for the numerical solution in some limit cases. Prohl and Schmuck [10] used finite element method for spatial discretization and an implicit temporal discrete scheme which preserves non-negativity of the ionic concentrations. They also considered a Chorin's type projection method, which is easier-to-implement, but does not preserve physically relevant properties.

In this paper, we aim at proposing and analyzing some efficient methods for numer-

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ical solutions of the NSNPP equations. The main ingredient of the work includes: (1) investigate the weak form of the problem and derive some stability properties for the weak solution; (2) construct several time stepping schemes, and demonstrate some different properties, such as non-negativity of the discrete concentrations, stability condition, or unconditional stability; (3) propose a fully discrete approach based on the spectral method for the spatial discretization and a semi-implicit second order difference scheme for the temporal discretization; (4) a series of numerical tests to validate the proposed methods and confirm the analytical results.

2 Model problem

Let Ω be a bounded domain in $\mathbb{R}^2$. The boundary of Ω, denoted by $\partial\Omega$, is Lipschitz continuous. Given the potential of the external electric field $\Psi_1(\boldsymbol{x},t)$ in $\Omega\times(0,T]$, $T>0$, and the initial conditions $\boldsymbol{u}(\boldsymbol{x},0)=\boldsymbol{u}_0(\boldsymbol{x})$, $n^+(\boldsymbol{x},0)=n_0^+(\boldsymbol{x})$, $n^-(\boldsymbol{x},0)=n_0^-(\boldsymbol{x})$, we consider the following Navier-Stokes-Nernst-Planck-Poisson equations (NSNPP equation for short): find $\boldsymbol{u}(\boldsymbol{x},t)$, $p(\boldsymbol{x},t)$,$n^+(\boldsymbol{x},t)$, $n^-(\boldsymbol{x},t)$, and $\Psi_0(\boldsymbol{x},t)$, such that

$$\frac{\partial \boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}-\triangle\boldsymbol{u}+\nabla p+(n^+-n^-)\nabla\Psi=0, \qquad \text{in } \Omega\times(0,T), \tag{2.1a}$$

$$\nabla\cdot\boldsymbol{u}=0, \qquad \text{in } \Omega\times(0,T), \tag{2.1b}$$

$$\boldsymbol{u}=0, \qquad \text{on } \partial\Omega\times(0,T), \tag{2.1c}$$

$$\frac{\partial n^+}{\partial t}-\nabla\cdot(n^+\nabla\Psi)-\triangle n^++(\boldsymbol{u}\cdot\nabla)n^+=0, \qquad \text{in } \Omega\times(0,T), \tag{2.2a}$$

$$-n^+\frac{\partial\Psi}{\partial\boldsymbol{n}}-\frac{\partial n^+}{\partial\boldsymbol{n}}+n^+(\boldsymbol{u}\cdot\boldsymbol{n})=0, \qquad \text{on } \partial\Omega\times(0,T), \tag{2.2b}$$

$$\frac{\partial n^-}{\partial t}+\nabla\cdot(n^-\nabla\Psi)-\triangle n^-+(\boldsymbol{u}\cdot\nabla)n^-=0, \qquad \text{in } \Omega\times(0,T), \tag{2.2c}$$

$$n^-\frac{\partial\Psi}{\partial\boldsymbol{n}}-\frac{\partial n^-}{\partial\boldsymbol{n}}+n^-(\boldsymbol{u}\cdot\boldsymbol{n})=0, \qquad \text{on } \partial\Omega\times(0,T), \tag{2.2d}$$

$$-\triangle\Psi_0=n^+-n^-, \qquad \text{in } \Omega\times(0,T), \tag{2.3a}$$

$$\frac{\partial\Psi_0}{\partial\boldsymbol{n}}=0, \qquad \text{on } \partial\Omega\times(0,T), \tag{2.3b}$$

where $\boldsymbol{u}$ is the velocity of the fluid field, p is the pressure of the flow, n^+ and n^- are the concentration of positive and negative ions respectively. $\Psi=\Psi_0+\Psi_1$ is the sum of the internal and external electrostatic potentials. In the above system, Eq. (2.1) is the Navier-Stokes equations modified to take into account of the electrical force generated by the interaction between the ionic concentration and the electric potential field. In the absence of chemical reactions, the ionic concentration distribution is described by Eq. (2.2), which is usually called the Nernst-Planck equations. The third part of the NSNPP equations, i.e., Eq. (2.3), is the Poisson equation, which determines the internal potential in the domain

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of interest through the charged particles. Without loss of generality, we only consider the problem without external electric field $\Psi_1 \equiv 0$. That is $\Psi = \Psi_0$.

We consider the variational formulation of the NSNPP problem (2.1)-(2.3) as follows: given $\boldsymbol{u}_0(\boldsymbol{x}) \in L^2(\Omega)^2$, $n_0^+(\boldsymbol{x})$, $n_0^-(\boldsymbol{x}) \in L^2(\Omega)$, which satisfy $\nabla \cdot \boldsymbol{u}_0 = 0$ in Ω, $\boldsymbol{u}_0 = 0$ on $\partial\Omega$, and $n_0^+(\boldsymbol{x}) - n_0^-(\boldsymbol{x}) \in L_0^2(\Omega)$, find $\boldsymbol{u}(\boldsymbol{x},t) \in H_0^1(\Omega)^2$, $p(\boldsymbol{x},t) \in L_0^2(\Omega)$, $n^{\pm}(\boldsymbol{x},t) \in L^2(\Omega)$, $\Psi(\boldsymbol{x},t) \in H^1(\Omega) \cap L_0^2(\Omega)$, such that $\boldsymbol{u}(\boldsymbol{x},0) = \boldsymbol{u}_0(\boldsymbol{x})$, $\boldsymbol{n}^{\pm}(\boldsymbol{x},0) = n_0^{\pm}(\boldsymbol{x})$, and for all $t \in (0,T]$,

$$\left(\frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{\varphi}\right) + (\boldsymbol{u} \cdot \nabla \boldsymbol{u}, \boldsymbol{\varphi}) + (\nabla \boldsymbol{u}, \nabla \boldsymbol{\varphi}) - (p, \nabla \cdot \boldsymbol{\varphi}) + \left((n^+ - n^-)\nabla \Psi, \boldsymbol{\varphi}\right) = 0, \quad \forall \boldsymbol{\varphi} \in H_0^1(\Omega)^2, \tag{2.4a}$$

$$-(q, \nabla \cdot \boldsymbol{u}) = 0, \quad \forall q \in L^2(\Omega), \tag{2.4b}$$

$$\left(\frac{\partial n^+}{\partial t}, v\right) + (\nabla \Psi n^+, \nabla v) + (\nabla n^+, \nabla v) - (\boldsymbol{u} n^+, \nabla v) = 0, \qquad \forall v \in H^1(\Omega), \tag{2.5a}$$

$$\left(\frac{\partial n^-}{\partial t}, w\right) - (\nabla \Psi n^-, \nabla w) + (\nabla n^-, \nabla w) - (\boldsymbol{u} n^-, \nabla w) = 0, \qquad \forall w \in H^1(\Omega), \tag{2.5b}$$

$$(\nabla \Psi, \nabla \psi) = (n^+ - n^-, \psi), \quad \forall \psi \in H^1(\Omega) \cap L_0^2(\Omega). \tag{2.6}$$

It has been proved in [13] that the weak problem (2.4)-(2.6) is well-posed, and the solution satisfies:

$$\boldsymbol{u} \in L^2(0,T; H_0^1(\Omega)^2) \cap L^\infty(0,T; L^2(\Omega)^2), \qquad p \in L^2(0,T; L_0^2(\Omega)),$$
$$n^{\pm} \in L^2(0,T; H^1(\Omega)) \cap L^\infty(0,T; L^2(\Omega)), \qquad \Psi \in L^2(0,T; H^2(\Omega) \cap L_0^2(\Omega)) \cap L^\infty(0,T; H^1(\Omega)).$$

The following lemma was also given in [13], which will be found useful in proving the stability of the weak solution of (2.4)-(2.6).

Lemma 2.1. *If the initial condition $n_0^{\pm}$ is non-negative almost everywhere in Ω, then $n^{\pm}(\boldsymbol{x},t) \geq 0$ a.e. $\boldsymbol{x} \in \Omega$, $t \in [0,T]$.*

Remark 2.1. Note that the compatibility condition of the solution of (2.4)-(2.6) is preserved, i.e.,

$$\int_\Omega \left(n^+(\boldsymbol{x},t) - n^-(\boldsymbol{x},t)\right) d\boldsymbol{x} = 0, \ \forall t \in (0,T]. \tag{2.7}$$

In fact, taking $v = 1$, $w = -1$ in (2.5) and summing them up gives immediately:

$$\frac{d}{dt} \int_\Omega \left(n^+(\boldsymbol{x},t) - n^-(\boldsymbol{x},t)\right) d\boldsymbol{x} = 0.$$

Remark 2.2. From the classical theory of Poisson equation; see, e.g., [5, 6, 11], it is well known that for $f \in H^{-1}(\Omega) \cap L_0^2(\Omega)$, the solution $\phi \in H^1(\Omega) \cap L_0^2(\Omega)$ of the problem

$$(\nabla \phi, \nabla \psi) = (f, \psi), \quad \forall \psi \in H^1(\Omega) \cap L_0^2(\Omega) \tag{2.8}$$

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belongs to the space $H^2(\Omega)$, and there is a constant $C_p(\Omega)$, such that

$$\|\phi\|_1 \leq C_p \|f\|_0. \tag{2.9}$$

Moreover, ϕ is also the solution of the following problem:

$$\begin{aligned} -\Delta\phi &= f, \quad \text{in } \Omega, \\ \frac{\partial\phi}{\partial \boldsymbol{n}} &= 0, \quad \text{on } \partial\Omega. \end{aligned}$$

Therefore it is not hard to verify that Eq. (2.8) holds for all test function $\psi \in W^{1,\frac{4}{3}}(\Omega)$.

