Modeling, Analysis, and Numerics in Electrohydrodynamics

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Preface

The main subject of this thesis is to analyze the incompressible Navier-Stokes-Nernst-Planck-Poisson system for bounded domains $\Omega \subset \mathbb{R}^3$. Such a system is used as a model in electrohydrodynamics or physicochemical models. First, we verify existence of weak and strong solutions. Moreover, we are able to characterize the weak solutions by an energy and an entropy law. The concentrations in the Nernst-Planck equations additionally are non-negative and bounded in $L^\infty(\Omega_T)$. These results motivate to construct convergent space-time discretizations based on low order finite elements, where solutions of the discrete problem preserve the characteristic properties from the continuous context.
For this purpose, we first introduce an energy based and an entropy based approximation for the simpler Nernst-Planck-Poisson sub-system which is also called the van Roosbroeck equations in the semiconductor theory. The main focus is to study qualitative properties of the two discretization strategies at finite discretization scales, like conservation of mass, non-negativity, discrete maximum principle, decay of discrete energies and entropies to study long-time asymptotics. The energy based scheme uses the M-matrix property to prove non-negativity and boundedness of iterates. Here, we have to assume more regular initial data in order to verify a perturbed entropy law. This deficiency for the entropy behavior is resolved by an entropy based scheme allowing for an entropy inequality without any additional assumptions. However, in turn, the latter scheme suffers from weaker results, such as quasi-non-negativity, and the lack of a discrete maximum principle.
These results suggest to follow the energy based approach for the coupled incompressible Navier-Stokes-Nernst-Planck-Poisson system. The main obstacle here is the lack of regularity of velocity fields from the Navier-Stokes equations which makes the verification of the M-matrix property in the Nernst-Planck-Poisson part more difficult. We therefore regularize the discrete momentum equation by an additional term such that the incompressible Navier-Stokes equations arise as the limit of the discrete problem. Main results then include non-negativity, conservation of mass, and a discrete maximum principle for concentrations, and a discrete energy and (in two dimensions) a discrete entropy law for iterates which solve a nonlinear algebraic problem: A fixed-point scheme is introduced for both, theoretical and practical purposes to solve the nonlinear problem together with an appropriate stopping criterion. Overall convergence of solutions to weak solutions of the incompressible Navier-Stokes-Nernst-Planck-Poisson equations is shown. We conclude with the verification of optimal convergence rates for a suggested time-splitting scheme whose iterates converge to (locally existing) strong solutions of the electrohydrodynamic system.
At the end we compare the energy based scheme and the splitting scheme by numerical experiments.

Zusammenfassung

In dieser Arbeit werden unter den Aspekten der Modellierung, Analysis, und Numerik die grundlegenden elektrohydrodynamischen Gleichungen im Fall wässriger Lösungen untersucht. Diese Gleichungen werden hergeleitet und notwendige Annahmen für deren Gültigkeit spezifiziert. Der analytische Teil der Arbeit verifiziert die Existenz von schwachen und starken Lösungen, für die ein Energie- und Entropieprinzip nachgewiesen werden; zusätzlich sind die Lösungen der Nernst-Planck Gleichungen beschränkt in $L^\infty(\Omega_T)$ und nicht-negativ.
Das Ziel der Arbeit ist es nun, diese charakteristischen Eigenschaften der Lösungen aus dem kontinuierlichen Kontext ins Diskrete zu übertragen mithilfe einer raumzeitlichen Diskretisierung, die finite Elemente niedriger Ordnung verwendet. Dafür führen wir ein energie- und ein entropiebasiertes Verfahren für das Nernst-Planck-Poisson Teilsystem ein. Die Verifikation der M-Matrix Eigenschaft einer Fixpunkt-Iteration zur Lösung der diskreten Nernst-Planck Gleichungen liefert die Nicht-Negativität und die Beschränktheit in $L^\infty(\Omega_T)$ der zugehörigen Lösungen. Anschliessenden verifizieren wir ein diskretes Energie- und Entropieprinzip. Da das Entropiegesetz leicht gestört ist, untersuchen wir ein zweites entropiebasiertes Verfahren, welches ein ungestörtes Entropieprinzip ermöglicht. Jedoch bekommen wir nur noch Quasi-Nicht-Negativität der Konzentrationen, und ein diskretes Maximumprinzip fehlt.
Wegen seiner stärkeren Resultate erweitern wir das energiebasierte Verfahren auf das ganze elektrohydrodynamische System und können damit alle charakteristischen Eigenschaften schwacher Lösungen auf die finiten Elemente Lösungen übertragen. Die Hauptresultate sind damit Nicht-Negativität, Massenerhaltung, und die Beschränktheit der Konzentrationen, und ein diskretes Energie- und (in zwei Dimensionen auch) ein diskretes Entropiegesetz für die Iterierten, welche ein nichtlineares algebraisches Problem lösen: Wir verwenden einen Fixpunktalgorithmus zusammen mit einer geeigneten Abbruchbedingung um sowohl theoretische als auch numerische Resultate zu erhalten. Es wird die Konvergenz der so erhaltenen Lösungen gegen schwache Lösungen der inkompressiblen Navier-Stokes-Nernst-Planck-Poisson Gleichungen gezeigt. Anschliessend verifizieren wir optimale Konvergenzraten für ein effizientes Splitting-Verfahren, dessen Iterierte gegen starke Lösungen konvergieren.
Am Ende vergleichen wir mittels numerischer Experimente den energiebasierten Fixpunktalgorithmus mit dem Splitting-Verfahren.

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Contents

Chapter 1

Introduction

1.1 The Model

We introduce the electrohydrodynamic model that consists of the incompressible Navier-Stokes equations

$$
\begin{aligned}
\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \Delta\mathbf{u} + \nabla p &= \mathbf{f}_C && \text{in } \Omega_T \\
\operatorname{div}\mathbf{u} &= 0 && \text{in } \Omega_T \\
\mathbf{u} &= 0 && \text{on } \partial\Omega\times(0,T)
\end{aligned}
\tag{1.1.1}
$$

where $\mathbf{f}_C := -\big(n^+ - n^-\big)\nabla\psi$ is the Coulomb force, and $\psi = \psi_0 + \psi_1$, the sum of the internal and external electrostatic potential. To macroscopically describe the density of charged particles, we use the Nernst-Planck equations

$$
\begin{aligned}
\partial_t n^+ - \operatorname{div}\big(n^+\nabla\psi\big) - \Delta n^+ + (\mathbf{u}\cdot\nabla)\,n^+ &= 0 && \text{in } \Omega_T \\
\langle J_{n^+}, \mathbf{n}\rangle &= 0 && \text{on } \partial\Omega\times(0,T) \\
\partial_t n^- + \operatorname{div}\big(n^-\nabla\psi\big) - \Delta n^- + (\mathbf{u}\cdot\nabla)\,n^- &= 0 && \text{in } \Omega_T \\
\langle J_{n^-}, \mathbf{n}\rangle &= 0 && \text{on } \partial\Omega\times(0,T)
\end{aligned}
\tag{1.1.2}
$$

where $J_{n^\pm} := \pm n^\pm\nabla\psi - \nabla n^\pm + \mathbf{u}n^\pm$ are the fluxes of $n^\pm$. Finally, the quasi-electrostatic potential produced by the concentrations n^+ and n^- is obtained by the Poisson equation

$$
\begin{aligned}
-\Delta\psi_0 &= n^+ - n^- && \text{in } \Omega_T \\
\langle\nabla\psi_0, \mathbf{n}\rangle &= 0 && \text{on } \partial\Omega\times(0,T)\,.
\end{aligned}
\tag{1.1.3}
$$

The derivation of the system (1.1.1)–(1.1.3) is given in Chapter 2 (Navier-Stokes equations) and in Chapter 3.1.1 (Nernst-Planck-Poisson equations). This electrokinetic model finds applications in the areas of colloidal chemistry, micro- and nano-fluids, also known as electrohydrodynamics. In colloidal chemistry, one is mainly interested in an accurate description of the aggregation-, separation-, and sedimentation behavior of charged colloidal particles. The research in micro- and nano-fluids or electrohydrodynamics is forced to optimize the micro- and nano-fluidic devices fulfilling separation, mixing and pumping tasks due to the growing demand of complexity. Hence, there is a great interest in computational models to improve the design of such devices. The success of these research fields bases heavily on a better understanding of the electroosmotic and electrophoretic phenomena occurring in such fluids. These phenomena are explained in Chapter 5.1. The main interest in the investigations in Chapter 3 through 5 is to provide finite element based discretizations that converge to weak solutions of the model (1.1.1)–(1.1.3) on one hand while preserving relevant properties of weak solutions in a fully discrete setting, and to propose an efficient finite element scheme to approximate strong solutions of the system (1.1.1)–(1.1.3) at optimal rates on the other hand.

1.2 Available and New Results

A related earlier work is [64], where a simplified model based on the additional volume additivity constraint $n^+ + n^- = 1$ is studied – which e.g. immediately implies the boundedness of $n^\pm$ in $L^\infty(\Omega_T)$. This property of the solutions yields the estimates to verify existence and uniqueness of weak solutions. Chapter 3 presents for the first time existence of weak and strong solutions, an energy, and an entropy law, where such a volume additivity is neglected. There are no results in the literature concerning the numerics of the whole system (1.1.1)–(1.1.3). However, by considering only certain parts, as the Navier-Stokes equations or as the Nernst-Planck-Poisson system, one finds the following analytical and numerical results.

For the analysis of the incompressible Navier-Stokes equations we refer to P.L. Lions [50] and R. Temam [75]. The weak convergence of iterates of (1.1.1) using implicit Euler schemes and stable finite elements can be found in the book of R. Temam [75]. The strong convergence of implicit and stable (space-) discretizations with optimal rates are shown in the article [38] of J.G. Heywood and R. Rannacher. Finally, optimal convergence rates of the splitting scheme introduced by A. Chorin respectively R. Temam in 1960 are verified in the book of A. Prohl [61].

The Nernst-Planck-Poisson system (1.1.2)–(1.1.3) is analyzed in [14, 32]. This system is also referred to as the van Roosbroeck equations in the context of semiconductors. The numerical analysis mainly concentrates on the stationary version of (1.1.2)–(1.1.3) in [3, 5, 17] so far. In the instationary situation, there are some finite volume discretizations of C. Chainais-Hillairet and F. Filbet [20] and C. Chainais-Hillairet, J.-G. Liu and Y.-J. Peng [21]. We are only aware of the article of H. Gajewski and K. Gärtner [33] that recovers energy and entropy properties of the Nernst-Planck-Poisson part from the continuous context to the discrete setting in the context of finite volumes. But there is no reliable finite element discretization so far. Especially for the whole system (1.1.1)–(1.1.3), this work provides the first numerical analysis for this electrohydrodynamic system.

1.3 Analytical Investigation

To establish the existence of weak solutions to the system (1.1.1)–(1.1.3), we define a fixed point map to decouple the system into single solvable equations. Then, Schauder's fixed point theorem gives the existence of weak solutions which are unique by a standard Gronwall argument. Moreover, the weak solutions of the equations (1.1.2) show non-negativity by testing (1.1.2) with $[n^\pm]^-$, where $[x]^- := -\min\{0, x\}$ and $x = [x]^+ - [x]^-$ for $x \in \mathbb{R}$. Moreover, the $n^\pm$ are bounded in $L^\infty(\Omega_T)$ for $\Omega_T := \Omega \times (0, T)$. This is an important property for the analysis and bases on the Moser iteration. The structure of the system (1.1.2)–(1.1.3) allows some cancellations and therefore enables to shorten this iteration procedure, see Lemma 3.3.6 in Chapter 3.3.1. Finally, the weak solutions are characterized for almost every $t \in [0, T]$, where $0 < T < \infty$, by the energy principle

$$\begin{aligned}
&\frac{1}{2}\Big[\|\mathbf{u}(\cdot,t)\|_{L^2}^2 + \|\nabla\psi_0(\cdot,t)\|_{L^2}^2\Big] + \int_0^t \Big\{\|\nabla\mathbf{u}\|_{L^2}^2 + \|n^+ - n^-\|_{L^2}^2 \\
&+ \int_\Omega (n^+ + n^-)|\nabla\psi_0|^2 dx\Big\} ds \leq \frac{1}{2}\Big[\|\mathbf{u}(\cdot,0)\|_{L^2}^2 + \|\nabla\psi_0(\cdot,0)\|^2\Big] \\
&+ \int_0^t \int_\Omega (n^+ + n^-)|\nabla\psi_1\mathbf{u}| + (n^+ + n^-)|\nabla\psi_1\nabla\psi_0| dx ds
\end{aligned} \tag{1.3.1}$$

and the entropy principle

$$
\begin{aligned}
&\int_\Omega n^\pm(\cdot,t)\big(\log\big(n^\pm(\cdot,t)\big)-1\big)+2dx+\frac{1}{2}\|\nabla\psi_0(\cdot,t)\|_{L^2}^2+\frac{1}{2}\|\mathbf{u}(\cdot,t)\|_{L^2}^2\\
&+\int_0^t\|\nabla\mathbf{u}\|_{L^2}^2ds+\int_0^t\int_\Omega n^\pm\big[\nabla\big(\log(n^\pm)-\psi\big)\big]^2dxds\\
&\quad\le\int_\Omega n^\pm(\cdot,0)\big(\log\big(n^\pm(\cdot,0)\big)-1\big)+2dx+\frac{1}{2}\|\nabla\psi_0(\cdot,0)\|_{L^2}^2+\frac{1}{2}\|\mathbf{u}(\cdot,0)\|_{L^2}^2\\
&\quad+\int_0^t\int_\Omega|\nabla\psi_0\nabla\psi_1|dxds\,.
\end{aligned}
\tag{1.3.2}
$$

We remark that the verification of the existence and uniqueness of weak solutions does not require these two characterizations. Moreover, the energy principle is not even necessary for global existence which is already obtained by the $L^\infty(\Omega_T)$-boundedness and standard a priori estimates. But exactly this energy law provides the necessary uniform bounds to study long-time asymptotics in the discrete finite element setting. Only the entropy principle provides an additional characterization as the convergence behavior of the instationary solutions to its steady states. We conclude by establishing the existence of strong solutions. This is achieved by standard test function strategies under suitable assumptions on the domain and data. The analysis of the above statements is provided in the Chapter 3.