Lemma 2.2. *If $\boldsymbol{u} \in H^1(\Omega)^2$, $\nabla\cdot\boldsymbol{u} = 0$ a.e. in Ω, and $\boldsymbol{u}\cdot\boldsymbol{n} = 0$ on $\partial\Omega$, then the following identity holds,*

$$(\boldsymbol{u}\cdot\nabla v, v) = 0, \quad \forall v \in H^1(\Omega).$$

Proof. Applying integration by parts, we have, $\forall v \in H^1(\Omega)$,

$$\begin{aligned} (\boldsymbol{u}\cdot\nabla v, v) &= -(\nabla\cdot(v\boldsymbol{u}), v) + \int_{\partial\Omega} v^2 \boldsymbol{u}\cdot\boldsymbol{n} \\ &= -(v\nabla\cdot\boldsymbol{u}, v) - (\boldsymbol{u}\cdot\nabla v, v) \\ &= -(\boldsymbol{u}\cdot\nabla v, v). \end{aligned}$$

Thus $(\boldsymbol{u}\cdot\nabla v, v) = 0$. □

Theorem 2.1. *Assume that the initial ionic concentrations $n_0^{\pm}$ are non-negative almost everywhere in Ω. Then the solution of the weak problem* (2.4)-(2.6) *satisfies the following stability inequalities: $\forall t \in (0,T)$,*

$$\|n^+(t)\|_0^2 + \|n^-(t)\|_0^2 + 2\int_0^t \left(\|\nabla n^+(\tau)\|_0^2 + \|\nabla n^-(\tau)\|_0^2\right) d\tau \leq \|n_0^+\|_0^2 + \|n_0^-\|_0^2, \tag{2.10}$$

$$\|\nabla\Psi(t)\|_0^2 + \|\boldsymbol{u}(t)\|_0^2 + 2\int_0^t \left(\|(n^+ - n^-)(\tau)\|_0^2 + \|\nabla\boldsymbol{u}(\tau)\|_0^2\right) d\tau \leq C_\Omega \|n_0^+ - n_0^-\|_0^2 + \|\boldsymbol{u}_0\|_0^2, \tag{2.11}$$

where C_Ω is a positive constant depending only on the area of Ω.

Proof. Firstly, we know from Lemma 2.1 that the solution $n^{\pm}$ satisfies the non-negativity. Taking $v = 2n^+$, $w = 2n^-$ in equations (2.5a) and (2.5b) respectively, summing them up, and applying Lemma 2.2, we obtain

$$\frac{d}{dt}\|n^+\|_0^2 + \frac{d}{dt}\|n^-\|_0^2 + 2\|\nabla n^+(\tau)\|_0^2 + 2\|\nabla n^-(\tau)\|_0^2 + I_1 = 0,$$

where

$$I_1 = \left(\nabla\Psi, \nabla(n^+)^2 - \nabla(n^-)^2\right).$$

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Noticing that $n^{\pm}\in H^1(\Omega)$, by the embedding theorem it holds $(n^{\pm})^2\in W^{1,\frac{4}{3}}(\Omega)$. Then it follows from Remark 2.2 and the non-negativity of $n^{\pm}$,

$$I_1=\big(n^+-n^-,(n^+)^2-(n^-)^2\big)=\big((n^+-n^-)^2,n^++n^-\big)\geq 0.$$

Thus

$$\frac{d}{dt}\|n^+\|_0^2+\frac{d}{dt}\|n^-\|_0^2+2\|\nabla n^+(\tau)\|_0^2+2\|\nabla n^-(\tau)\|_0^2\leq 0.$$

Integrating the above inequality with respect to t results in (2.10). Now we turn to prove (2.11). Taking $\boldsymbol{\varphi}=2\boldsymbol{u}$, $q=2p$, $v=2\Psi$, $w=-2\Psi$ in (2.4) and (2.5), and summing them up, we obtain

$$\frac{d}{dt}\|\boldsymbol{u}\|_0^2+2\|\nabla\boldsymbol{u}\|_0^2+2\Big(\frac{\partial}{\partial t}(n^+-n^-),\Psi\Big)+2(\nabla n^+-\nabla n^-,\nabla\Psi)+2(n^++n^-,|\nabla\psi|^2)=0. \tag{2.12}$$

Furthermore, using (2.6) gives

$$\begin{aligned}2\Big(\frac{\partial}{\partial t}(n^+-n^-),\Psi\Big)&=2\frac{d}{dt}(n^+-n^-,\Psi)-2\Big(n^+-n^-,\frac{\partial\Psi}{\partial t}\Big)\\&=2\frac{d}{dt}\|\nabla\Psi\|_0^2-2\Big(\nabla\Psi,\frac{\partial}{\partial t}(\nabla\Psi)\Big)\\&=\frac{d}{dt}\|\nabla\Psi\|_0^2,\end{aligned} \tag{2.13}$$

and

$$2(\nabla n^+-\nabla n^-,\nabla\Psi)=2\|n^+-n^-\|_0^2. \tag{2.14}$$

On the other hand, the non-negativity of $n^{\pm}$ yields

$$2(n^++n^-,|\nabla\psi|^2)\geq 0. \tag{2.15}$$

Using (2.13)-(2.15) in (2.12) gives

$$\frac{d}{dt}\|\boldsymbol{u}\|_0^2+\frac{d}{dt}\|\nabla\Psi\|_0^2+2\|\nabla\boldsymbol{u}\|_0^2+2\|n^+-n^-\|_0^2\leq 0. \tag{2.16}$$

Now we integrate (2.16) with respect to the time variable to get

$$\|\nabla\Psi(t)\|_0^2+\|\boldsymbol{u}(t)\|_0^2+2\int_0^t\big(\|(n^+-n^-)(\tau)\|_0^2+\|\nabla\boldsymbol{u}(\tau)\|_0^2\big)d\tau\leq\|\nabla\Psi(0)\|_0^2+\|\boldsymbol{u}_0\|_0^2. \tag{2.17}$$

Furthermore, applying the inequality (2.9) in Remark 2.2, and noticing the equivalence between the H^1 semi-norm and H^1 norm in the space $H^1(\Omega)\cap L_0^2(\Omega)$, we obtain

$$\|\nabla\Psi(0)\|_0^2\leq C_\Omega\|n_0^+-n_0^-\|_0^2, \tag{2.18}$$

where C_Ω is a constant depending on Ω.

Finally we obtain (2.11) by combining (2.18) with (2.17). □

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3 Time discretization and stability

It is very hard to construct a stable explicit time stepping scheme for the system (2.4)-(2.6) due to its non-linear and coupling features. On the other hand, a full implicit scheme could be more stable, but would result in some non-linear coupled equations to be solved at each time step. As a consequence, full implicit schemes would be very expensive for a system like (2.4)-(2.6). In this section, we aim at proposing and analyzing some semi-implicit schemes for the time discretization of (2.4)-(2.6).

Let $\tau = T/M$ be the time step size with M the number of total time steps. We start with proposing a first-order scheme as follows:

• Scheme A

Given the initial values $\boldsymbol{u}^0, n^{\pm,0}$, find $\Psi^0 \in H^1(\Omega)\cap L_0^2(\Omega)$ by the following equation:

$$(\nabla\Psi^0,\nabla\psi) = (n^{+,0}-n^{-,0},\psi), \quad \forall\psi\in H^1(\Omega)\cap L_0^2(\Omega). \tag{3.1}$$

Then for $m=0,1,\cdots$, successively find $n^{\pm,m+1}\in H^1(\Omega)$, $\Psi^{m+1}\in H^1(\Omega)\cap L_0^2(\Omega)$, $\boldsymbol{u}^{m+1}\in H_0^1(\Omega)^2$, and $p^{m+1}\in L_0^2(\Omega)$, such that

$$\begin{aligned}\frac{1}{\tau}(n^{+,m+1}-n^{+,m},v)+(\nabla\Psi^m n^{+,m+1},\nabla v)+(\nabla n^{+,m+1},\nabla v)\\ -(\boldsymbol{u}^m n^{+,m+1},\nabla v)=0, \quad \forall v\in H^1(\Omega);\end{aligned} \tag{3.2a}$$

$$\begin{aligned}\frac{1}{\tau}(n^{-,m+1}-n^{-,m},w)-(\nabla\Psi^m n^{-,m+1},\nabla w)+(\nabla n^{-,m+1},\nabla w)\\ -(\boldsymbol{u}^m n^{-,m+1},\nabla w)=0, \quad \forall w\in H^1(\Omega);\end{aligned} \tag{3.2b}$$

$$(\nabla\Psi^{m+1},\nabla\psi) = (n^{+,m+1}-n^{-,m+1},\psi), \quad \forall\psi\in H^1(\Omega)\cap L_0^2(\Omega); \tag{3.3}$$

$$\begin{aligned}\frac{1}{\tau}(\boldsymbol{u}^{m+1}-\boldsymbol{u}^m,\boldsymbol{\varphi})+(\boldsymbol{u}^m\cdot\nabla\boldsymbol{u}^{m+1},\boldsymbol{\varphi})+(\nabla\boldsymbol{u}^{m+1},\nabla\boldsymbol{\varphi})-(p^{m+1},\nabla\cdot\boldsymbol{\varphi})\\ +(\nabla\Psi^{m+1}(n^{+,m+1}-n^{-,m+1}),\boldsymbol{\varphi})=0, \quad \forall\boldsymbol{\varphi}\in H_0^1(\Omega)^2,\end{aligned} \tag{3.4a}$$

$$-(q,\nabla\cdot\boldsymbol{u}^{m+1})=0, \quad \forall q\in L_0^2(\Omega). \tag{3.4b}$$

In order to analyze the above scheme, we use the idea in [13] and introduce an auxiliary subsystem as follows:

$$\begin{aligned}\frac{1}{\tau}(n^{+,m+1}-n^{+,m},v)+(\nabla\Psi^m[n^{+,m+1}]^+,\nabla v)+(\nabla n^{+,m+1},\nabla v)\\ -(\boldsymbol{u}^m n^{+,m+1},\nabla v)=0, \quad \forall v\in H^1(\Omega);\end{aligned} \tag{3.5a}$$

$$\begin{aligned}\frac{1}{\tau}(n^{-,m+1}-n^{-,m},w)-(\nabla\Psi^m[n^{-,m+1}]^+,\nabla w)+(\nabla n^{-,m+1},\nabla w)\\ -(\boldsymbol{u}^m n^{-,m+1},\nabla w)=0, \quad \forall w\in H^1(\Omega),\end{aligned} \tag{3.5b}$$

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where, for a given function f, $[f]^+(x)=\sup\{f(x),0\}$. Obviously, if the auxiliary system (3.5) admits the solutions $n^{\pm,m}$, $m=0,1,\cdots,M$, which are non-negative almost everywhere in Ω, then they are also solutions of the original problem (3.2).

Lemma 3.1. *Given the initial value $n^{\pm,0}$ is non-negative almost everywhere in Ω, then the solutions of system* (3.2) *satisfy the non-negativity, that means*

$$n^{\pm,m}\geq 0 \text{ a.e. in } \Omega, \quad \forall m=1,2,\cdots,M. \tag{3.6}$$

Proof. By similarity, we only prove the non-negativity of $n^{+,m}$. We do it by the mathematical induction: suppose $n^{+,m}\geq 0$ a.e. in Ω is true for a given $m\geq 0$, we want to prove that $n^{+,m+1}\geq 0$ a.e. in Ω. Let $N^{+,m+1}:=\sup\{n^{+,m+1},0\}, N^{-,m+1}:=\sup\{-n^{+,m+1},0\}$, then we have $n^{+,m+1}=N^{+,m+1}-N^{-,m+1}$. Taking $v=-2N^{-,m+1}$ in (3.5a), using the properties of $N^{\pm,m+1}$ and $\nabla N^{\pm,m+1}$(refer to [4]), and Lemma 2.2, we get

$$-\int_\Omega \frac{2}{\tau}\left[(N^{+,m+1}-N^{-,m+1})-n^{+,m}\right]N^{-,m+1}d\boldsymbol{x}+2\|\nabla N^{-,m+1}\|_0^2=0. \tag{3.7}$$

Noticing that $N^{+,m+1}N^{-,m+1}\equiv 0$, we obtain

$$\int_\Omega \frac{2}{\tau}(N^{-,m+1}+n^{+,m})N^{-,m+1}d\boldsymbol{x}+2\|\nabla N^{-,m+1}\|_0^2=0.$$

Reformulating the first term gives

$$\frac{1}{\tau}\left(\|N^{-,m+1}\|_0^2+\|N^{-,m+1}+n^{+,m}\|_0^2-\|n^{+,m}\|_0^2\right)+2\|\nabla N^{-,m+1}\|_0^2=0. \tag{3.8}$$

We now prove $n^{+,m+1}\geq 0$ a.e. in Ω by contradiction. If there exists a non zero-measure subdomain $\tilde{\Omega}\subset\Omega$, such that

$$n^{+,m+1}(\boldsymbol{x})<0, \quad \forall \boldsymbol{x}\in\tilde{\Omega},$$

then

$$\|N^{-,m+1}\|_0^2>0, \text{ and } \|N^{-,m+1}+n^{+,m}\|_0^2-\|n^{+,m}\|_0^2\geq 0.$$

This obviously contradicts with (3.8). Thus $n^{+,m+1}\geq 0$ a.e. in Ω. The proof is completed. □

Theorem 3.1. *Given initial values $\boldsymbol{u}^0\in L^2(\Omega)^2$ and $n^{\pm,0}\in L^2(\Omega)$ that satisfy $\nabla\cdot\boldsymbol{u}^0=0$ in Ω, $\boldsymbol{u}^0=0$ on $\partial\Omega$, $n^{+,0}-n^{-,0}\in L_0^2(\Omega)$ in Ω, and $n^{\pm,0}\geq 0$ a.e in Ω. Then the scheme A is stable under condition $\tau\leq\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}^{-1}$ in the sense that the following inequalities hold for all $m=1,2,\cdots,M$:*

$$\|n^{+,m+1}\|_0^2+\|n^{-,m+1}\|_0^2+2\tau\|\nabla n^{+,m+1}\|_0^2+2\tau\|\nabla n^{-,m+1}\|_0^2\leq\|n^{+,m}\|_0^2+\|n^{-,m}\|_0^2, \tag{3.9}$$

$$\|\nabla\Psi^{m+1}\|_0^2+\|\boldsymbol{u}^{m+1}\|_0^2+2\tau\|n^{+,m+1}-n^{-,m+1}\|_0^2+2\tau\|\nabla\boldsymbol{u}^{m+1}\|_0^2\leq\|\nabla\Psi^m\|_0^2+\|\boldsymbol{u}^m\|_0^2. \tag{3.10}$$

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Proof. Firstly, we show that the inequality (3.9) holds. Taking $v=2\tau n^{+,m+1}$, $w=2\tau n^{-,m+1}$ in (3.2), and then summing them up, we get

$$\|n^{+,m+1}\|_0^2-\|n^{+,m}\|_0^2+\|n^{-,m+1}\|_0^2-\|n^{-,m}\|_0^2 \\ +2\tau\|\nabla n^{+,m+1}\|_0^2+2\tau\|\nabla n^{-,m+1}\|_0^2+I_a+I_b=0, \quad (3.11)$$

where

$$I_a=\|n^{+,m+1}-n^{+,m}\|_0^2+\|n^{-,m+1}-n^{-,m}\|_0^2,$$
$$I_b=\tau\int_\Omega \nabla\Psi^m\cdot\nabla\left[(n^{+,m+1})^2-(n^{-,m+1})^2\right]d\boldsymbol{x}.$$

Let $e^m:=n^{+,m}-n^{-,m}, m=1,2,\cdots$. It follows from the non-negativity of $n^{\pm,m+1}$ and (3.3) with $\psi=(n^{\pm,m+1})^2$ that

$$\begin{aligned} I_b&=\tau\int_\Omega e^{m+1}e^m(n^{+,m+1}+n^{-,m+1})d\boldsymbol{x}\\ &=-\frac{\tau}{2}\int_\Omega(n^{+,m+1}+n^{-,m+1})\left((e^{m+1}-e^m)^2-(e^m)^2-(e^{m+1})^2\right)d\boldsymbol{x}\\ &\geq-\frac{\tau}{2}\int_\Omega(n^{+,m+1}+n^{-,m+1})(e^{m+1}-e^m)^2d\boldsymbol{x}\\ &\geq-\tau\int_\Omega(n^{+,m+1}+n^{-,m+1})\left((n^{+,m+1}-n^{+,m})^2+(n^{-,m+1}-n^{-,m})^2\right)d\boldsymbol{x}\\ &\geq-\tau\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}\left(\|n^{+,m+1}-n^{+,m}\|_0^2+\|n^{-,m+1}-n^{-,m}\|_0^2\right). \end{aligned}$$