1.4 Numerical Schemes for the Nernst-Planck-Poisson Part

Since we cannot apply results from the literature to obtain a finite element based discretization of the sub-system (1.1.2)–(1.1.3) with $\mathbf{u}=\mathbf{0}$, we first establish reliable schemes in this simplified context. The details for the subsequent statements can be found in the Chapter 4. We propose in the following an energy based and an entropy based approach. For these two strategies we choose fully implicit schemes which are necessary to recover the energy law providing uniform bounds for the corresponding finite element solutions. Afterwards, these bounds allow to study long-time behavior of the iterates and to investigate their convergence behavior to its steady states by a suitable entropy law. However, this implicit character requires a convenient fixed point iteration in each timestep that ends after a finite number of steps where a suitable stopping criterion is met. Subsequently, we denote by V_h the piecewise affine finite element space. Further, we indicate with $(\cdot,\cdot)_h$ the use of reduced integration.

The energy based strategy is given by the following finite element scheme for strongly acute meshes:

Let $(P^0,N^0)\in\big[V_h\big]^2$, *such that* $\big(P^0-N^0,1\big)=0$. *For every* $j\ge 1$, *find iterates* $(P^j,N^j,\Psi^j)\in\big[V_h\big]^3$, *where* $\big(\Psi^j,1\big)=0$, *such that for all* $(\Phi_1,\Phi_2,\Phi_3)\in\big[V_h\big]^3$

$$
\begin{aligned}
&\big(d_tP^j,\Phi_1\big)_h+\Big(P^j\nabla\Psi^j,\nabla\Phi_1\Big)+\big(\nabla P^j,\nabla\Phi_1\big)=0\,,\\
&\big(d_tN^j,\Phi_2\big)_h-\Big(N^j\nabla\Psi^j,\nabla\Phi_2\Big)+\big(\nabla N^j,\nabla\Phi_2\big)=0\,,\\
&\big(\nabla\Psi^j,\nabla\Phi_3\big)=\big(P^j-N^j,\Phi_3\big)_h\,.
\end{aligned}
\tag{1.4.1}
$$

Since the scheme (1.4.1) is fully implicit and nonlinear, we linearize the scheme (1.4.1) by a fixed point algorithm. The idea is now to verify the M-matrix property of the system matrix corresponding to the following fully practical algorithm:

1. *Let* $(P^0, N^0) \in [V_h]^2$, *such that* $(P^0 - N^0, 1) = 0$. *For* $j \geq 1$, *set* $(P^{j,0}, N^{j,0}) := (P^{j-1}, N^{j-1})$, *and* $\ell := 0$.
2. *For* $\ell \geq 1$, *compute* $(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}) \in [V_h]^3$, *where* $(\Psi^{j,\ell}, 1) = 0$, *such that for all* $(\Phi_1, \Phi_2, \Phi_3) \in [V_h]^3$

$$\begin{aligned}
&\frac{2}{k}\big(P^{j,\ell}, \Phi_1\big)_h + \Big(P^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi_1\Big) + \Big(\nabla P^{j,\ell}, \nabla\Phi_1\Big) = \frac{1}{k}\Big(P^{j-1} + P^{j,\ell-1}, \Phi_1\Big)_h, \\
&\frac{2}{k}\big(N^{j,\ell}, \Phi_2\big)_h - \Big(N^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi_2\Big) + \Big(\nabla N^{j,\ell}, \nabla\Phi_2\Big) = \frac{1}{k}\Big(N^{j-1} + N^{j,\ell-1}, \Phi_2\Big)_h, \\
&\Big(\nabla\Psi^{j,\ell}, \nabla\Phi_3\Big) = \Big(P^{j,\ell} - N^{j,\ell}, \Phi_3\Big)_h .
\end{aligned} \tag{1.4.2}$$

3. *For fixed* $\theta > 0$, *stop if*

$$\|\nabla\{\Psi^{j,\ell} - \Psi^{j,\ell-1}\}\|_{L^2} + \frac{1}{k}\Big[\|P^{j,\ell} - P^{j,\ell-1}\|_h + \|N^{j,\ell} - N^{j,\ell-1}\|_h\Big] \leq \theta, \tag{1.4.3}$$

set $(P^j, N^j, \Psi^j) := (P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell})$, *and go to 4.; otherwise, set* $\ell \leftarrow \ell + 1$ *and continue with 2.*

4. *Stop if* $j + 1 = J$; *set* $j \leftarrow j + 1$ *and go to 1. otherwise.*

The M-matrix property is guaranteed by a dimensional argument which requires sufficiently small mesh parameters $h > 0$ and $k > 0$ corresponding to the space and time discretization. Due to the monotonicity property of the M-matrix, we immediately have non-negativity of $n^\pm$. Also the $L^\infty(\Omega_T)$-boundedness is a direct consequence of a discrete maximum principle which also bases on the M-matrix property. Further, we obtain the existence and uniqueness of iterates via Banach's fixed point theorem. Since the algorithm (1.4.2) converges to scheme (1.4.1) for $\theta \to 0$, we immediately have non-negativity and $L^\infty(\Omega_T)$-boundedness of iterates of the scheme (1.4.1). The discrete counterparts of the energy law (1.3.1) and the entropy law (1.3.2) can only be verified for such a fully implicit scheme. After choosing the test functions $\Phi_1 = \Psi$, $\Phi_2 = -\Psi$ and $\Phi_3 = P^j - N^j$, the energy is an immediate result of a subsequent summation, i.e.,

$$E(\Psi^J) + \frac{k^2}{2}\sum_{j=1}^{J}\|\nabla d_t\Psi^j\|_{L^2}^2 + k\sum_{j=1}^{J}\Big(P^j + N^j, |\nabla\Psi^j|^2\Big) + k\sum_{j=1}^{J}\|P^j - N^j\|_h^2 = E(\Psi^0). \tag{1.4.4}$$

Finally, the entropy principle (1.3.2) can only be verified in a perturbed way. The reason is that we have to choose the linearized test functions $\mathcal{I}_h\big[F'(\Phi_i + \delta)\big]$ for $i = 1, 2$, $\Phi_1 = P^j$, $\Phi_2 = N^j$ and $F(x) := x\big(\log(x) - 1\big) + 1$. The operator $\mathcal{I}_h$ is the linear, nodal interpolation. In contrast to the continuous case, we cannot let $\delta \to 0$ at the end. Hence, we have to control an additional perturbation term depending on $\delta > 0$. This requires to derive additional a priori estimates requiring initial data P^0, $N^0 \in H^1(\Omega)$. At the end, we obtain the entropy law

$$\begin{aligned}
&W^{j'} - W^j + \frac{k^2}{2}\sum_{\ell=j+1}^{j'}\|\nabla d_t\Psi^\ell\|_{L^2}^2 + k\sum_{\ell=j+1}^{j'}\Big[\Big(P^\ell, \Big|\nabla\big\{\Psi^\ell + \mathcal{I}_h\big[F'(P^\ell)\big]\big\}\Big|^2\Big) \\
&\quad + \Big(N^\ell, \Big|\nabla\big\{\Psi^\ell - \mathcal{I}_h\big[F'(N^\ell)\big]\big\}\Big|^2\Big)\Big] \leq Ch\delta^{-4}\Big[E(\Psi^0) + \|\nabla P^0\|_{L^2}^2 + \|\nabla N^0\|_{L^2}^2\Big]^2,
\end{aligned} \tag{1.4.5}$$

where $W^j := \int_\Omega \mathcal{I}_h\Big[F(P^j) + F(N^j)\Big] + \frac{1}{2}|\nabla\Psi^j|^2 dx$.

Since the energy based scheme allows only a perturbed entropy law and hence requires the stronger H^1-assumption on the initial data, we introduce a second entropy based scheme for general meshes:

Fix $0 < \varepsilon < 1$, and let $\big(P^0, N^0\big) \in \big[V_h\big]^2$, such that $\big(P^0 - N^0, 1\big) = 0$. For every $j \geq 1$, find iterates $\big(P^j, N^j, \Psi^j\big) \in \big[V_h\big]^3$, where $(\Psi^j, 1) = 0$ such that for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$

$$
\begin{aligned}
\big(d_t P^j, \Phi_1\big)_h + \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_\varepsilon(P^j)\nabla\Phi_1\Big) + \big(\nabla P^j, \nabla\Phi_1\big) &= 0\,, \\
\big(d_t N^j, \Phi_2\big)_h - \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_\varepsilon(N^j)\nabla\Phi_2\Big) + \big(\nabla N^j, \nabla\Phi_2\big) &= 0\,, \\
\big(\nabla\Psi^j, \nabla\Phi_3\big) &= \big(P^j - N^j, \Phi_3\big)_h\,.
\end{aligned}
\tag{1.4.6}
$$

We call the function $\boldsymbol{\mathcal{S}}_\varepsilon$ entropy-provider, since it allows for the same cancellation effects in the derivation of the entropy law as in the continuous context. In fact, the entropy-provider $\boldsymbol{\mathcal{S}}_\varepsilon$ is defined by $\boldsymbol{\mathcal{S}}_\varepsilon(P^j)\nabla\mathcal{I}_h\big[F'(P^j)\big] = \nabla P^j$ which imitates the continuous situation $n^+\nabla\log(n^+) = \nabla n^+$. The scheme (1.4.6) improves (1.4.1) such that we do not have to require any additional assumptions on the data to even obtain the following unperturbed entropy law

$$
\begin{aligned}
&W^J + \frac{k^2}{2}\sum_{\ell=1}^{J}\|\nabla d_t\Psi^\ell\|_{L^2}^2 + 2k\sum_{j=1}^{J}\|P^j - N^j\|_h^2 + k\sum_{j=1}^{J}\Big(\nabla\Psi^j, [\boldsymbol{\mathcal{S}}_\varepsilon(P^j) + \boldsymbol{\mathcal{S}}_\varepsilon(N^j)]\nabla\Psi^j\Big) \\
&\quad + k\sum_{j=1}^{J}\Big[\Big(\boldsymbol{\mathcal{S}}_\varepsilon(P^j)\nabla\mathcal{I}_h\big[F_\varepsilon'(P^j)\big], \nabla\mathcal{I}_h\big[F_\varepsilon'(P^j)\big]\Big) \\
&\quad + \Big(\boldsymbol{\mathcal{S}}_\varepsilon(N^j)\nabla\mathcal{I}_h\big[F_\varepsilon'(N^j)\big], \nabla\mathcal{I}_h\big[F_\varepsilon'(N^j)\big]\Big)\Big] \leq W^0\,,
\end{aligned}
\tag{1.4.7}
$$

where W^J is defined as in (1.4.5). Also the energy law is obtained as in the energy based approach and looks like

$$
\begin{aligned}
&E\big(\Psi^J\big) + \frac{k^2}{2}\sum_{j=1}^{J}\|\nabla d_t\Psi^j\|_{L^2}^2 + k\sum_{j=1}^{J}\Big(\nabla\Psi^j, \big[\boldsymbol{\mathcal{S}}_\varepsilon(P^j) + \boldsymbol{\mathcal{S}}_\varepsilon(N^j)\big]\nabla\Psi^j\Big) \\
&\quad + k\sum_{j=1}^{J}\|P^j - N^j\|_h^2 = E\big(\Psi^0\big)\,.
\end{aligned}
\tag{1.4.8}
$$

However, the existence and uniqueness of the entropy based scheme follows directly by Brouwer's fixed point theorem and requires no linearizing algorithm. Therefore, the proof is not constructive; hence, we do not verify an M-matrix property for the scheme (1.4.6). As a consequence, the non-negativity is replaced by a quasi-non-negativity statement which is defined in the following sense:

For a given space discretization parameter $h > 0$ there exists a lower bound $\sigma(h) > 0$ such that $\sigma(h) \to 0$ for $h \to 0$. Then, the iterates of scheme (1.4.6) are called quasi-non-negative if they satisfy $-\sigma(h) \leq P^j,\ N^j$.

The verification of this quasi-non-negativity relies on the entropy principle. The idea comes from the entropy-mobility construction introduced in the context of thin films by G. Grün and M. Rumpf in [36]. Hence, the entropy based approach convinces by no additional regularity requirements and an entropy inequality not requiring any coupling of mesh parameters. The disadvantage is that we only obtain quasi-non-negativity and no discrete maximum principle in a direct approach, i.e., without verifying the M-matrix property.

1.5 Convergent, properties-preserving finite-element based Discretization of the Electrohydrodynamic Model

We now consider the whole system (1.1.1)–(1.1.3), i.e. $\mathbf{u} \neq \mathbf{0}$. Hence, we additionally have to control the convective term $\operatorname{div}\big(\mathbf{u}n^{\pm}\big)$, and to suitably discretize the incompressible Navier-Stokes equations. For this purpose, we use the MINI-element characterized by the pair $(\,\mathbf{V}_h,\, M_h\,)$. We denote by Y_h the piecewise affine finite element space. We follow the energy based approach implying the scheme:

(1). Set $\mathbf{U}^0 = J_{\mathbf{V}_h}\mathbf{u}_0$ *and* $\big((N^+)^0, (N^-)^0\big) := \big(J_{Y_h}n_0^+, J_{Y_h}n_0^-\big)$ *with* $\big(n_0^+ - n_0^-, 1\big) = 0$.