It is readily seen that $I_a+I_b\geq 0$ if $\tau\leq\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}^{-1}$. This gives the inequality (3.9). Next we prove (3.10). Taking $\boldsymbol{\varphi}=2\tau\boldsymbol{u}^{m+1}$, $q=2\tau p^{m+1}$ in (3.4), and $v=2\tau\Psi^{m+1}$, $w=-2\tau\Psi^{m+1}$ in (3.2), adding all resulting equations, and using the fact that

$$\begin{aligned} &(e^{m+1},\Psi^{m+1})=\|\nabla\Psi^{m+1}\|_0^2, \quad (\nabla e^{m+1},\nabla\Psi^{m+1})=\|e^{m+1}\|_0^2,\\ &(e^m,\Psi^{m+1})=(\nabla\Psi^m,\nabla\Psi^{m+1}), \end{aligned} \quad (3.12)$$

we obtain

$$\left(\|\nabla\Psi^{m+1}\|_0^2-\|\nabla\Psi^m\|_0^2+\|\boldsymbol{u}^{m+1}\|_0^2-\|\boldsymbol{u}^m\|_0^2\right)+2\tau\|e^{m+1}\|_0^2+2\tau\|\nabla\boldsymbol{u}^{m+1}\|_0^2 \\ +\left(\|\nabla\Psi^{m+1}-\nabla\Psi^m\|_0^2+\|\boldsymbol{u}^{m+1}-\boldsymbol{u}^m\|_0^2\right)+I_c+I_d=0, \quad (3.13)$$

where

$$I_c=\tau(n^{+,m+1}+n^{-,m+1},2\nabla\Psi^{m+1}\cdot\nabla\Psi^m),$$
$$I_d=\tau(n^{+,m+1}-n^{-,m+1},2(\boldsymbol{u}^{m+1}-\boldsymbol{u}^m)\cdot\nabla\Psi^{m+1}).$$

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These two quantities can be estimated as follows:

$$\begin{aligned}
I_c &= \tau\big(n^{+,m+1}+n^{-,m+1},-|\nabla\Psi^{m+1}-\nabla\Psi^m|^2+|\nabla\Psi^m|^2+|\nabla\Psi^{m+1}|^2\big)\\
&\geq -\tau\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}\|\nabla\Psi^{m+1}-\nabla\Psi^m\|_0^2+\tau\big(n^{+,m+1}+n^{-,m+1},|\nabla\Psi^{m+1}|^2\big),\\
I_d &\geq -\tau\big(|n^{+,m+1}-n^{-,m+1}|,|\boldsymbol{u}^{m+1}-\boldsymbol{u}^m|^2\big)-\tau\big(|n^{+,m+1}-n^{-,m+1}|,|\nabla\Psi^{m+1}|^2\big)\\
&\geq -\tau\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}\|\boldsymbol{u}^{m+1}-\boldsymbol{u}^m\|_0^2-\tau\big(n^{+,m+1}+n^{-,m+1},|\nabla\Psi^{m+1}|^2\big).
\end{aligned}$$

Combining the above inequalities yields

$$I_c+I_d\geq -\tau\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}\big(\|\nabla\Psi^{m+1}-\nabla\Psi^m\|_0^2+\|\boldsymbol{u}^{m+1}-\boldsymbol{u}^m\|_0^2\big). \tag{3.14}$$

Bringing (3.14) into (3.13), we obtain (3.10) under the condition $\tau\leq\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}^{-1}$. □

Although the scheme A decouples the NSNPP system into three parts which are relatively independent, the velocity and pressure remain coupled in the Navier-Stokes equation. In the next scheme we want to further decouple the velocity and pressure by employing some well-known decoupling approaches for the Navier-Stokes equation, i.e., the projection-type schemes [2,7,15].

• Scheme B

Given initial values $\boldsymbol{u}^0,n^{\pm,0}$, find $\Psi^0\in H^1(\Omega)\cap L_0^2(\Omega)$ by solving:

$$(\nabla\Psi^0,\nabla\psi)=(n^{+,0}-n^{-,0},\psi),\quad \forall\psi\in H^1(\Omega). \tag{3.15}$$

Then, given an approximate initial pressure p^0, find $n^{\pm,m+1}\in H^1(\Omega)$, $\Psi^{m+1}\in H^1(\Omega)\cap L_0^2(\Omega)$, $\tilde{\boldsymbol{u}}^{m+1}\in H_0^1(\Omega)^2$, $\boldsymbol{u}^{m+1}\in H^1(\Omega)^2$, $p^{m+1}\in H^1(\Omega)\cap L_0^2(\Omega)$, such that

$$\begin{aligned}
&\frac{1}{\tau}(n^{+,m+1}-n^{+,m},v)+(\nabla\Psi^m n^{+,m+1},\nabla v)+(\nabla n^{+,m+1},\nabla v)\\
&\qquad -(\boldsymbol{u}^m n^{+,m+1},\nabla v)=0,\quad \forall v\in H^1(\Omega);
\end{aligned} \tag{3.16a}$$

$$\begin{aligned}
&\frac{1}{\tau}(n^{-,m+1}-n^{-,m},w)-(\nabla\Psi^m n^{-,m+1},\nabla w)+(\nabla n^{-,m+1},\nabla w)\\
&\qquad -(\boldsymbol{u}^m n^{-,m+1},\nabla w)=0,\quad \forall w\in H^1(\Omega);
\end{aligned} \tag{3.16b}$$

$$(\nabla\Psi^{m+1},\nabla\psi)=(n^{+,m+1}-n^{-,m+1},\psi),\quad \forall\psi\in H^1(\Omega); \tag{3.17}$$

$$\begin{aligned}
&\frac{1}{\tau}(\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m,\boldsymbol{\varphi})+(\boldsymbol{u}^m\cdot\nabla\tilde{\boldsymbol{u}}^{m+1},\boldsymbol{\varphi})+(\nabla\tilde{\boldsymbol{u}}^{m+1},\nabla\boldsymbol{\varphi})-(p^m,\nabla\cdot\boldsymbol{\varphi})\\
&\qquad +(\nabla\Psi^{m+1}(n^{+,m+1}-n^{-,m+1}),\boldsymbol{\varphi})=0,\quad \forall\boldsymbol{\varphi}\in H_0^1(\Omega)^2;
\end{aligned} \tag{3.18a}$$

$$\tau(\nabla p^{m+1}-\nabla p^m,\nabla q)+(q,\nabla\cdot\tilde{\boldsymbol{u}}^{m+1})=0,\quad \forall q\in H^1(\Omega); \tag{3.18b}$$

$$\boldsymbol{u}^{m+1}=\tilde{\boldsymbol{u}}^{m+1}-\tau(\nabla p^{m+1}-\nabla p^m). \tag{3.18c}$$

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Remark 3.1. From (3.18a)-(3.18c), it is not hard to check that the scheme B maintains the incompressibility of the flow and the homogeneous Dirichlet boundary condition, i.e.,

$$\nabla\cdot\boldsymbol{u}^{m+1}=0 \text{ in } \Omega, \quad \text{and} \quad \boldsymbol{u}^{m+1}\cdot\boldsymbol{n}=0 \text{ on } \partial\Omega.$$

The non-negativity of the discrete ionic concentration solution of the scheme B can be proved by following exactly the same lines as in Lemma 3.1, while the stability of the solution is proved in Theorem 3.2.

Theorem 3.2. *Given the initial values $\boldsymbol{u}^0\in L^2(\Omega)^2$, $p^0\in H^1(\Omega)\cap L_0^2(\Omega)$, and $n^{\pm,0}\in L^2(\Omega)$, such that $\nabla\cdot\boldsymbol{u}^0=0$ in Ω, $\boldsymbol{u}^0\cdot\boldsymbol{n}=0$ on $\partial\Omega$, $n^{+,0}-n^{-,0}\in L_0^2(\Omega)$, and $n^{\pm,0}\geq 0$ in Ω. Then the following energy inequalities hold for $m=0,1,\cdots,M-1$ under the constraint $\tau\leq\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}^{-1}$:*

$$\|n^{+,m+1}\|_0^2+\|n^{-,m+1}\|_0^2+2\tau\|\nabla n^{+,m+1}\|_0^2+2\tau\|\nabla n^{-,m+1}\|_0^2\leq\|n^{+,m}\|_0^2+\|n^{-,m}\|_0^2, \tag{3.19}$$

$$\begin{aligned}\|\nabla\Psi^{m+1}\|_0^2+\|\boldsymbol{u}^{m+1}\|_0^2+\tau^2\|\nabla p^{m+1}\|_0^2+2\tau\|n^{+,m+1}-n^{-,m+1}\|_0^2+2\tau\|\nabla\tilde{\boldsymbol{u}}^{m+1}\|_0^2\\ \leq\|\nabla\Psi^m\|_0^2+\|\boldsymbol{u}^m\|_0^2+\tau^2\|\nabla p^m\|_0^2.\end{aligned} \tag{3.20}$$