(2). For $j = 1, \dots, J$, *let* $\mathbf{F}_C^j := -((N^+)^j - (N^-)^j)\nabla\Psi^j$. *Find* $(\,\mathbf{U}^j,\, \Pi^j,\, (N^+)^j,\, (N^-)^j,\, \Psi^j) \in \mathbf{V}_h \times M_h \times [Y_h]^3$, *where* $(\Psi^j, 1) = 0$, *such that for all* $(\,\mathbf{V},\, \Phi^{\pm},\, \Phi,\, Q\,) \in \mathbf{V}_h \times [Y_h]^3 \times M_h$

(1.5.1)
$$\begin{aligned}
&(d_t\mathbf{U}^j, \mathbf{V}) + (\nabla\mathbf{U}^j, \nabla\mathbf{V}) + \epsilon(\nabla d_t\mathbf{U}^j, \nabla\mathbf{V}) + \big((\mathbf{U}^{j-1}\cdot\nabla)\mathbf{U}^j, \mathbf{V}\big) + \frac{1}{2}\big((\operatorname{div}\mathbf{U}^{j-1})\mathbf{U}^j, \mathbf{V}\big)\\
&\qquad\qquad - (\Pi^j, \operatorname{div}\mathbf{V}) = (\mathbf{F}_C^j, \mathbf{V})\,,\\
&(\operatorname{div}\mathbf{U}^j,\, Q) = 0\,,\\
&(d_t(N^{\pm})^j, \Phi^{\pm})_h + (\nabla(N^{\pm})^j, \nabla\Phi^{\pm}) \pm \big((N^{\pm})^j\nabla\Psi^j, \nabla\Phi^{\pm}\big) - (\mathbf{U}^j(N^{\pm})^j, \nabla\Phi^{\pm}) = 0\,,\\
&(\nabla\Psi^j, \nabla\Phi) = ((N^+)^j - (N^-)^j, \Phi)_h\,,
\end{aligned}$$

where $\epsilon := h^{\alpha}$ *with* $0 < \alpha < \frac{6-N}{3}$ *and* $(\Psi^j, 1) = 0$.

Later on, we will see that we have to require the following compatibility condition

$$Y_h/\mathbb{R} \subseteq M_h \tag{1.5.2}$$

between Y_h and M_h, which represents the coupling character of (1.1.1)–(1.1.3). To verify that the above scheme (1.5.1) is reliable, that means that it allows to recover all the characteristic properties for iterates as non-negativity, $L^\infty(\Omega_T)$-boundedness, energy and entropy principles from the continuous context to the discrete setting, we adapt the ideas from the energy based scheme (1.4.1). This procedure is not straightforward as one can already recognize by the ϵ-regularization. The scheme (1.5.1) is again fully implicit to be able to verify the energy and entropy properties. In practice, we linearize the fully implicit scheme (1.5.1) by the following implementable algorithm:

1. *Let* $(\mathbf{U}^0, (N^+)^0, (N^-)^0) \in \mathbf{V}_h \times [Y_h]^2$ *such that* $((N^+)^0 - (N^-)^0, 1) = 0$. *For* $j \geq 1$, *set* $\Big((N^+)^{j,0}, (N^-)^{j,0}\Big) := \Big((N^+)^{j-1}, (N^-)^{j-1}\Big)$, *and* $\ell := 0$.

2. For $\ell \geq 1$*, compute* $\Big(\mathbf{U}^{j,\ell}, (N^+)^{j,\ell}, (N^-)^{j,\ell}, \Psi^{j,\ell-1}, \Pi^{j,\ell}\Big) \in \mathbf{V}_h \times [V_h]^3 \times M_h$ *that solve for all* $\Big(\mathbf{V}, \Phi^\pm, \Phi, Q\Big) \in \mathbf{V}_h \times [Y_h]^3 \times M_h$*, and* $\mathbf{F}_C^{j,\ell-1} := -\big((N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}\big)\nabla\Psi^{j,\ell-1}$,

$$\begin{aligned}
&\Big(\nabla\Psi^{j,\ell-1}, \nabla\Phi\Big) = \Big((N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}, \Phi\Big)_h\,,\\
&\frac{1}{k}\Big(\mathbf{U}^{j,\ell}, \mathbf{V}\Big) + \frac{\epsilon}{k}\Big(\nabla\mathbf{U}^{j,\ell}, \nabla\mathbf{V}\Big) + \Big(\nabla\mathbf{U}^{j,\ell}, \nabla\mathbf{V}\Big) + \epsilon\Big(\nabla d_t\mathbf{U}^{j,\ell}, \nabla\mathbf{V}\Big)\\
&\quad + \Big((\mathbf{U}^{j-1}\cdot\nabla)\mathbf{U}^{j,\ell}, \mathbf{V}\Big) + \frac{1}{2}\Big((\mathrm{div}\mathbf{U}^{j-1})\mathbf{U}^{j,\ell}, \mathbf{V}\Big) = \Big(\Pi^{j,\ell}, \mathrm{div}\mathbf{V}\Big) + \Big(\mathbf{F}_C^{j,\ell-1}, \mathbf{V}\Big)\\
&\quad + \frac{1}{k}\Big(\mathbf{U}^{j-1}, \mathbf{V}\Big) + \frac{\epsilon}{k}\Big(\nabla\mathbf{U}^{j-1}, \nabla\mathbf{V}\Big)\,,\\
&\frac{1}{k}\Big((N^\pm)^{j,\ell}, \Phi^\pm\Big)_h \pm \Big((N^\pm)^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi^\pm\Big) + \Big(\nabla(N^\pm)^{j,\ell}, \nabla\Phi^\pm\Big)\\
&\qquad - \Big(\mathbf{U}^{j,\ell-1}(N^\pm)^{j,\ell}, \nabla\Phi^\pm\Big) = \frac{1}{k}\Big((N^\pm)^{j-1}, \Phi^\pm\Big)_h\,,\\
&\Big(\mathrm{div}\,\mathbf{U}^{j,\ell}, Q\Big) = 0\,,
\end{aligned} \tag{1.5.3}$$

where $(\Psi^{j,\ell-1}, 1) = 0$*.* 3. *Stop, if for fixed* $\theta > 0$ *we have*

$$\begin{aligned}
&\|\mathbf{U}^{j,\ell} - \mathbf{U}^{j,\ell-1}\|_{L^2} + \|\nabla\{\Psi^{j,\ell} - \Psi^{j,\ell-1}\}\|_{L^2}\\
&+ \Big(\|(N^+)^{j,\ell} - (N^+)^{j,\ell-1}\|_{L^\infty} + \|(N^-)^{j,\ell} - (N^-)^{j,\ell-1}\|_{L^\infty}\Big) \leq \theta
\end{aligned} \tag{1.5.4}$$

and go to 4.; set $\ell \leftarrow \ell + 1$ *and continue with 2. otherwise.*
4. *Stop, if* $j + 1 = J$*; set* $j \leftarrow j + 1$ *and go to 1. otherwise.*

This algorithm (1.5.3) allows us to recover in a constructive way all the results from the continuous context (Section 1.3) to the discrete finite element setting. Existence and uniqueness of iterates of algorithm (1.5.3) follow from Banach's fixed point theorem under the mild mesh constraint $k < Ch^{\frac{N}{3}+\sigma}$ for $\sigma > 0$. Further, we verify that the system matrix for the concentrations in algorithm (1.5.3) is an M-matrix. In contrast to the case $\mathbf{U}^j = \mathbf{0}$, the lack of regularity of $\mathbf{U}^j$ prevents a straightforward verification. As a consequence, the term $\epsilon d_t\nabla\mathbf{U}^j$ also appears in the scheme (1.5.1) and the algorithm (1.5.3). Hence, testing the Navier-Stokes equation in scheme (1.5.1) with $\mathbf{V} = \mathbf{U}^j$ provides the necessary regularity to establish the M-matrix property by a dimensional argument which guarantees the dominating influence of the stiffness matrix. But afterwards, this additional ϵ-term in the scheme (1.5.1) complicates the derivation of the necessary time-regularity to obtain compactness by Aubin-Lions' theorem. Therefore, we define the test function $\mathbf{W}^j \in \mathbf{V}_h$ in (1.5.1) with the help of the solution of

$$\frac{1}{\epsilon}\Big(\nabla\mathbf{W}^j, \nabla\mathbf{\Phi}\Big) = \Big(d_t\mathbf{U}^j, \mathbf{\Phi}\Big) \qquad \text{for all } \mathbf{\Phi} \in \mathbf{V}_h\,, \tag{1.5.5}$$

in order to gain the necessary bounds for the compactness. The M-matrix property implies non-negativity and boundedness of the concentrations in algorithm (1.5.3). These iterates converge to solutions of the scheme (1.5.1) by sending $\theta \to 0$ in the stopping criterion (1.5.4). In addition to the assumptions for the M-matrix property, we now have to require the compatibility property (1.5.2) between Y_h and M_h to verify the boundedness of $(N^\pm)^j$. Let us remark that a straightforward analysis using inverse estimates instead of the ϵ-regularization ends up in conflicting coupling constraints of the mesh parameters. For the energy functional

$E(\mathbf{U}^j,\Psi^j) := \frac{1}{2}\Big[\|\mathbf{U}^j\|^2_{L^2} + \|\nabla\Psi^j\|^2_{L^2}\Big]$, we have the following energy law

$$
\begin{aligned}
&E(\mathbf{U}^J,\Psi^J) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^J\|^2_{L^2} + k\sum_{j=1}^{J}\|\nabla\mathbf{U}^j\|^2_{L^2} + k^2\sum_{j=1}^{J}\Big\{E(d_t\mathbf{U}^j,d_t\Psi^j) + \frac{\epsilon}{2}\|d_t\nabla\mathbf{U}^j\|^2_{L^2}\Big\} \\
&+ k\sum_{j=1}^{J}\Big[\|\nabla\mathbf{U}^j\|^2_{L^2} + \|(N^+)^j - (N^-)^j\|^2_h\Big] = E(\mathbf{U}^0,\Psi^0) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^0\|^2_{L^2}\,,
\end{aligned}
\tag{1.5.6}
$$

which is obtained by choosing the testfunctions $\mathbf{V} = \mathbf{U}^j$, $\Phi^\pm = \pm N^\pm$ and $\Phi = N^+ - N^-$. The scheme (1.5.1) allows only a perturbed entropy law requiring more regular initial data as the energy based scheme (1.4.1) for the Nernst-Planck-Poisson system. Since the derivation of an unperturbed entropy law would be straightforward thanks to the already derived results for the entropy based scheme (1.4.6) and the unsatisfying results as quasi-non-negativity, no discrete maximum principle, necessity of several applications of the entropy-provider $\boldsymbol{\mathcal{S}}_\epsilon$ and the non-constructive proof, we do not provide any details to such an approach, see also Chapter 5.5.3. By choosing the testfunctions $\mathbf{V} = \mathbf{U}^j$ and $\Phi^\pm = \mathcal{I}_h\big[F'(N^\pm)\big] - \nabla\Psi^j$, we obtain the perturbed entropy law in two dimensions

$$
\begin{aligned}
&W^{j'} + \frac{k^2}{2}\sum_{l=j+1}^{j'}\Big[\|\nabla d_t\Psi^l\|^2_{L^2} + \epsilon\|d_t\nabla\mathbf{U}^l\|^2_{L^2}\Big] + k\sum_{l=j+1}^{j'}\Big[\big((N^+)^l, \big|\nabla\Psi^l + \mathcal{I}_h\big[F'((N^+)^l)\big]\big|^2\big) \\
&\qquad + \|\nabla\mathbf{U}^l\|^2_{L^2} + \big((N^-)^l, \big|\nabla\big\{\Psi^l - \mathcal{I}_h\big[F'((N^-)^l)\big]\big\}\big|^2\big)\Big] \\
&\qquad\qquad \le W^j + Ch\delta^{-4}\Big[E(\mathbf{U}^0,\Psi^0) + \|\nabla(N^+)^0\|^2_{L^2} + \|\nabla(N^-)^0\|^2_{L^2}\Big]^2\,,
\end{aligned}
\tag{1.5.7}
$$

where

$$
W^J := E\big(\mathbf{U}^J,\Psi^J\big) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^J\|^2_{L^2} + \int_\Omega\Big\{\mathcal{I}_{Y_h}\Big[F\Big((N^+)^J\Big) + F\Big((N^-)^J\Big)\Big] + 2\Big\}\,dx\,.
$$

To approximate strong solutions, we analyze a time-splitting scheme based on Chorin's projection method [22]. In this scheme, the computation of iterates is fully decoupled in every time-step which leads to significantly reduced computational resurces. But this strategy sacrifices the discrete energy and entropy inequalities, which are relevant tools to characterize long-time asymptotics and convergence towards weak solutions. Therefore, the related numerical analysis requires the existence of (local) strong solutions which is verified in Chapter 3.

We propose the following efficient time-splitting scheme:

Given $\big\{\mathbf{u}^{j-1},(n^\pm)^{j-1}\big\}$*, determine* $\big\{\mathbf{u}^j,(n^\pm)^j,\psi^j\big\} \in \mathbf{S}$ *in the following way:*

1. *Start with* $\mathbf{u}^0 = \mathbf{u}_0$, $(n^\pm)^0 = n_0^\pm$. *Then the following steps determine the iterates for* $j \ge 1$.
2. *Compute* ψ^{j-1} *from*

$$
\begin{aligned}
-\Delta\psi^{j-1} &= (n^+)^{j-1} - (n^-)^{j-1} \\
\langle\nabla\psi^{j-1},\mathbf{n}\rangle &= 0 \quad \text{on } \partial\Omega\,.
\end{aligned}
$$

3. *Compute* $(n^{\pm})^j$ *via*

$$\begin{aligned} \frac{1}{k}\big\{(n^{\pm})^j - (n^{\pm})^{j-1}\big\} - \Delta(n^{\pm})^j \pm \mathrm{div}((\mathrm{n}^{\pm})^{\mathrm{j}}\nabla\psi^{\mathrm{j}-1}) + (\mathbf{u}^{\mathrm{j}-1}\cdot\nabla)(\mathrm{n}^{\pm})^{\mathrm{j}} &= 0 \\ \langle\nabla(n^{\pm})^j \pm (n^{\pm})^j\nabla(n^{\pm})^{j-1} + \mathbf{u}^{j-1}(n^{\pm})^j, \mathbf{n}\rangle &= 0 \quad \textit{on } \partial\Omega\,. \end{aligned}$$

4. *Find* $\tilde{\mathbf{u}}^j$ *by solving*

$$\begin{aligned} \frac{1}{k}\big\{\tilde{\mathbf{u}}^j - \mathbf{u}^{j-1}\big\} - \Delta\tilde{\mathbf{u}}^j + (\mathbf{u}^{j-1}\cdot\nabla)\tilde{\mathbf{u}}^j &= -\Big((n^+)^j - (n^-)^j\Big)\nabla\psi^{j-1} \\ \tilde{\mathbf{u}}^j &= 0 \quad \textit{on } \partial\Omega\,. \end{aligned}$$

5. *Determine the tuple* $\big\{\mathbf{u}^j, (N^+)^j\big\} \in V^{0,2} \times H^1/\mathbb{R}$ *that solves the system*

$$\frac{1}{k}\big\{\mathbf{u}^j - \tilde{\mathbf{u}}^j\big\} + \nabla p^j = 0 \tag{1.5.8}$$

$$\mathrm{div}\,\mathbf{u}^j = 0, \qquad \mathbf{u}^j\cdot\mathbf{n} = 0, \quad \textit{on } \partial\Omega\,. \tag{1.5.9}$$

To analyze this scheme, we introduce several auxiliary problems taking care of each error caused by the single splitting steps. The analysis succeeds thanks to an inductive argument on the error control over the time steps $0 \le j \le J$ to compensate for the lack of a discrete energy law. As a consequence of these techniques, the iterates of our time-splitting scheme converge to strong solutions at optimal rates. These results are generalized to a fully discrete setting in a last step.

Finally, we compare the energy based and the splitting scheme by computational experiments. The computational demand of the fixed point iterations used in the energy based algorithm is up to six iterations. The comparison of this algorithm with the splitting scheme indicates through all computations that the time-splitting scheme requires only half of the computational time than the energy based algorithm. Especially, if small time scales are needed to obtain more accurate results, then the fixed point iterations consume a significant amount of CPU-time. Therefore, it is reasonable to only use the energy based algorithm A_1, if physical relevant properties such as non-negativity, discrete maximum principle, energy and entropy characterizations have necessarily to be preserved.

The chapters are organized in the following way: In Chapter 2, we give some motivations and provide the necessary assumptions to apply the electrohydrodynamic system (1.1.1)–(1.1.3). Existence, uniqueness of solutions to (1.1.1)–(1.1.3) and additional characterizations of weak solutions are shown in Chapter 3. We provide an energy based and an entropy based finite element approximation converging to weak solutions of the Nernst-Planck-Poisson system in Chapter 4. The extension to the whole electrohydrodynamic system is given in Chapter 5. In the same chapter, we propose an efficient time-splitting scheme based on Chorin's projection method to approximate strong solutions, and we verify convergence of iterates to strong solutions at optimal rates.

This Ph.D. thesis summarizes the three research papers [62, 63, 71].

Chapter 2

Physical Introduction and Model Assumptions

First, we explain the setting on which we base the considerations leading toward the later on analyzed electrokinetic model.

2.1 Fluid and Flow Properties

We regard the fluid as a single continuum phase that is continuously and indefinitely divisible. This ensures that all macroscopic physical, chemical, and thermodynamic quantities, such as momentum, energy, density, and temperature, are finite and uniformly distributed over any infinitesimally small volume, and allows to talk about the value of the quantity "at a point". Moreover, we assume that the characteristic macroscopic flow scale is large compared with the molecular length scale characterizing the structure of the fluid.

Since our fluids of interest are regarded as continuous, the distinction between liquids and gases is not fundamental with respect to the dynamics, provided compressibility may be neglected. A gas is much less dense and much more compressible than a liquid as long as it is not too close to or above the critical temperature at which it can be liquefied. The behavior of a gas flow with small pressure changes is essentially the same as that of an "incompressible" liquid flow. Then the density in a flowing compressible gas can be regarded as essentially constant if the changes in pressure are small. Therefore, we emphasize that one should not interpret "incompressible" with "constant density". As an example, a low-speed flow of air may be regarded a constant density flow despite the fact that air is a highly compressible fluid.

We consider fluids that support viscous effects, usually termed transport effects. These include diffusion of mass, heat, and charge. Transport effects together with non-equilibrium effects, such as finite-rate chemical reactions and phase changes, have their roots in the molecular behavior of the fluid and are dissipative. Dissipative phenomena are associated with thermodynamic irreversibility and an increase in the global entropy. But in the following we neglect thermodynamic effects.

2.1.1 Newton's Viscosity Law in Two Dimensions

Let us first examine Newton's law of viscosity. It states that there is a linear relation between the shear stresses and rates of strain. Let us first examine this law for the case of simple shear where there is only one strain component. For an intuitive understanding, we consider the planar

Figure 2.1.1: Shear flow between two parallel plates (left) and forces on a fluid element (right), see [78]. ($x = x_1$, $y = x_2$)

Couette problem [73, p. 27] with the velocity field

$$u_1 = \dot{\gamma} x_2 \quad u_2 = 0 \quad u_3 = 0\,, \tag{2.1.1}$$

arising by the parallel motion of one infinite plate at a constant speed $\dot{\gamma}$ with respect to a second fixed infinite plate, the plates being separated by a small distance $2h$ with the pressure p constant throughout the fluid. The role of boundary conditions in a viscous flow is critical, and we assume the *no-slip condition*, i.e., the fluid 'sticks' to both plates. A tangential force is required to maintain the motion of the moving plate, and this force must be in equilibrium with the frictional forces in the fluid. Hence, a force balance for the fluid element in Figure 2.1.1 gives for the net force acting on the element in the x_1 direction

$$\sum_{i=1}^{4} F_{x_1}^i = \Big(\frac{\partial \tau_{x_2 x_1}}{\partial x_2}\Big) \Delta x_2 \Delta x_1 A\,, \tag{2.1.2}$$

where A is the unit area of the fluid element, hence $A = 1$, and

$$\begin{aligned} F_{x_1}^1 &:= -\tau_{x_2 x_1} \\ F_{x_1}^2 &:= p \Delta x_2 \Delta x_1 = \tau_{x_1 x_2} \\ F_{x_1}^3 &:= \tau_{x_2 x_1} + \frac{\partial \tau_{x_2 x_1}}{\partial x_2} \Delta x_2 \Delta x_1 \\ F_{x_1}^4 &:= -p \Delta x_2 \Delta x_1 = -\tau_{x_1 x_2}\,. \end{aligned} \tag{2.1.3}$$

Here, $\tau_{x_2 x_1}$ is the shear stress exerted in the x_1 direction on a fluid surface of constant center of mass (x_1, x_2). In (2.1.3) we applied the following convention: On a positive x_2 face the shear is positive in the positive x_1 direction, and on a negative x_2 face the shear is positive in the negative x_1 direction.

For the mass density ρ and the material derivative $\frac{D}{Dt}$ that corresponds to the total time derivative by the equation

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i},$$

we obtain from Newton's second law applied on a fluid element with the volume $V = \Delta x_1 \Delta x_2$ the relation

(2.1.4)
$$\frac{\sum_{i=1}^{4} F^i_{x_1}}{V} = \rho \frac{Du}{Dt}\,.$$

For steady flows, i.e. $\dot{\gamma} = \text{const.}$, with plates infinite in x_1 direction implies $\frac{\partial}{\partial t} = 0$ and $\frac{\partial}{\partial x_1} = 0$. As a consequence, we obtain the velocities as in the shear plate problem (2.1.1). Hence, $\frac{D}{Dt} = 0$, and with (2.1.2) we obtain

(2.1.5)
$$\frac{\sum_{i=1}^{4} F^i_{x_1}}{V} = \frac{\partial \tau_{x_2 x_1}}{\partial x_2} = 0$$

and hence throughout the fluid

(2.1.6)
$$\tau_{x_2 x_1} = \text{const.}\,.$$

For most fluids the shear stress is a unique function of the strain rate. The constitutive relation of Newton assumes the shear stress to be linear in the strain rate. In the Couette problem (2.1.1) there is only the single strain-rate component $\frac{\partial u_1}{\partial x_2} = \dot{\gamma}$ and single stress component $\tau_{x_2 x_1}$, therefore the Newtonian viscosity law reads as

(2.1.7)
$$\tau_{x_2 x_1} = \eta \frac{\partial u_1}{\partial x_2} = \eta \dot{\gamma}\,.$$

The quantity η is the viscosity coefficient of a *Newtonian fluid*, i.e. a fluid following the law (2.1.7). It is an intensive property and is generally a function of temperature and pressure, although under most conditions for simple fluids it is a function of temperature alone. Polymeric fluids and suspensions may not follow the Newtonian law (2.1.7), and when they do not they are termed *non-Newtonian fluids.* In viscous flows the ratio

$$\nu = \frac{\eta}{\rho}$$

frequently occurs and is termed the *kinematic viscosity.* Of importance is that ν has the same dimensions as the coefficient of diffusion in a mass transfer problem and may be interpreted as a diffusion coefficient for momentum. An important point to observe is that for gases the viscosity increases with temperature, whereas for liquids the viscosity usually decreases. The dependence on the pressure is not strong.

The reason for the different behaviors of viscosity with temperature lies in the different mechanisms of momentum transport in gases, where the molecules are on average relatively far apart, and in liquids, where they are close together. The origin of shear stress arises from molecular motions in which molecules that move from a region of higher average transverse velocity toward a region of lower average transverse velocity carry more momentum than those moving in the opposite direction. This transfer of excess molecular momentum manifests itself as a macroscopic shear. In a gas the momentum transport of the molecules from a region of lower to higher velocity, or vice versa, is proportional to the random thermal motion or mean molecular speed. Calculation leads to a coefficient of kinematic viscosity

$$\nu \sim \bar{c} l\,,$$

where l is the mean free path between collisions and $\bar{c}$ is the mean molecular speed, a quantity that increases as the square root of the absolute temperature.

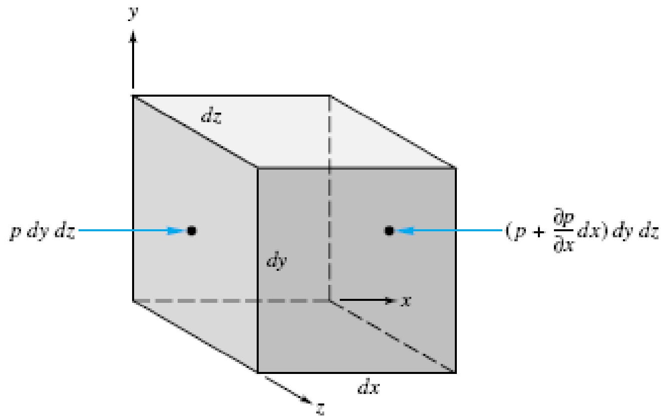


Figure 2.1.2: Net x force on an element due to pressure variation, see [78].

For a liquid we considerably have a different situation. The molecules have a preferred motion because, due to the close molecular packing, they acquire sufficient activation energy to "jump" to a neighboring vacant lattice site. With the activation energy ΔG of the molecule to escape to a vacant site in the fluid, we obtain the proportionality

$$\tau_{x_2x_1}\exp\Big(-\frac{\Delta G}{RT}\Big) \sim \frac{\partial u_1}{\partial x_2}\,, \tag{2.1.8}$$

where $\frac{\partial u_1}{\partial x_2}$ is the velocity gradient normal to the main direction of motion, R is the gas constant, and T is the absolute temperature. The exponential term characterizes the probability of a molecule in a fluid at rest escaping into an adjoining "hole". For a fluid flowing in the direction of the molecular jump, this probability is increased in proportion to the shear stress because of the additional work done on the molecules by the fluid motion. Newton's viscosity law (2.1.7) applied to (2.1.8) implies

$$\eta \sim \exp\Big(\frac{\Delta G}{RT}\Big)\,.$$

This exponential decrease of viscosity with temperature agrees with the observed behavior of most liquids.