Proof. The proof of (3.19) is same as for (3.9). We only need to prove (3.20). Using (3.16) with $v=2\tau\Psi^{m+1}$ and $w=-2\tau\Psi^{m+1}$, and noticing (3.12), we get

$$\begin{aligned}\|\nabla\Psi^{m+1}\|_0^2-\|\nabla\Psi^m\|_0^2+\|\nabla\Psi^{m+1}-\nabla\Psi^m\|_0^2+2\tau\|e^{m+1}\|_0^2\\ +2\tau(\nabla\Psi^{m+1}\cdot\nabla\Psi^m,n^{+,m+1}+n^{-,m+1})-2\tau(\boldsymbol{u}^m e^{m+1},\nabla\Psi^{m+1})=0.\end{aligned} \tag{3.21}$$

Then using (3.18a) with $\boldsymbol{\varphi}=2\tau\tilde{\boldsymbol{u}}^{m+1}$ we obtain

$$\begin{aligned}\|\tilde{\boldsymbol{u}}^{m+1}\|_0^2-\|\boldsymbol{u}^m\|_0^2+\|\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m\|_0^2+2\tau\|\nabla\tilde{\boldsymbol{u}}^{m+1}\|_0^2\\ -2\tau(p^m,\nabla\cdot\tilde{\boldsymbol{u}}^{m+1})+2\tau(\tilde{\boldsymbol{u}}^{m+1}e^{m+1},\nabla\Psi^{m+1})=0.\end{aligned} \tag{3.22}$$

Furthermore, rewrite (3.18c) as

$$\boldsymbol{u}^{m+1}+\tau\nabla p^{m+1}=\tilde{\boldsymbol{u}}^{m+1}+\tau\nabla p^m,$$

and take the L^2-inner product of above with itself on both sides give

$$\|\boldsymbol{u}^{m+1}\|_0^2-\|\tilde{\boldsymbol{u}}^{m+1}\|_0^2+\tau^2(\|\nabla p^{m+1}\|_0^2-\|\nabla p^m\|_0^2)+2\tau(\nabla\cdot\tilde{\boldsymbol{u}}^{m+1},p^m)=0. \tag{3.23}$$

Now we combine (3.21)-(3.23) together to get

$$\begin{aligned}\|\boldsymbol{u}^{m+1}\|_0^2-\|\boldsymbol{u}^m\|_0^2+\|\nabla\Psi^{m+1}\|_0^2-\|\nabla\Psi^m\|_0^2+\|\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m\|_0^2+\|\nabla\Psi^{m+1}-\nabla\Psi^m\|_0^2\\ +2\tau\big(\|\nabla\tilde{\boldsymbol{u}}^{m+1}\|_0^2+\|e^{m+1}\|_0^2\big)+\tau^2\big(\|\nabla p^{m+1}\|_0^2-\|\nabla p^m\|_0^2\big)+I_e=0,\end{aligned} \tag{3.24}$$

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where

$$\begin{aligned}I_e&=2\tau(n^{+,m+1}+n^{-,m+1},\nabla\Psi^m\cdot\nabla\Psi^{m+1})+2\tau\big((\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m)e^{m+1},\nabla\Psi^{m+1}\big)\\&\geq\tau\big(n^{+,m+1}+n^{-,m+1},-|\nabla\Psi^{m+1}-\nabla\Psi^m|^2+|\nabla\Psi^{m+1}|^2+|\nabla\Psi^m|^2\big)\\&\quad-\tau\big(n^{+,m+1}+n^{-,m+1},|\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m|^2+|\nabla\Psi^{m+1}|^2\big)\\&\geq-\tau\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}\big(\|\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m\|_0^2+\|\nabla\Psi^{m+1}-\nabla\Psi^m\|_0^2\big).\end{aligned}$$

Hence, (3.20) holds if $\tau\leq\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}^{-1}$. □

Theorems 3.1 and 3.2 indicate that the both scheme A and B are conditionally stable. In the following we want to show that by adding a stabilization term it is possible to construct an unconditionally stable scheme.

• Scheme C

Given $\boldsymbol{u}^0,n^{\pm,0}$, find $\Psi^0\in H^1(\Omega)\cap L_0^2(\Omega)$, such that:

$$(\nabla\Psi^0,\nabla\psi)=(n^{+,0}-n^{-,0},\psi),\quad\forall\psi\in H^1(\Omega).\tag{3.25}$$

Given p^0, find $n^{\pm,m+1}\in H^1(\Omega)$, $\Psi^{m+1}\in H^1(\Omega)\cap L_0^2(\Omega)$, $\tilde{\boldsymbol{u}}^{m+1}\in H_0^1(\Omega)^2$, $\boldsymbol{u}^{m+1}\in H^1(\Omega)^2$, $p^{m+1}\in H^1(\Omega)\cap L_0^2(\Omega)$, such that

$$\begin{aligned}&\big(s^{m+1}+\frac{1}{\tau}\big)(n^{+,m+1}-n^{+,m},v)+(\nabla\Psi^m n^{+,m+1},\nabla v)+(\nabla n^{+,m+1},\nabla v)\\&\qquad-(\boldsymbol{u}^m n^{+,m+1},\nabla v)=0,\quad\forall v\in H^1(\Omega);\end{aligned}\tag{3.26a}$$

$$\begin{aligned}&\big(s^{m+1}+\frac{1}{\tau}\big)(n^{-,m+1}-n^{-,m},w)-(\nabla\Psi^m n^{-,m+1},\nabla w)+(\nabla n^{-,m+1},\nabla w)\\&\qquad-(\boldsymbol{u}^m n^{-,m+1},\nabla w)=0,\quad\forall w\in H^1(\Omega);\end{aligned}\tag{3.26b}$$

$$(\nabla\Psi^{m+1},\nabla\psi)=(n^{+,m+1}-n^{-,m+1},\psi),\quad\forall\psi\in H^1(\Omega);\tag{3.27}$$

$$\begin{aligned}&\big(s^{m+1}+\frac{1}{\tau}\big)(\tilde{\boldsymbol{u}}^{m+1}-\boldsymbol{u}^m,\boldsymbol{\varphi})+(\boldsymbol{u}^m\cdot\nabla\tilde{\boldsymbol{u}}^{m+1},\boldsymbol{\varphi})+(\nabla\tilde{\boldsymbol{u}}^{m+1},\nabla\boldsymbol{\varphi})\\&\qquad-(p^m,\nabla\cdot\boldsymbol{\varphi})+(\nabla\Psi^{m+1}(n^{+,m+1}-n^{-,m+1}),\boldsymbol{\varphi})=0,\quad\forall\boldsymbol{\varphi}\in H_0^1(\Omega)^2;\end{aligned}\tag{3.28a}$$

$$\frac{\tau}{s^{m+1}\tau+1}(\nabla p^{m+1}-\nabla p^m,\nabla q)+(q,\nabla\cdot\tilde{\boldsymbol{u}}^{m+1})=0;\quad\forall q\in H^1(\Omega);\tag{3.28b}$$

$$\boldsymbol{u}^{m+1}=\tilde{\boldsymbol{u}}^{m+1}-\frac{\tau}{s^{m+1}\tau+1}(\nabla p^{m+1}-\nabla p^m),\tag{3.28c}$$

where s^{m+1} is a stabilization constant.

Theorem 3.3. *Under the same conditions as in Theorem* 3.2 *for the initial values* $\boldsymbol{u}^0$, p^0, *and* $n^{\pm,0}$, *then for* $m=0,1,\cdots,M-1$, *the non-negativity of the concentration functions* $n^{\pm,m+1}$ *are*

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maintained if $s^{m+1}\geq 0$. *Moreover, if* $s^{m+1}\geq\frac{\tau}{4}\|n^{+,m+1}+n^{-,m+1}\|_{L^\infty}^2$, *then the solution of the scheme C satisfies the following energy inequalities without any constraint on* τ*:*

$$\|n^{+,m+1}\|_0^2+\|n^{-,m+1}\|_0^2+\frac{2\tau}{1+s^{m+1}\tau}\big(\|\nabla n^{+,m+1}\|_0^2+\|\nabla n^{-,m+1}\|_0^2\big)\leq\|n^{+,m}\|_0^2+\|n^{-,m}\|_0^2; \tag{3.29}$$

$$\|\nabla\Psi^{m+1}\|_0^2+\|\boldsymbol{u}^{m+1}\|_0^2+\frac{\tau^2}{(1+s^{m+1}\tau)^2}\|\nabla p^{m+1}\|_0^2+\frac{2\tau}{1+s^{m+1}\tau}\big(\|n^{+,m+1}-n^{-,m+1}\|_0^2+\|\nabla\tilde{\boldsymbol{u}}^{m+1}\|_0^2\big)\leq\|\nabla\Psi^m\|_0^2+\|\boldsymbol{u}^m\|_0^2+\frac{\tau^2}{(1+s^{m+1}\tau)^2}\|\nabla p^m\|_0^2. \tag{3.30}$$

The proof of Theorem 3.3 is quite similar to that of Lemma 3.1 and Theorem 3.2. We omit the details to avoid repetition.