2.1.2 Extension of Newton's Viscosity Law to Three Dimensions

We generalize the Newton viscosity law to three dimensions. In two dimensions we just considered the case of constant pressure p. Hence let us first generalize the balance equation (2.1.2) to the non-constant pressure case. To do so, we complete the force balance (2.1.2) with the balance of the pressure force varying in x direction as depicted in Figure 2.1.2 under neglect of the $z = x_3$ direction. Therefore, we only have to modify the force

$$F^2_{x_1} \qquad \text{to} \qquad F^2_{x_1} := \Big(-p - \frac{\partial p}{\partial x_1}\Big)\Delta x_2 \Delta x_1\,. \tag{2.1.9}$$

For a general fluid, the pressure variation can be present in all three space dimensions. Hence, the stresses on the sides of the control surface of the the fluid element, called surface forces and subsequent denoted by $\mathbf{f}_{\text{surf}}$, are the sum of the hydrostatic pressure p plus the viscous stresses $\tau_{x_ix_j}$ which arise from motion with velocity gradients

$$\sigma_{ij} := \begin{bmatrix} -p + \tau_{x_1x_1} & \tau_{x_2x_1} & \tau_{x_3x_1} \\ \tau_{x_1x_2} & -p + \tau_{x_2x_2} & \tau_{x_3x_2} \\ \tau_{x_1x_3} & \tau_{x_2x_3} & -p + \tau_{x_3x_3} \end{bmatrix}, \tag{2.1.10}$$

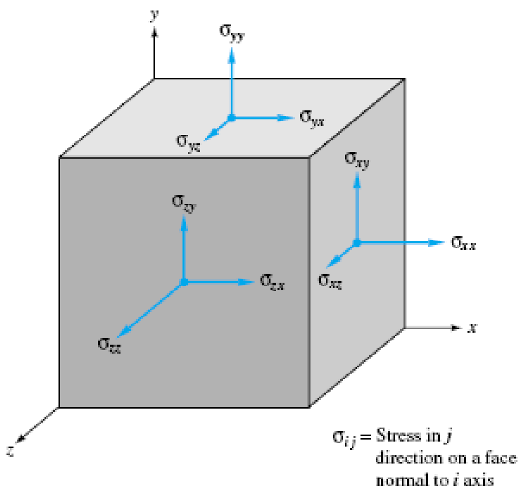


Figure 2.1.3: Connection between a fluid element and the entries of the stress tensor σ_{ij}, see [78]

and therefore $\sigma_{ij} := -p\delta_{ij} + \tau_{x_j x_i}$ for δ_{ij} the Kronecker symbol being 1 for $i = j$ and else 0. The matrix (2.1.10) is called *stress tensor*. The shear terms $\tau_{x_j x_i}$ are symmetric, i.e. $\tau_{x_j x_i} = \tau_{x_i x_j}$ for $i \neq j$. As a consequence, the stress tensor σ has only six independent components.

Assumptions on a Newtonian fluid [8]:

i) The fluid is isotropic; that is, the properties are independent of direction.

ii) In a static or inviscid fluid the stress tensor must reduce to the hydrostatic pressure condition; that is $\sigma_{ij} = -p\delta_{ij}$.

iii) The stress tensor σ_{ij} is at most a linear function of the shear tensor $\tau_{x_j x_i}$.

One recognizes that condition ii) is already satisfied. Moreover, with these assumptions it can be shown, that the shear tensor $\tau_{x_j x_i}$ in a Newtonian fluid becomes

(2.1.11) $$\tau_{x_j x_i} := 2\eta\Big(\epsilon_{ij} - \frac{1}{3}\mathrm{div}\,\mathbf{u}\,\delta_{ij}\Big)\,,$$

where the rate-of-strain tensor ϵ_{ij} is defined as

(2.1.12) $$\epsilon_{ij} := \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big)\,,$$

and $\mathbf{u} := [u_1, u_2, u_3]'$. Finally, conservation of momentum as expressed through Newton's second law (2.1.4) applied to a fluid particle may be written as

(2.1.13) $$\rho\frac{D\mathbf{u}}{Dt} = \mathbf{f}_{\mathrm{body}} + \mathbf{f}_{\mathrm{surf}}\,,$$

where the applied force per unit volume on the fluid particle is divided into surface and body forces. The body forces are proportional to the total volume or mass of the fluid element, examples of which are the gravitational, electrical or electromagnetic body force. Here, especially the electrical body force is considered, which per unit volume is

$$\mathbf{f}_{\mathrm{body}} := -\rho_q \nabla\psi\,,$$

where $\nabla\psi$ is the electrical field corresponding to the electrostatic potential ψ and ρ_q is the charge density in the fluid. The surface forces are given by the external stresses defined by (2.1.10) and by Gauss's theorem as

$$\begin{aligned}\mathbf{f}_{\mathrm{surf}} := \operatorname{div}\sigma_{ij} &= \frac{\partial\sigma_{ij}}{\partial x_j}\\ &= -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left\{\eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{u_k}{\partial x_k}\right)\right\}.\end{aligned}$$

The equation (2.1.13) is usually referred to as the *Navier-Stokes equation*. It is called incompressible, if $\operatorname{div}\mathbf{u} = \frac{\partial u_k}{\partial x_k} = 0$. Further, if the viscosity η is constant, the the Navier-Stokes equation reduces for $\operatorname{div}\mathbf{u} = 0$ to

$$\rho\frac{D\mathbf{u}}{Dt} = -\nabla p + \eta\Delta\mathbf{u} - \rho_q\nabla\psi\,. \tag{2.1.14}$$

2.2 Particles and their Geometry

We deal with suspensions of small "particles", including macromolecules, colloids, cells, and flocs. Generally, we will consider macromolecules to represent the smallest dispersed phase that is not considered as a single component. Subsequent, we precise the term macro molecule and provide examples motivated by their interest in practical applications.

A *macro molecule* is a large molecule composed of many small, simple chemical units called structural units. It may be either biological or synthetic. Biological macromolecules contain numerous structural units, in contrast to synthetic macromolecules. Sometimes all macromolecules are referred to as *polymers*, although a polymer may be distinguished as a macro molecule made up of repeating units. Polyethylene, for example, is a synthetic polymer built up from a single repeating unit, the ethylene group. Each structural unit in the polyethylene polymer is connected to two other structural units such that these structures together build a linear chain.

A special biological macro molecule is a *protein*. It is composed of amino acid residues of the 20 common amino acids, joined consecutively by peptide bonds. *Hemoglobin*, the oxygen-carrying protein in red blood cells, is nearly spherical, with a diameter of about 5 nm [70]. A model of a hemoglobin molecule as deduced in [59] from x-ray diffraction studies is built up from blocks representing the electron density patterns at various levels in the molecule. A larger protein, one that is fundamental to the blood-clotting process, is *fibrinogen*, a long slender molecule with a length of about 50 nm [70]. On a scale often an order of magnitude larger are viruses, which are very symmetric rigid macromolecules consisting of infectious nucleic acids surrounded by coats made up of protein subunits. The structure of a *tobacco* mosaic virus of length about 300 nm is given in Figure 2.2.1. However, the fibrinogen protein and the tobacco virus are not further considered here because of the geometrical shape which is of interest in the following part.

Given a variety of particles and their diverse shapes, the question arises how they are represented or modeled in a rational treatment of their interactions in fluid systems. The interactions of these particles with the fluid system depends highly on their geometry. Often their shapes are complex. Here we choose the most often used sphere shaped geometry in the Euclidean sense. Many protein macromolecules can be regarded as spherical to motivate our assumption on the geometry. For example, hemoglobin in Figure 2.2.2, synthetic polymers dispersed in suspension, like the polystyrene latex particles shown in the electron micrograph of Figure 2.2.3, are spherical or very nearly spherical, as are the particles of numerous colloidal systems.

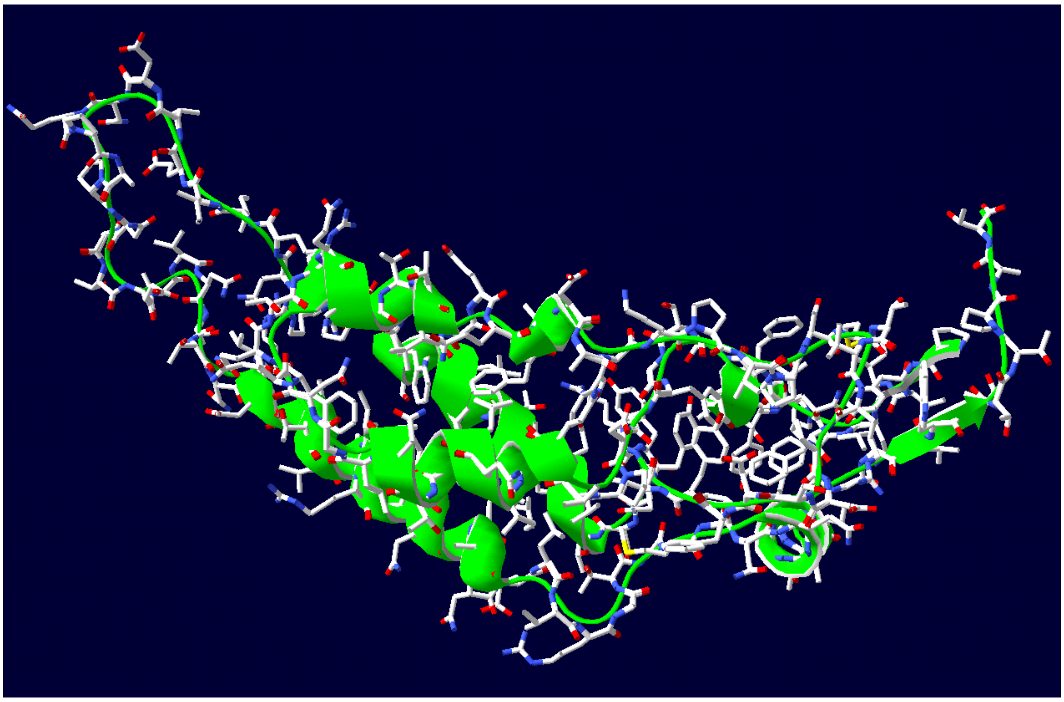


Figure 2.2.1: The Tobacco mosaic virus (TMV) is an RNA virus that infects plants.
(from `http://commons.wikimedia.org/wiki/Image:Tobacco_MosaicVirus_structure.png`)

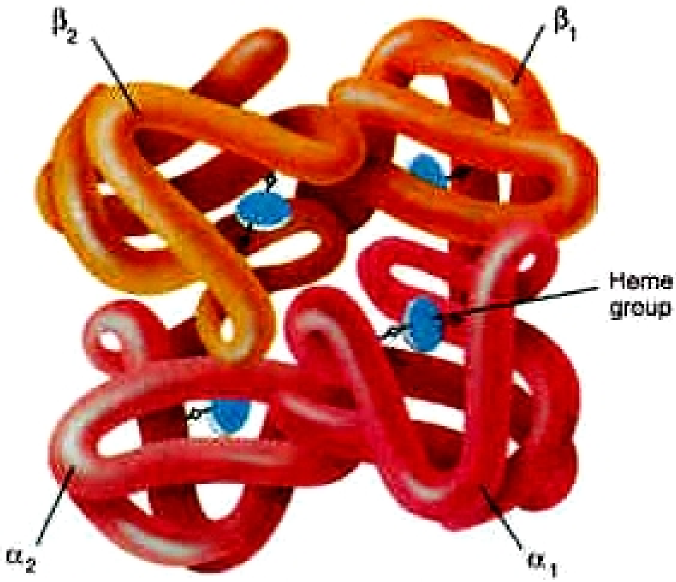


Figure 2.2.2: The hemoglobin model from Perutz (1964).
(from `http://www.daviddarling.info/encyclopedia/H/hemoglobin.html`)

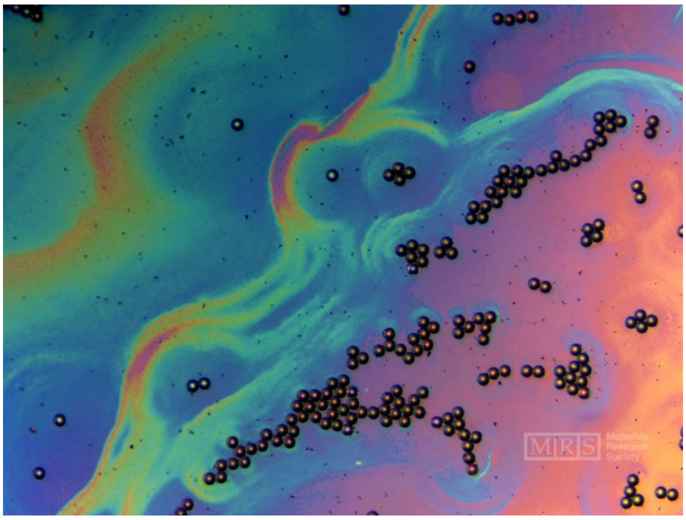


Figure 2.2.3: The aggregation of polystyrene latex particles.
(from http://www.mrs.org/s_mrs/doc.asp?CID=1920&DID=171434)

A relatively simple geometric description seem amenable, in many cases, to individual particles of which we have spoken. However, in solution, particles may floc or aggregate due to random particle-particle and particle-floc collisions, and generally complex shapes arise that belie the much simpler shape of the original particle. The Figure 2.2.4 shows an irreversible aggregate formed in suspension of spherical gold particles with diameter 15 nm. The treelike cluster of such a gold aggregate is one of a general class of shapes named *fractals* by Mandelbrot [52]. For such clusters we have to assume low-speed, inertia free flow (low Reynolds number flow) such that the sphere shape is an applicable model assumption on the particles. First, we draw around an arbitrary point of the cluster a sphere of radius r. Then the number of particles N is counted. For r ranging from about the particle size to the cluster size, it is found that $N(r) \sim (r)^{1.75}$ [76]. Now, [77] theoretically argue that the hydrodynamic interactions of such a cluster in flows with low Reynolds number Re are as if the cluster were a hard sphere of radius a spanning the cluster. Since the geometrical representation of particles is closely related to the representation of *porous media*, we motivate that in certain cases we can also apply our model for such a system. Examples of porous media are packed beds of particles, soils, sedimentary rock, gels, membranes, and many biological systems. Porous media are generally heterogeneous and characterized by three-dimensional random networks. They often exhibit a fractal nature, as in geophysical environments, such as sedimentary rocks, and in biological environments, such as the lung and capillary systems.

We shall assume the porous media, for which we want our model to be justified, to be homogeneous. This enables to be consistent with the above approach on the particle geometry. Moreover, we would have to model the media by simple geometrical means such as bundles or assemblages of straight capillaries or beds of discrete geometrically defined particles, such as spheres or cylinders. To enable such simplified models of a real porous media by appropriate defined geometrical averages to be representative, is a generally assumed property [2].

2.3 Conclusion

The previous considerations allow to summary the following assumptions on the electrokinetic model (1.1.1)–(1.1.3):

Assumptions on a Newtonian fluid [8]:

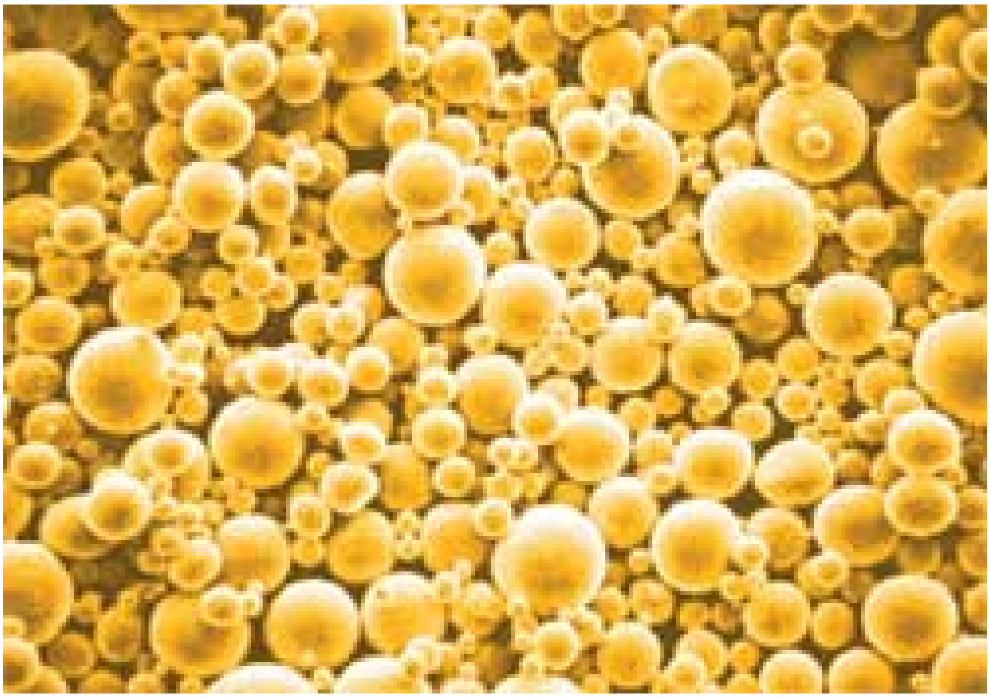


Figure 2.2.4: The aggregation of gold particles.
(from http://www.inbiogold.com/inbio_contact_us.html)

i) The fluid is isotropic; that is, the properties are independent of direction.

ii) In a static or inviscid fluid the stress tensor must reduce to the hydrostatic pressure condition; that is $\sigma_{ij} = -p\delta_{ij}$.

iii) The stress tensor σ_{ij} is at most a linear function of the shear tensor $\tau_{x_j x_i}$.

iv) The admissible particles or species are the ones which can rationally be represented by geometrical means implying spheres as discrete particle shape.

Finally, let us recall that under the characterization iv) of admissible particles belong the hemoglobin molecule, polysterene latex particles and spherical gold particles for example. Sometimes it is necessary to suppose additional assumptions as e.g. for the spherical gold particles a low Reynolds number flow is required.

The reason for the assumption iv) in the context of electrohydrodynamics is the use of Stokes law for the species considered as rigid spheres for which the drag force parallel to the direction of translation is

$$\mathbf{F} = 6\pi\eta R_h \mathbf{u}\,,$$

where η is the fluid viscosity and R_h the hydrodynamic radius of the particle. How this law enters in the derivation of the electrohydrodynamic model is motivated in Chapter 3.1.1.

Chapter 3

Analysis of the Navier-Stokes-Nernst-Planck-Poisson System

3.1 Introduction

We consider an isothermal, incompressible and viscous Newtonian fluid of uniform and homogeneous composition of a high number of positively and negatively charged particles ranging from colloidal to nano size. Electrokinetic flows can occur when a force (electrical, gravitational, shear or pressure gradient) acts on such a continuum. Moreover we assume an electrorheological behaviour of such continua. In fact, all transport properties of colloidal or nano particles are affected to some extent by the charge at the solid-liquid interface. The interplay between charges and the flow field around and between the particles constitute the electrokinetic effects in the presence of an electrical field. In the literature, the resulting effects (as electro-osmosis and electro-phoresis) are often described by the concept of the ζ-potential to explore the adsorption of charged species onto surfaces. In this context the particle geometry is also relevant. But to understand primarily the basic principles, we work with spheres as particle shape. Further we assume a dilute fluid and therefore we neglect electromagnetic forces. In [11, 19, 37, 45, 56], for example, such phenomena are considered.
The just explained phenomena are of great interest in the material sciences and electro chemistry. Researchers in these areas seek a serious theoretical understanding of solid-liquid interfaces and their interaction behaviour. Such knowledge allows to improve life time, charge cycles and capacity of lithium ion batteries and other fuel cells, see [10, 26, 27, 68, 69]. For further applications we refer to Section 3.1.2. Recently some models have been developed that concentrate on the particle configuration and a more precise charge location via the help of a profile function ϕ. In such a context one arrives at an anisotropic diffusion model, see [44, 45].
Our mesoscopic model describes the fluid velocity $\mathbf{u}(\mathbf{x}, t)$, which depends on the number densities of positively and negatively charged constituents $n^+(\mathbf{x}, t)$, $n^-(\mathbf{x}, t)$. These densities are again coupled through the Poisson equation for the quasi-electrostatic potential Ψ_0. The potential $\Psi_1(\mathbf{x}, t)$ is induced by an externally applied electrical field. Hence with $\Psi(\mathbf{x}, t) = \Psi_1(\mathbf{x}, t) + \Psi_0(\mathbf{x}, t)$ we define the potential for the whole system. We will show existence and uniqueness of the weak solutions ($\mathbf{u}$,n^+,n^-,Ψ_0) in dimension $N = 2$, and under additional assumptions also in $N = 3$. Moreover, we extend the concept of weak solutions to strong solutions in specific cases.

3.1.1 Model Construction

The following ideas are mainly inspired by [18, 37, 60]. The model is a mesoscopic fluiddynamical view of electrohydrodynamics. Let $\Omega_T := \Omega \times (0,T)$, where $\Omega \subset \mathbb{R}^N$ is bounded and has a $C^{1,1}$-boundary. For Dirichlet boundary conditions the fluid velocity $\mathbf{u} : \Omega_T \to \mathbb{R}^N$ solves the generally accepted incompressible Navier-Stokes equation

$$\begin{aligned} \mathbf{u}_t + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \eta\Delta\mathbf{u} + \nabla p &= \mathbf{f}_C, && \text{in } \Omega_T,\\ \operatorname{div}\mathbf{u} &= 0, && \text{in } \Omega_T,\\ \mathbf{u} &= 0, && \text{on } \partial\Omega \times (0,T), \end{aligned}$$

where η is the viscosity, $\mathbf{f}_C : \Omega_T \to \mathbb{R}^N$ the Coulomb force $\mathbf{f}_C = -\rho\mathbf{E}$ for a charge density $\rho : \Omega_T \to \mathbb{R}$ on an infinitesimal volume element of the fluid, and $\mathbf{E}$ is the electrical field $\nabla\Psi$ consisting of an internal $\nabla\Psi_0$ and an external electrical field $\nabla\Psi_1$. The incompressibility assumption is reasonable since either the contained particles and ions are assumed to have the same mass density or the fluid is very dilute.

The number densities $n_i : \Omega_T \to \mathbb{R}$ describe the transport of charge carriers and have to be explained more carefully. We apply the principle of mass conservation to them, i.e., the source or sink terms P_i satisfy $\sum_i P_i = 0$ and hence the concentrations n_i are the solutions of

$$\partial_t n_i + \operatorname{div}(n_i\mathbf{v}_i) = P_i, \tag{3.1.1}$$

where $\mathbf{v}_i : \Omega_T \to \mathbb{R}^N$ represents the average particle velocity of charged particles. To describe $\mathbf{v}_i$ we approximate the nano or colloidal particles as spheres moving in a continuum following the laws of an ideal gas of particles in the volume occupied by the fluid. Consider a charge carrier $i \in \mathbb{N}$ of charge $e_i \in \mathbb{R}$, which is a positive or negative integer of the absolute electron charge $e = 1.6 \times \exp\{-19\}\,C$, in a fluid at rest. There are three forces acting upon this particle i. One is the Coulomb force $e_i\mathbf{E}$, due to the presence of the electric field $\mathbf{E} : \Omega_T \to \mathbb{R}^N$. The next is a friction force, due to the surrounding fluid, which in our approximation is given by the Stokes law, i.e., $6\pi\eta R_h\mathbf{v}_i$, where $\eta \in \mathbb{R}_{>0}$ is the fluid viscosity, $R_h \in \mathbb{R}_{>0}$ the hydrodynamic radius of the particle and $\mathbf{v}_i : \Omega_T \to \mathbb{R}^N$ the relative velocity of the particle with respect to the liquid. The hydrodynamic radius is given by $R_h = \frac{kT}{6\pi\eta D}$. The third force is the pressure of other particles or ions upon the particle i, which according to the ideal gas law is given by $p_i = n_ikT \in \mathbb{R}$, with n_i the number density of particles or ions of the type i per unit volume.

Therefore Newton's law becomes

$$m_i\frac{d\mathbf{v}_i}{dt} = e_i\mathbf{E} - 6\pi\eta R_h\mathbf{v}_i - \frac{1}{n_i}\nabla\left(n_ik_BT\right).$$

Here we can neglect the inertia term $m_i\frac{d\mathbf{v}_i}{dt}$. This term compared to the friction term provides the time τ needed for the constituent to reach its limit velocity in the fluid. Even for fluids such as water, for which $\eta = 10^{-3}kgm^{-1}s^{-1}$ we have for an ion such as OH^-, with the ionic radius of the order of $2\cdot 10^{-10}$, a value $\tau \sim 10^{-14}s$. Hence the inertia term is negligible. Consequently, the velocity of the ion in a fluid at constant temperature is given by

$$\mathbf{v}_i = \mu_i\mathbf{E} - \frac{\mu_ik_BT}{e_i}\frac{1}{n_i}\nabla n_i, \tag{3.1.2}$$

where we have introduced the mobility $\mu_i \in \mathbb{R}$ given by

$$\mu_i = \frac{e_i}{6\pi\eta R_h}.$$

We remark that μ_i carries the sign of the charge. We justify the use of the Stokes formula with the low Reynolds number Re for the flow

$$Re = \frac{\rho\eta u}{R_h} \ll 1.$$

We can write the friction force term in (3.1.2) as a diffusion term, i.e.,

$$\mathbf{v}_i = \mu_i \mathbf{E} - D_i \frac{1}{n_i} \nabla n_i,$$

with $D_i \in \mathbb{R}$ the coefficient of molecular diffusion. For a liquid at rest in thermodynamic equilibrium, it holds $\mathbf{v}_i = 0$. Also, according to Boltzmann's law we have $n_i \propto \exp(-e_i \Psi k_B T)$, and from (3.1.2), by taking into account that $\mathbf{E} = -\nabla\Psi$ and defining the positive constant $D_i := \frac{\mu_i k_B T}{e_i} \frac{1}{n_i}$, we obtain Einstein's relation

$$\frac{D_i}{\mu_i} = \frac{k_B T}{e_i},$$

with k_B the Boltzmann constant.