4 A higher order scheme and full discretization

In this section, we consider a spectral method for the spatial discretization. For ease of presentation, we assume $\Omega=(-1,1)^2$. Let $I\!P_K(\Omega)$ be the space of polynomials of degree $\leq K$ with respect to each variable in Ω. We introduce the following approximation spaces:

$$\begin{aligned}&\boldsymbol{V}_K=\big(H_0^1(\Omega)\cap I\!P_K(\Omega)\big)^2,\\&M_K=L_0^2(\Omega)\cap I\!P_{N-2}(\Omega),\\&Y_K=H^1(\Omega)\cap I\!P_K(\Omega),\\&Z_K=H^1(\Omega)\cap L_0^2(\Omega)\cap I\!P_K(\Omega).\end{aligned}$$

We denote by x_i and ω_i, $i=0,1,\cdots,K$ the one-dimensional Legendre-Gauss-Lobatto (LGL) points and weights respectively in $[-1,1]$. The LGL points and weights in the 2-dimensional domain Ω is:

$$\boldsymbol{x}_{ij}=(x_i,x_j),\quad \omega_{ij}=\omega_i\omega_j,\quad i,j=0,1,\cdots,K. \tag{4.1}$$

Then we use them to define the discrete inner product:

$$(\phi,\varphi)_K=\sum_{i,j=0}^{K}\phi(\boldsymbol{x}_{ij})\varphi(\boldsymbol{x}_{ij})\omega_{ij},$$

and the associated discrete norm: $\|\phi\|_{0,K}=\sqrt{(\phi,\phi)_K}$.

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We first consider the spatial discretization for the continuous problem (2.4)-(2.6): given initial functions $\boldsymbol{u}_K(0)$ and $n_K^{\pm}(0)$, find, for all $t\in(0,T)$, $\boldsymbol{u}_K(t)\in\boldsymbol{V}_K$, $p_K(t)\in M_K$, $n_K^{\pm}(t)\in Y_K$, and $\Psi_K(t)\in Z_K$, such that

$$\left(\frac{\partial \boldsymbol{u}_K}{\partial t},\boldsymbol{\varphi}\right)_K+(\boldsymbol{u}_K\cdot\nabla\boldsymbol{u}_K,\boldsymbol{\varphi})_K+(\nabla\boldsymbol{u}_K,\nabla\boldsymbol{\varphi})_K-(p_K,\nabla\cdot\boldsymbol{\varphi})_K$$
$$+\left((n_K^+-n_K^-)\nabla\Psi_K,\boldsymbol{\varphi}\right)_K=0,\quad \forall\boldsymbol{\varphi}\in\boldsymbol{V}_K, \tag{4.2a}$$
$$-(q,\nabla\cdot\boldsymbol{u}_K)_K=0,\quad \forall q\in M_K; \tag{4.2b}$$

$$\left(\frac{\partial n_K^+}{\partial t},v\right)_K+(\nabla\Psi_K n_K^+,\nabla v)_K+(\nabla n_K^+,\nabla v)_K-(\boldsymbol{u}_K n_K^+,\nabla v)_K=0,\qquad \forall v\in Y_K; \tag{4.3a}$$

$$\left(\frac{\partial n_K^-}{\partial t},w\right)_K-(\nabla\Psi_K n_K^-,\nabla w)_K+(\nabla n_K^-,\nabla w)_K-(\boldsymbol{u}_K n_K^-,\nabla w)_K=0,\qquad \forall w\in Y_K; \tag{4.3b}$$

$$(\nabla\Psi_K,\nabla\psi)_K=(n_K^+-n_K^-,\psi)_K,\quad \forall\psi\in Z_K. \tag{4.4}$$

Lemma 4.1. *If the initial condition $n_K^{\pm}(0)\geq 0$ in Ω, then the solution $n_K^{\pm}(t)$ of the spectral discrete problem* (4.2)-(4.4) *is also non-negative in Ω for all $t>0$.*

Proof. We only prove the non-negativity of n_K^+. Similar to the proof of Lemma 3.1, we introduce the auxiliary equation:

$$\left(\frac{\partial n_K^+}{\partial t},v\right)_K+(\nabla\Psi_K[n_K^+]^+,\nabla v)_K+(\nabla n_K^+,\nabla v)_K-(\boldsymbol{u}_K[n_K^+]^+,\nabla v)_K=0,\quad \forall v\in Y_K. \tag{4.5}$$

Then we just need to prove that the above solution is non-negative. To this end, let $N^-=\sup\{-n_K^+,0\}$, $N^+=\sup\{n_K^+,0\}$. Taking $v=-2N^-$ in (4.5) gives

$$2\left(\frac{\partial N^-}{\partial t},N^-\right)_K+2(\nabla N^-,\nabla N^-)_K=0.$$

That is

$$\frac{d}{dt}\|N^-\|_{0,K}^2+2\|\nabla N^-\|_{0,K}^2=0.$$

Integrating with respect to time on $(0,t)$ for $t\in(0,T)$, we get

$$\|N^-(t)\|_{0,K}^2-\|N^-(0)\|_{0,K}^2+2\int_0^t\|\nabla N^-\|_{0,K}^2d\tau=0.$$

The assumption $n_K^+(0)\geq 0$ in Ω means $N^-(0)\equiv 0$. Therefore

$$\|N^-(t)\|_{0,K}\leq 0,\ \forall t\in(0,T).$$

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By virtue of the equivalence between the discrete norm $\|\cdot\|_{0,K}$ and the continuous norm $\|\cdot\|_0$ in the space $IP_K(\Omega)$, we obtain

$$\|N^-(t)\|_0 \leq 0, \ \ \forall t \in (0,T).$$

Thus

$$n_K^+(t) \geq 0 \ \ a.e. \text{ in } \Omega, \ \forall t \in (0,T).$$

This ends the proof. □

Now we consider full discretization of the problem (2.4)-(2.6). Clearly all the three first-order schemes A, B and C can be used to discretize the spectral approximation problem (4.2)-(4.4) in time, and the resulting full discrete problems would satisfy similar stability properties as Theorems 3.1, 3.2, and 3.3 for the semi-discrete problems A, B and C respectively. The details of these full discrete schemes and their stability analysis will not be reported here in order to avoid repetition (also to limit the length of the paper).

Up to now we have only considered schemes of first order in time. Next we try to construct a second-order time stepping scheme for the NSNPP system. Usually high order schemes have more demand than low order schemes in practical applications. The former is often more efficient over the latter in one side, but much more difficult to analyze on the other side.

Roughly, the second-order scheme we are constructing will make use of the second-order backward differentiation for the time derivatives and semi-implicit/extrapolation treatment for the non-linear convection terms. Precisely, the full discrete version of the second-order scheme in time/spectral method in space reads: Given initial values $\boldsymbol{u}_K^0, p_K^0$, and $n_K^{\pm,0}$, find $n_K^{\pm,m+1} \in Y_K$, $\Psi_K^{m+1} \in Z_K$, $\tilde{\boldsymbol{u}}_K^{m+1} \in \boldsymbol{V}_K$, $\boldsymbol{u}_K^{m+1} \in \boldsymbol{V}_K$, and $p_K^{m+1} \in M_K$, such that

$$\begin{aligned}
&\frac{1}{2\tau}(3n_K^{+,m+1}-4n_K^{+,m}+n_K^{+,m-1},v)_K+\big((2\nabla\Psi_K^m-\nabla\Psi_K^{m-1})n_K^{+,m+1},\nabla v\big)_K \\
&\qquad +(\nabla n_K^{+,m+1},\nabla v)_K-\big((2\boldsymbol{u}_K^m-\boldsymbol{u}_K^{m-1})n_K^{+,m+1},\nabla v\big)_K=0, \quad \forall v\in Y_K; \qquad (4.6a)\\
&\frac{1}{2\tau}(3n_K^{-,m+1}-4n_K^{-,m}+n_K^{-,m-1},w)_K-\big((2\nabla\Psi_K^m-\nabla\Psi_K^{m-1})n_K^{-,m+1},\nabla w\big)_K \\
&\qquad +(\nabla n_K^{-,m+1},\nabla w)_K-\big((2\boldsymbol{u}_K^m-\boldsymbol{u}_K^{m-1})n_K^{-,m+1},\nabla w\big)_K=0, \quad \forall w\in Y_K; \qquad (4.6b)\\
&(\nabla\Psi_K^{m+1},\nabla\psi)_K=(n_K^{+,m+1}-n_K^{-,m+1},\psi)_K, \quad \forall\psi\in Z_K; \qquad (4.7)\\
&\frac{1}{2\tau}(3\tilde{\boldsymbol{u}}_K^{m+1}-4\boldsymbol{u}_K^m+\boldsymbol{u}_K^{m-1},\boldsymbol{\varphi})_K+\big((2\boldsymbol{u}_K^m-\boldsymbol{u}_K^{m-1})\cdot\nabla\tilde{\boldsymbol{u}}_K^{m+1},\boldsymbol{\varphi}\big)_K+(\nabla\tilde{\boldsymbol{u}}_K^{m+1},\nabla\boldsymbol{\varphi})_K \\
&\qquad -(p_K^m,\nabla\cdot\boldsymbol{\varphi})_K+\big(\nabla\Psi_K^{m+1}(n_K^{+,m+1}-n_K^{-,m+1}),\boldsymbol{\varphi}\big)_K=0, \quad \forall\boldsymbol{\varphi}\in\boldsymbol{V}_K; \qquad (4.8a)\\
&\qquad \frac{2}{3}\tau(\nabla p_K^{m+1}-\nabla p_K^m,\nabla q)_K+(q,\nabla\cdot\tilde{\boldsymbol{u}}_K^{m+1})_K=0, \quad \forall q\in M_K; \qquad (4.8b)\\
&\qquad \boldsymbol{u}_K^{m+1}=\tilde{\boldsymbol{u}}_K^{m+1}-\frac{2}{3}\tau(\nabla p_K^{m+1}-\nabla p_K^m). \qquad (4.8c)
\end{aligned}$$