Until now the fluid is considered to be at rest. For a fluid in motion the ions are advected with the bulk flow velocity $\mathbf{u} : \Omega_T \to \mathbb{R}^N$. Then, each charge carrier moves in the liquid with the average velocity $\mathbf{v}_i$, which is the sum of three terms

$$\mathbf{v}_i = \mu_i \mathbf{E} - D_i \frac{\nabla n_i}{n_i} + \mathbf{u}. \tag{3.1.3}$$

In most circumstances the ionic charge carriers originate from dissociation of impurities in the bulk, and/or are injected into the liquid. Now we are able to write the conservation equation (3.1.1) for the i-th particle in full length as

$$\partial_t n_i - \mu_i \mathrm{div}\,(n_i \nabla\Psi) - D_i \Delta n_i + \mathbf{u}\nabla n_i = P_i, \qquad i \in \{1, \dots, L\}, \tag{3.1.4}$$

where we assume that the chemical reactions (sources or sinks P_i) between the $L \in \mathbb{N}$ particles are cancelling each other out. Finally every particle i will now be distinguished according to its surface charge (if it is not a molecule or ion), i.e., we define the collection of positively charged objects by n^+ and the negatively charged ones by n^-. More precisely we introduce

$$n^+ := \sum_{i=1}^{L} e_i n_i \chi_{\{e_i \text{ positive charge}\}}, \qquad n^- := \sum_{i=1}^{L} |e_i| n_i \chi_{\{e_i \text{ negative charge}\}}, \tag{3.1.5}$$

and in the same way $P^\pm$. By respecting the signs in equation (3.1.4) and with (3.1.5) we obtain

$$\partial_t n^\pm \mp \mu^\pm \mathrm{div}\left(n^\pm \nabla\Psi\right) - \Delta n^\pm + \mathbf{u}\nabla n^\pm = P^\pm, \quad \text{in } \Omega, \tag{3.1.6}$$

$$\langle J_\pm, \mathbf{n} \rangle = 0, \quad \text{in } \partial\Omega \times (0, T), \tag{3.1.7}$$

where $J_\pm := \mp n^\pm \nabla\Psi - \nabla n^\pm + \mathbf{u} n^\pm$ and

$$\mu^+ := \frac{e_i}{6\pi\eta R_h} \chi_{\{e_i \text{ positive charge}\}}, \qquad \mu^- := \frac{e_i}{6\pi\eta R_h} \chi_{\{e_i \text{ negative charge}\}}. \tag{3.1.8}$$

Further, we assume $P^+ = P^- = 0$. Hence we neglect reactions as combinations and recombinations. Finally, the positive and negative charge densities are coupled via the Poisson equation

$$-\epsilon \Delta\Psi_0 = n^+ - n^- \; (= \rho) \quad \text{in } \Omega_T, \tag{3.1.9}$$

$$\langle \nabla\Psi_0^\pm, \mathbf{n} \rangle = 0, \quad \text{in } \partial\Omega \times (0, T). \tag{3.1.10}$$

Since we assume the constants to be the same for all i's, we set them all equal to 1, that is $D_i = \mu_i = \epsilon = 1$ in (3.1.6) and (3.1.9). At this point we are able to define the charge density $\rho : \Omega_T \to \mathbb{R}$ as $\rho := n^+ - n^-$.

Remark 3.1.1. 1) The equations (3.1.6) are the Nernst-Planck equations modified by the convective term $(\mathbf{u} \cdot \nabla)\, n^{\pm}$. These equations (3.1.6) are generally used to describe a binary symmetric electrolyte [56, 60], but are also very accurate to model particle concentrations in dilute solutions [37].
2) The Nernst-Planck equations (3.1.6) can be modified to an anisotropic diffusion model [44, 45]. For a chosen profile function ϕ, let $\mathbf{n} = -\frac{\nabla \phi}{|\nabla \phi|}$, what allows to write the new equations as

$$n_t - \operatorname{div}\left[(\mathbb{1} - \mathbf{n} \otimes \mathbf{n})\,(\nabla n + n \nabla \Psi)\right] + (\mathbf{u} \cdot \nabla) n = 0. \tag{3.1.11}$$

This additional term $(\mathbb{1} - \mathbf{n} \otimes \mathbf{n})$, where $\mathbb{1}$ is the identity matrix, guarantees that there is no penetration of ions into colloids explicitly without using artificial potentials.

3.1.2 The Nernst-Planck Equation and its Applications

Roubicek [67, 66] describes a different model of similar equations. In contrast to our model, he considers a purely ion-depending fluid, including mixture-behaviour. A pointwise a priori normalization $n := \sum_i n_i = 1$, called volume additivity on the number densities of positively or negatively charged constituents, plays a central role in his works. Such a volume additivity allows to immediately obtain a uniform control on $\|n\|_{L^2}$ and $\|\nabla n\|_{L^2}$. This enables to directly achieve global existence of weak solutions ([66]). According to Remark 4.3 in [66], this article may be the first step to establish mathematical analysis in the area of electrohydrodynamics (EHD), which drops the volume additivity constraint. Jerome [40] establishes a semigroup approach to a similar system.

The Nernst-Planck equations (3.2.4)-(3.2.7) below are also applied in other fields: One application is the semiconductor theory (see [32] or [14]), which is essentially described by the same equations without the convective terms $(\mathbf{u} \cdot \nabla)\, n^{\pm}$. Equations in this context are often called van Roosbroeck equations.

Furthermore, the equations (3.2.4)-(3.2.7) below provide also a basis for models in chemotaxis (see [24]). The parabolic-elliptic system (1.2) in [24] corresponds to our Nernst-Planck-Poisson system for n^+-charged particles, but with different sign in front of the nonlinear term. For such systems only describing n^+-charged particles, blow-up can occur (see [14]) for supercritical initial data.

Finally the already mentioned equations (3.2.4)-(3.2.7) provide a possible model in the neurosciences investigating the function of neurons in the context of electrical and chemical conduction (see [43]). Since the membrane potential, called Nernst-potential (which corresponds to the electrostatic potential), is the principal state variable used for rapid intercellular communication in neurons, this equation is fundamental for the understanding of the membrane behaviour.

3.2 Analytical Investigation Of The Model

For given initial data $(\mathbf{u}_0, n_0^+, n_0^-)$, pure Neumann boundary conditions defined precisely later and $\mathbf{f}_C := -\,(n^+ - n^-)\,\nabla \Psi$, let us consider on $\Omega_T := \Omega \times (0,T)$, for $\Omega \subset \mathbb{R}^N$ bounded, convex and $N \leq 3$, the following set of equations

$$\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \Delta\mathbf{u} + \nabla p = \mathbf{f}_C \quad \text{in } \Omega_T \tag{3.2.1}$$
$$\operatorname{div}\mathbf{u} = 0 \quad \text{in } \Omega_T \tag{3.2.2}$$
$$\mathbf{u} = 0 \quad \text{on } \partial\Omega\times(0,T) \tag{3.2.3}$$

$$\partial_t n^+ - \operatorname{div}\left(n^+\nabla\Psi\right) - \Delta n^+ + (\mathbf{u}\cdot\nabla)\,n^+ = 0 \quad \text{in } \Omega_T \tag{3.2.4}$$
$$\langle J_{n^+}, \mathbf{n}\rangle = 0 \quad \text{on } \partial\Omega\times(0,T) \tag{3.2.5}$$
$$\partial_t n^- + \operatorname{div}\left(n^-\nabla\Psi\right) - \Delta n^- + (\mathbf{u}\cdot\nabla)\,n^- = 0 \quad \text{in } \Omega_T \tag{3.2.6}$$
$$\langle J_{n^-}, \mathbf{n}\rangle = 0 \quad \text{on } \partial\Omega\times(0,T) \tag{3.2.7}$$

$$-\Delta\Psi_0 = n^+ - n^- \quad \text{in } \Omega_T \tag{3.2.8}$$
$$\langle\nabla\Psi_0, \mathbf{n}\rangle = 0 \quad \text{on } \partial\Omega\times(0,T) \tag{3.2.9}$$

where $J_{n_\pm} := \pm n^\pm\nabla\Psi - \nabla n^\pm + \mathbf{u}n^\pm$ and the electrical potential $\Psi := \Psi_0 + \Psi_1$, with Ψ_0 the internal electrical potential obtained via (3.2.8), and Ψ_1 an externally applied potential.

Remark 3.2.1. For (3.2.4) and (3.2.6) we can apply standard parabolic existence theory. Therefore we introduce the notation

$$\partial_t n^+ - \Delta n^+ + \overline{b}^j_+(\mathbf{x},t)\partial_j n^+ + \overline{c}^+(\mathbf{x},t)n^+ \;=\; 0, \tag{3.2.10}$$
$$\partial_t n^- - \Delta n^- + \overline{b}^j_-(\mathbf{x},t)\partial_j n^- + \overline{c}^-(\mathbf{x},t)n^- \;=\; 0, \tag{3.2.11}$$

where $\overline{b}^j_\pm(\mathbf{x},t) := (\overline{\mathbf{u}})^{(j)} \mp \partial_j\overline{\Psi}$ and $\overline{c}^\pm(\mathbf{x},t) := \mp\Delta\overline{\Psi}$ and the bar-notation is introduced in view of the existence proof to point out decoupling and linearization strategies unlike the original equations (3.2.4) and (3.2.6).

3.2.1 Main Results

In Section 3.2.2 we provide definitions of terms used in the following theorems.

Theorem 3.2.2. (Existence) *For $N \leq 3$, and $\Omega \subset \mathbb{R}^N$ open, bounded and convex, $n_0^\pm \in L^\infty(\Omega, \mathbb{R}_{\geq 0})$, $\mathbf{u}_0 \in V^{0,2}(\Omega, \mathbb{R}^N)$ and $0 < T < \infty$, the system (3.2.1)-(3.2.9) has a global weak solution $(\mathbf{u}, n^+, n^-, \Psi_0)$, defined in* Definition 3.2.6.

The next result is mainly restricted by the Navier-Stokes equation (3.2.1).

Theorem 3.2.3. (Uniqueness) *Under the assumption $(\Psi, 1) = 0$, the solutions obtained in* Theorem 3.2.2 *are unique for $N = 2$, and without the convective term $(\mathbf{u}\cdot\nabla)\mathbf{u}$ in (3.2.1) also for $N = 3$.*

The regularity of our weak solution obtained in Theorem 3.2.2 will be improved in the way of

Theorem 3.2.4. (Strong solutions) *For the stronger boundary condition $\langle\nabla n^\pm, \mathbf{n}\rangle = 0$ and dimension $N \leq 3$, the weak solutions obtained in* Theorem 3.2.3 *are unique strong solutions defined in* Definitions 3.2.6 *and* 3.2.7 *below, i.e., $n_0^\pm \in H^1(\Omega, \mathbb{R}_{\geq 0})$ and $\mathbf{u}_0 \in V^{1,2}(\Omega, \mathbb{R}^N)$. In dimension $N = 3$, this existence is only local.*

Remark 3.2.5. The stronger boundary condition in Theorem 3.2.4 is not restrictive, since it still guarantees the physically relevant no-flux boundary conditions.

3.2.2 Preliminaries and Definitions

Let us introduce some standard notations (see [50]) for often used spaces as

$$\tilde{\mathcal{D}}(\Omega) := \{\mathbf{u} \in C_0^\infty(\Omega, \mathbb{R}^N); \quad \operatorname{div} \mathbf{u} = 0\}, \tag{3.2.12}$$

$$V^{0,2}(\Omega) := \text{the closure of } \tilde{\mathcal{D}} \text{ in } L^2 = \overline{\tilde{\mathcal{D}}}^{L^2}, \tag{3.2.13}$$

$$V^{1,2}(\Omega) := \text{the closure of } \tilde{\mathcal{D}} \text{ in } H_0^1 = \overline{\tilde{\mathcal{D}}}^{H_0^1}, \tag{3.2.14}$$

where the assumption on $\Omega \subset \mathbb{R}^N$ is distinguished between the
Assumption on the domain for weak solutions

(A1) $\Omega \subset \mathbb{R}^N$ is open, bounded and has a $C^{1,1}$-boundary. If $N = 2$, it suffices to assume that Ω is convex.

and the *Assumption on the domain for strong solutions*

(A2) $\Omega \subset \mathbb{R}^N$ is open, bounded and has a $C^{2,2}$-boundary.

The dimension of the space is $N \leq 3$. The space $V^{0,2}(\Omega)$ is equipped with the scalar product $(\cdot,\cdot)$ induced by $L^2(\Omega)$; the space $V^{1,2}(\Omega)$ is a Hilbert space with the scalar product

$$((\mathbf{u}, \mathbf{v})) = \sum_{i=1}^{N} (\mathrm{D}_i \mathbf{u}, \mathrm{D}_i \mathbf{u}),$$

since Ω is bounded. Obviously, $V^{1,2}(\Omega)$ is contained in $V^{0,2}(\Omega)$, is dense in $V^{0,2}(\Omega)$ and the injection is continuous. Moreover, by Riesz representation theorem, we can identify $V^{0,2}$ and $\left(V^{0,2}\right)^*$, and we arrive at the inclusions

$$V^{1,2} \subset V^{0,2} \equiv \left(V^{0,2}\right)^* \subset V^{-1,2} \equiv \left(V^{1,2}\right)^*,$$

where each space is dense in the following one, and the injections are continuous. Further we will use $c > 0$ for all generic constants and where it is necessary $c_S > 0$ for constants depending on the dimension in Sobolev inequalities.