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For the time being, we are unable to prove the stability of the above scheme. The main obstacle is in the analysis of the discrete ionic concentrations: the non-negativity of the discrete ionic concentrations, which is a key property to establish the energy inequality, can't be proved for the second order stepping scheme. Nevertheless, the proposed method (4.6)-(4.8) will be numerically investigated in the next section, and the obtained numerical result seems to confirm the non-negativity property of the high accurate ionic concentrations.

5 Numerical Test

The numerical test has purpose to validate the proposed schemes in terms of stability and accuracy. Some suitable forcing terms are added in the equations such that the problem admits the following exact solution:

$$\boldsymbol{u}=\begin{pmatrix}\sin(2\pi x)\cos(2\pi y)\sin t\\ -\sin(2\pi y)\cos(2\pi x)\sin t\end{pmatrix},\quad p=\sin(2\pi x)\sin(2\pi y)\sin t,$$
$$\Psi_0=\frac{1}{\pi^2}\cos(\pi x)\cos(\pi y)\sin t,$$
$$n^+=3\cos(\pi x)\cos(\pi y)\sin t,\quad n^-=\cos(\pi x)\cos(\pi y)\sin t.$$

Notice that the above solution is quite artificial because the ionic concentrations $n^{\pm}$ are even negative.

For the purpose of accuracy investigation, we first solve the problem (2.1)-(2.3) by employing spectral method for the space discretization and Scheme C with stabilizer $s^{m+1}=\tau^2\|n^{+,m}+n^{-,m}\|_{L^\infty}^2$ for the time stepping. All the numerical results reported in the figures below have been evaluated at $T=1$. Figs. 1-4 show the discrete L^2 errors of the ionic concentrations, electrostatic potential, and fluid velocity with respect to the time step size τ, where a logarithmic scale has been used for both τ-axis and error-axis. Two error curves corresponding to two polynomial degrees $N=23$ and $N=25$ are plotted in all these figures. The fact that the two curves completely overlap implies that the temporal error dominates the spatial error. As expected, Scheme C yields a first-order temporal approximation to all computed components, since the error curves are all straight lines parallel to the reference line of slope 1.

Next we repeat the same calculations by using the second order scheme in time. The spatial approximation uses always the same Legendre spectral method. The obtained results are plotted in Figs. 5-8. It is now observed that the error curves on $n^{\pm}$, Ψ, and $\boldsymbol{u}$ are all straight lines of slope 2 in the log-log scale. This clearly indicates the second order convergence rate with respect to the time step size.

Now we check the spatial accuracy with respect to the polynomial degree by fixing the time step size sufficiently small to avoid contamination of the temporal error. Only the second order scheme in time is used for this test since it allows use of not so small time step. In Figs. 9-12, we present the errors as a function of the polynomial degree N

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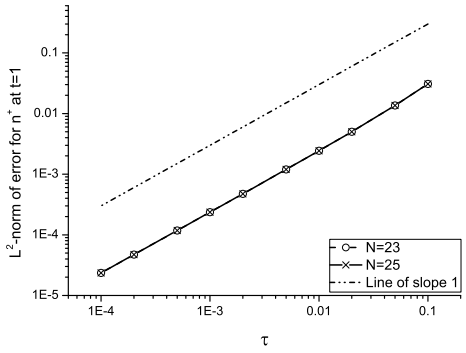


Figure 1: n^+-errors with respect to τ for N=23,25. Scheme C.

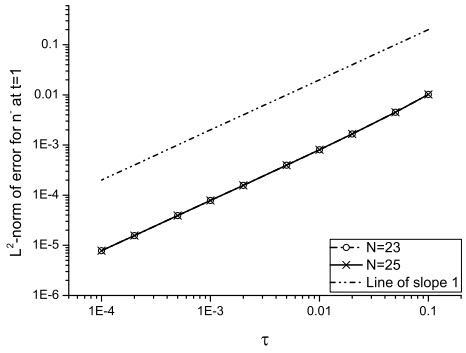


Figure 2: n^--errors with respect to τ for N=23,25. Scheme C.

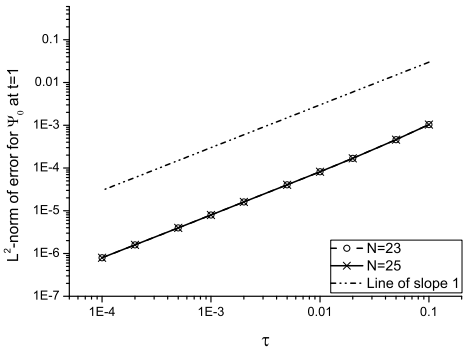


Figure 3: Ψ-errors with respect to τ for N=23,25. Scheme C.

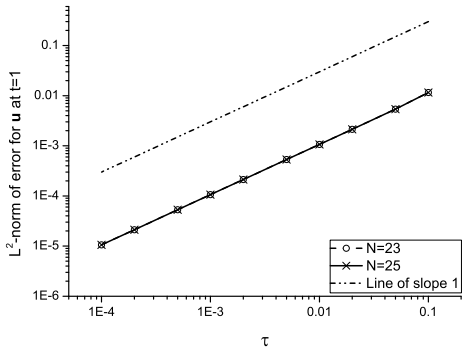


Figure 4: $\boldsymbol{u}$-errors with respect to τ for N=23,25. Scheme C.

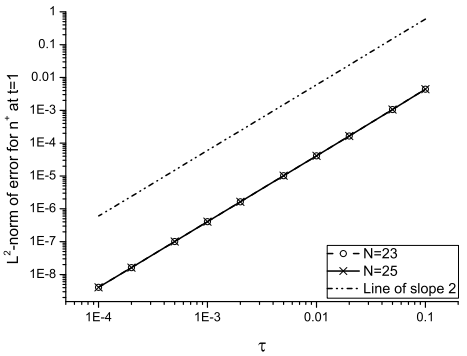


Figure 5: n^+-errors with the 2nd-order scheme in time.

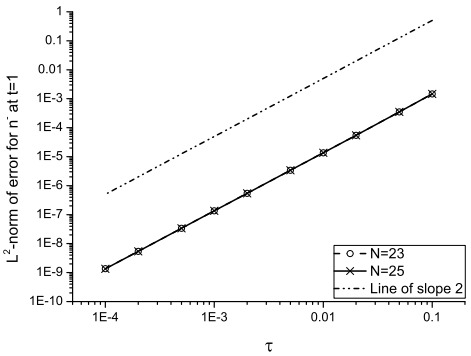


Figure 6: n^--errors with the 2nd-order scheme in time.

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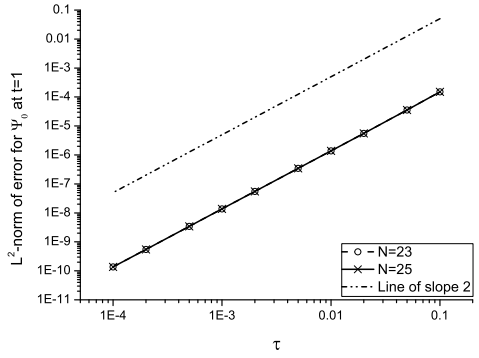


Figure 7: Ψ-errors with the 2nd-order scheme in time.

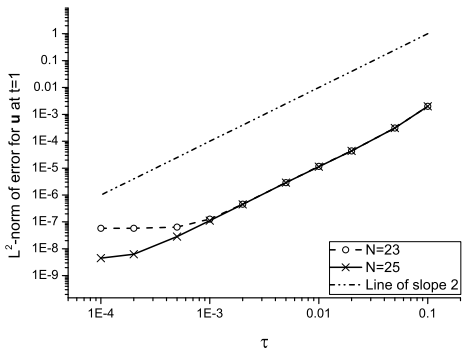


Figure 8: $\boldsymbol{u}$-errors with the 2nd-order scheme in time.

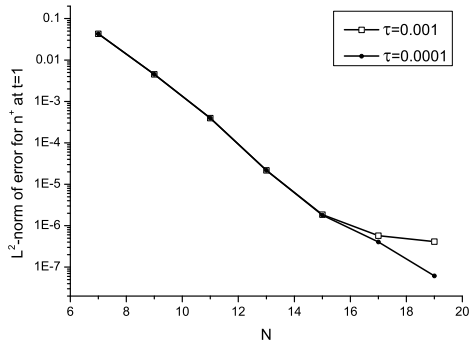


Figure 9: Errors of n^+ as a function of N for $\tau=0.001,0.0001$ using the 2nd-order scheme.

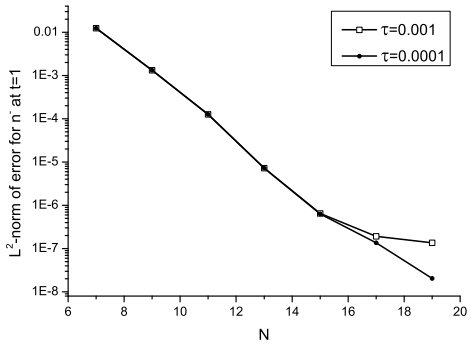


Figure 10: Errors of n^- as a function of N for $\tau=0.001,0.0001$ using the 2nd-order scheme.

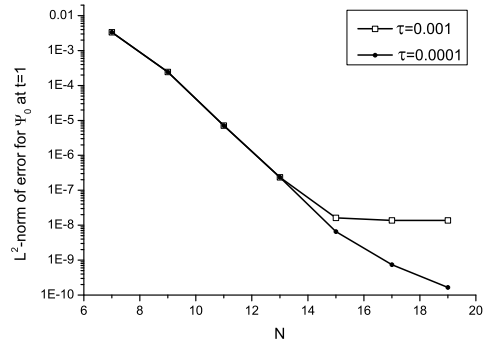


Figure 11: Errors of Ψ_0 as a function of N for $\tau=0.001,0.0001$ using the 2nd-order scheme.

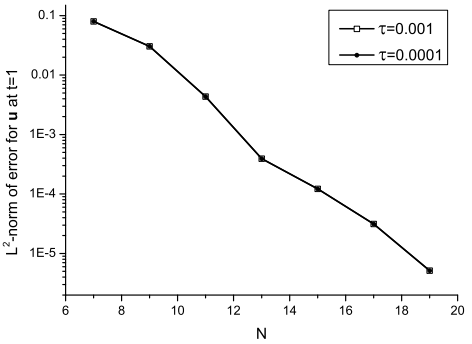


Figure 12: Errors of $\boldsymbol{u}$ as a function of N for $\tau=0.001,0.0001$ using the 2nd-order scheme.

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for two values of τ: 0.001 and 0.0001. A logarithmic scale is now used for the error-axis. Clearly, the errors show an exponential decay, since in these semi-log representations one observes that the error variations are essentially linear versus the polynomial degrees for all solution components. That is the so-called spectral accuracy as expected for smooth exact solutions.

Finally, we verify the non-negativity preserving property of the discrete concentrations. Both the first and second order time stepping schemes, combined with the spectral method in space, are applied to solve the NSNPP system with the following initial conditions:

$$\boldsymbol{u}_0 = \begin{pmatrix} 10\sin(2\pi x)\cos(2\pi y) \\ -10\sin(2\pi y)\cos(2\pi x) \end{pmatrix},$$
$$n_0^+ = \cos(2\pi x)+1, \quad n_0^- = \cos(2\pi y)+1,$$

where the initial ionic concentrations are set non-negative. We hope they will remain non-negative in the whole computational domain for all time. In the calculation, we take the time step $\tau = 0.001$ and polynomial degree $N = 23$. The ionic solutions at six instants between 0 and 0.5 are plotted in Fig. 13 and Fig. 14 for the first order scheme. It is observed that the ionic concentrations preserve the non-negativity at all captured instants. To better demonstrate the non-negativity preserving, zooms near the zero concentrations are presented in Fig. 15 and Fig. 16. This confirms our theoretical analysis provided in the previous sections.

The numerical results obtained by using the second order scheme are presented in Fig. 17 and Fig. 18, where the surfaces show the spatial distributions of the ionic concentrations at six different time instants. A close look at these figures confirms that the ionic concentrations remain non-negative. Although not yet proved theoretically, this numerical test tends to predict the non-negativity preserving of the second order scheme: a very desirable property of the NSNPP problem.

6 Concluding remarks

We have presented some numerical methods for the Navier-Stokes-Nernst-Planck-Poisson coupled equation. The proposed methods combine several finite difference schemes in time with a Legendre spectral method for the spatial discretization. For the methods using first-order time stepping schemes, a rigorous analysis was carried out, showing that the overall schemes are conditionally/unconditionally stable. A number of numerical examples were provided to confirm the theoretical claims. For the method using the second-order time stepping, although rigorous stability proof is not available, we have provided numerical tests to demonstrate the efficiency of the method. In particular, the obtained numerical results have shown that all the proposed methods preserve the non-negativity of the ionic concentration solutions, a property which is crucial for practical applications of the NSNPP problem.

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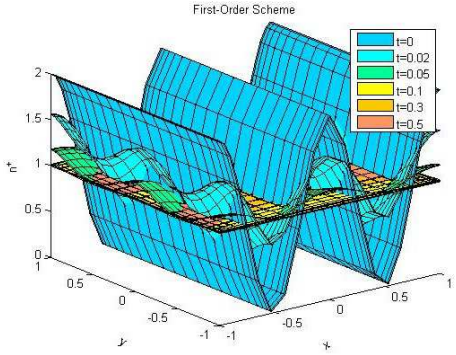


Figure 13: Ionic concentration n^+ at some different instants. 1st-order scheme with $N=23$, $\tau=0.001$.

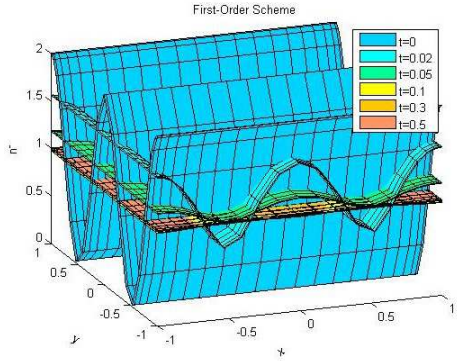


Figure 14: Ionic concentration n^- at some different instants. 1st-order scheme with $N=23$, $\tau=0.001$.

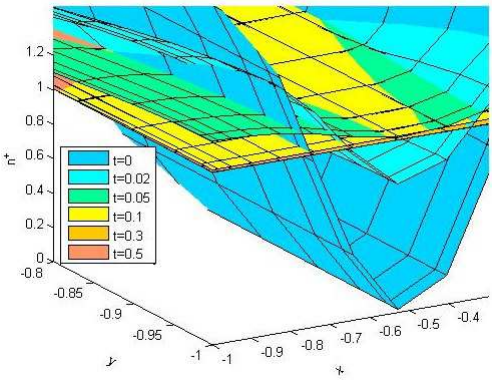


Figure 15: The partial enlarged detail of Fig. 13.

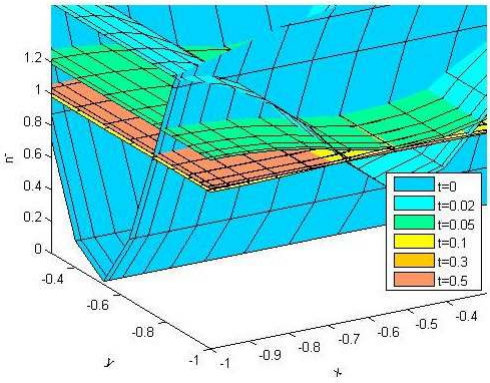


Figure 16: The partial enlarged detail of Fig. 14

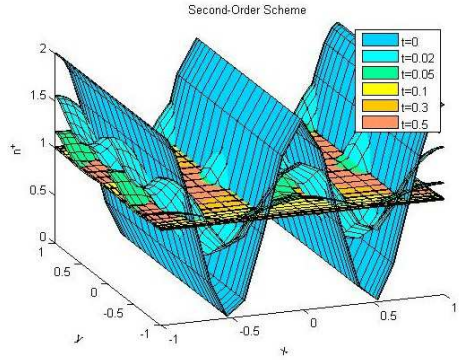


Figure 17: Ionic concentration n^+ at some different instants. 2nd-order scheme.

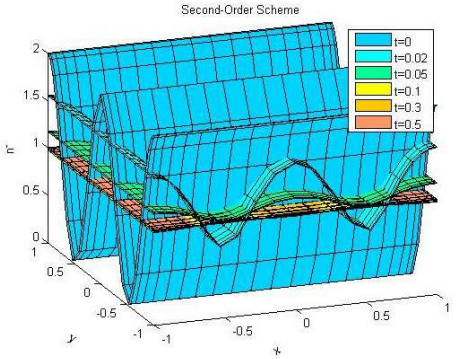


Figure 18: Ionic concentration n^- at some different instants. 2nd-order scheme.

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