First we repeat the **classical formulation** for the initial boundary value problem of the full Navier-Stokes equation: Find a vector function

$$\mathbf{u} : \Omega_T \to \mathbb{R}^N$$

and scalar functions

$$\begin{aligned} p : \Omega_T &\to \mathbb{R}, \\ n^\pm : \Omega_T &\to \mathbb{R}, \\ \Psi_0 : \Omega_T &\to \mathbb{R}, \end{aligned}$$

such that equations (3.2.1)-(3.2.9) are satisfied for every $(\mathbf{x}, t) \in \Omega_T$. Then we call $(\mathbf{u}, p, n^+, n^-, \Psi_0)$ a **classical solution**. Continuity and density of $C^\infty(\overline{\Omega_T})$ respectively $\tilde{\mathcal{D}}(\Omega)$ in $H^1(\Omega)$ respectively $V^{1,2}(\Omega)$ suggest the following **weak formulation**: For all $\tilde{\boldsymbol{\phi}} \in V^{1,2}(\Omega)$, $\phi \in H^1(\Omega)$ and almost every $0 < t < T$, there holds

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{u}, \tilde{\boldsymbol{\phi}}\right) + \left((\mathbf{u} \cdot \nabla)\,\mathbf{u}, \tilde{\boldsymbol{\phi}}\right) + \left(\nabla \mathbf{u}, \nabla \tilde{\boldsymbol{\phi}}\right) = \left(\mathbf{f}_C, \tilde{\boldsymbol{\phi}}\right), \tag{3.2.15}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(n^\pm, \phi\right) \pm \left(n^\pm \nabla \Psi, \nabla \phi\right) + \left(\nabla n^\pm, \nabla \phi\right) - \left(\mathbf{u} n^\pm, \nabla \phi\right) = 0. \tag{3.2.16}$$

From (3.2.15) we are able to formally define the trilinear form β and an operator B as

$$\beta(\mathbf{u},\mathbf{v},\mathbf{w}) := (B(\mathbf{u},\mathbf{v}),\mathbf{w}) := \sum_{i,j=1}^{N}\int_{\Omega}\mathbf{u}_i\partial_i\mathbf{v}_j\mathbf{w}_j dx = ((\mathbf{u}\cdot\nabla)\mathbf{v},\mathbf{w})\,. \tag{3.2.17}$$

We will see out of which spaces $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ are taken in our context. The following well-known ***properties of*** β will be used later on, see [75]:

β1) *β is trilinear and continuous on $V^{1,2}\times V^{1,2}\times V^{1,2}$ if Ω is bounded and $N\leq 4$.*

β2) *For Ω an open set, there holds*

$$\beta(\mathbf{u},\mathbf{v},\mathbf{v}) = 0, \qquad \forall\,\mathbf{u}\in V^{1,2},\ \mathbf{v}\in H_0^1(\Omega), \tag{3.2.18}$$

$$\beta(\mathbf{u},\mathbf{v},\mathbf{w}) = -\beta(\mathbf{u},\mathbf{w},\mathbf{v}), \qquad \forall\,\mathbf{u}\in V^{1,2},\ \mathbf{v},\ \mathbf{w}\in H_0^1(\Omega). \tag{3.2.19}$$

β3) Convergence property: *Suppose $\mathbf{v}_k\to\mathbf{v}$ weakly in $V^{1,2}$ and strongly in $V^{0,2}$. Then for any smooth $\mathbf{w}$, $\beta(\mathbf{v}_k,\mathbf{v}_k,\mathbf{w})\to\beta(\mathbf{v},\mathbf{v},\mathbf{w})$.*

Finally we consider the Poisson equation (3.2.8) in the weak formulation

$$(\nabla\Psi_0,\nabla\phi) - \int_{\partial\Omega}\nabla\Psi_0\phi\mathbf{n}\,\mathrm{d}x = \left(\left(n^+ - n^-\right),\phi\right)$$

for *a.e.* $t\in(0,T)$ and all $\phi\in H^1(\Omega)$. These formulations above motivate the following definition, which already includes essential characterizations gathered in the sense of [50].

Definition 3.2.6. *(Weak solution)* Let $\Psi_1\in L^2(0,T;H^3(\Omega))\cap L^\infty(0,T;H^2(\Omega))$, $N\leq 3$, and $0<T<\infty$. Assume $(A1)$.We call $(\mathbf{u},n^+,n^-,\Psi_0)$ a weak solution of (3.2.1)-(3.2.9), if

i) it satisfies for $p=2$, if $N=2$, or for $p=\frac{4}{3}$, if $N=3$, that

(3.2.20)
$$\mathbf{u}\in L^2(0,T;V^{1,2}(\Omega,\mathbb{R}^N))\cap L^\infty(0,T;V^{0,2}(\Omega,\mathbb{R}^N))\cap W^{1,p}(0,T;V^{-1,2}(\Omega,\mathbb{R}^N)),$$

(3.2.21)
$$n^\pm\in L^2(0,T;H^1(\Omega))\cap L^\infty(\Omega_T)\cap W^{1,\frac{6}{5}}(0,T;(H^1(\Omega))^*),$$

(3.2.22)
$$\Psi_0\in L^2(0,T;H^2(\Omega))\cap L^\infty(0,T;H^1(\Omega)),$$

ii) it solves equations (3.2.1)-(3.2.8) in the weak sense for initial data

$$\mathbf{u}_0 \in V^{0,2}(\Omega,\mathbb{R}^N),$$
$$n_0^\pm \in L^\infty(\Omega) \quad \text{and} \quad n_0^\pm\geq 0 \quad \text{a.e. in } \Omega,$$

where for $t\to 0$ there holds

$$\mathbf{u}(\cdot,t)\rightharpoonup\mathbf{u}_0 \quad \text{in } L^2(\Omega,\mathbb{R}^N) \tag{3.2.23}$$

$$n^\pm(\cdot,t)\rightharpoonup n_0^\pm \quad \text{in } L^2(\Omega), \tag{3.2.24}$$

iii) it satisfies the following boundary conditions in trace sense for a.e. $t \in [0,T]$, i.e.,

$$\langle J_{n^\pm}, \mathbf{n}\rangle\big|_{\partial\Omega\times\{t\}} = 0, \tag{3.2.25}$$

$$\text{and } \langle \nabla\Psi_0, \mathbf{n}\rangle\big|_{\partial\Omega\times\{t\}} = 0, \tag{3.2.26}$$

where $\mathbf{n}$ is the unit normal on the boundary of Ω,

iv) it fulfils for $t \in [0,T]$ the two energy inequalities

$$E(t) + \int_0^t e(s) + d(s)\,ds \le E(0) + \int_0^t L_{\mathbf{u}}(s) + L_\Psi(s)\,ds \tag{3.2.27}$$

$$W(t) + \int_0^t I^+(s) + I^-(s)\,ds \le W(0) + \int_0^t L_1(s)\,ds, \tag{3.2.28}$$

where $W(t) := W_{NPP}(t) + W_{INS}(t)$, for

$$\begin{aligned}
W_{NPP}(t) &:= \int_\Omega n^+\left(\log\left(n^+\right)-1\right) + n^-\left(\log\left(n^-\right)-1\right) + \frac{1}{2}\left|\nabla\Psi_0\right|^2 + 2\,\mathrm{d}x\\
W_{INS}(t) &:= \int_\Omega \frac{1}{2}|\mathbf{u}|^2\,dx + \int_0^t\int_\Omega |\nabla\mathbf{u}|^2\,dxds\\
I^\pm(t) &:= \int_\Omega n^\pm\left[\nabla\left(\log\left(n^\pm\right)-\Psi\right)\right]^2 dx\\
E(t) &:= \frac{1}{2}\|\mathbf{u}\|_{L^2}^2 + \|\nabla\Psi_0\|_{L^2}^2\\
e(t) &:= \|\nabla\mathbf{u}\|_{L^2}^2 + \left\|n^+ - n^-\right\|_{L^2}^2\\
d(t) &:= \int_\Omega \left(n^+ + n^-\right)|\nabla\Psi_0|^2\,dx\\
L_{\mathbf{u}}(t) &:= \int_\Omega \left(n^+ + n^-\right)\left|\langle\nabla\Psi_1, \mathbf{u}\rangle\right|\mathrm{d}x\\
L_\Psi(t) &:= \int_\Omega \left(n^+ + n^-\right)\left|\langle\nabla\Psi_1, \nabla\Psi_0\rangle\right|\mathrm{d}x\\
L_1(t) &:= \int_\Omega \left|\langle(\nabla\Psi_0)_t, \nabla\Psi_1\rangle\right|\mathrm{d}x
\end{aligned}$$

Next we study more regular solutions to (3.2.1)-(3.2.9), for $N \le 3$.

Definition 3.2.7. *(Strong solution)* Let $\Psi_1 \in L^\infty(0,T;H^3(\Omega))$ and assume $(A2)$. Then the weak solutions $(\mathbf{u}, n^+, n^-, \Psi_0)$, together with the pressure function $p : \Omega_T \to \mathbb{R}$ are called strong solutions of (3.2.1)-(3.2.9), if they satisfy

i)

$$\begin{aligned}
\mathbf{u} &\in L^2(0,T;V_0^{1,2}(\Omega,\mathbb{R}^N)\cap V^{2,2}(\Omega,\mathbb{R}^N))\cap W^{1,2}(0,T;V^{0,2}(\Omega,\mathbb{R}^N))\\
n^\pm &\in L^2(0,T;H^2(\Omega))\cap C(0,T;H^1(\Omega))\cap W^{1,2}(0,T;L^2(\Omega))\\
\Psi_0 &\in L^2(0,T;H^3(\Omega))\cap L^\infty(0,T;H^2(\Omega))\\
p &\in L^2(0,T;H^1(\Omega)/\mathbb{R}),
\end{aligned}$$

where in dimension $N = 3$ the time $T = T(\mathbf{u}_0) > 0$ is finite,

ii) the initial conditions

$$\mathbf{u}_0 \in V^{1,2}(\Omega, \mathbb{R}^N), \tag{3.2.29}$$

$$n_0^{\pm} \in H^1(\Omega) \cap L^\infty(\Omega), \tag{3.2.30}$$

where for $t \to 0$ there holds

$$\mathbf{u}(\cdot, t) \to \mathbf{u}_0 \quad \text{in } L^2(\Omega, \mathbb{R}^N), \tag{3.2.31}$$

$$n^{\pm}(\cdot, t) \to n_0^{\pm} \quad \text{in } L^2(\Omega), \tag{3.2.32}$$

iii) the stronger boundary condition $\langle \nabla n^{\pm}, \mathbf{n} \rangle|_{\partial\Omega \times \{t\}} = 0$,

iv) for $N \leq 3$ the energy identities

$$E(t) + \int_0^t e(s) + d(s)\, ds = E(0) - \int_0^t L_{\mathbf{u}}(s) + L_{\Psi}(s)\, ds, \tag{3.2.33}$$

$$W(t) + \int_0^t I^+(s) + I^-(s)\, ds = W(0) - \int_0^t L_1(s)\, ds, \tag{3.2.34}$$

where L_1, L_Ψ and $L_{\mathbf{u}}$ are integrated without taking the absolute values of their integrands.

3.3 Proof of the Main Results

Let us give an overview for the proof of Theorem 3.2.2, which also reflects the main ideas. Therefore we remark first that existence for each equation in decoupled form is already known. Here we check whether there exist solutions in the sense of Definition 3.2.6 respectively 3.2.7 for the coupled system.

A) *Local Existence of Weak Solutions*

1. *Properties of Weak Solutions* $(\mathbf{u}, n^+, n^-, \Psi_0)$
   i) Non-negativity for $n^{\pm}$ via an auxiliary problem
   ii) Energy Inequality I, see (3.2.27)
   iii) Energy Inequality II, see (3.2.28)
   iv) $L^\infty(\Omega_T)$-bound for $n^{\pm}$

2. *A Priori Estimates*
   Recall of standard results

3. *Local Existence of* $(\mathbf{u}, n^+, n^-, \Psi_0)$
   i) Definition of a continuous mapping $F : Y \to Y$, and $B_R \subset Y$

$$F : B_R \to B_R$$
$$\overline{\mathbf{y}} := (\overline{n}^+, \overline{n}^-) \mapsto \mathbf{y} := (n^+, n^-),$$

   such that $\mathbf{y}$ is the weak solution of the system (3.2.1)-(3.2.8) decoupled through $\overline{\mathbf{y}}$. In fact we obtain the corresponding fluid velocity $\mathbf{u}$ and the internal electrical potential Ψ_0 to the concentrations n^+ and n^- .
   ii) F allows to apply Schauder's Fixed Point Theorem, i.e., $\overline{\mathbf{y}} = \mathbf{y} \in B_R$ exists.

B) ***Global Existence***

1. *Standard Continuation Principle via Uniform Bounds*

In the subsequent sections we carry out these steps.

3.3.1 STEP A) (1): Properties of Weak Solutions

In order to prove the following Lemma 3.3.2, we introduce the auxiliary problem

$$\partial_t n^{\pm} \mp \operatorname{div}\left(\left[n^{\pm}\right]^{+} \nabla\Psi\right) - \Delta n^{\pm} + (\mathbf{u}\cdot\nabla)n^{\pm} = 0, \tag{3.3.1}$$

where $[x]^{+} := \sup\{x, 0\}$.

Remark 3.3.1. Any solution $n^{\pm}$ of the auxiliary problem (3.3.1) that satisfies $0 \leq n^{\pm}$ *a.e* in Ω_T is already a solution of our original system (3.2.4)-(3.2.6), see [32].

Lemma 3.3.2. (Non-negativity) *The weak solutions $n^{\pm} : \Omega_T \to \mathbb{R}$ of the Nernst-Planck equations (3.2.4) and (3.2.6) are non-negative a.e. in Ω_T.*

Proof. We establish the proof only for n^{+} (it can be done analogously for n^{-}). For the definitions $N^{-} :=\sup\{-n^{+}, 0\}$ and $N^{+} := \sup\{n^{+}, 0\}$ we can write n^{+} as $n^{+} = N^{+} - N^{-}$. Now we test (3.3.1) with N^{-}. After integration by parts we obtain

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left\|N^{-}\right\|_{L^2}^2 - \left\|\nabla N^{-}\right\|_{L^2}^2 \quad = \quad -\left(N^{+}\nabla N^{-}, \nabla\Psi\right) = 0,$$

where we used properties of $N^{\pm}$ and $\nabla N^{\pm}$ (compare [34]) and the fact $\left((\mathbf{u}\cdot\nabla)N^{-}, N^{-}\right) = 0$. Finally for $t \in [0, T]$, integration over $[0, t]$ yields to

$$\left\|N_0^{-}\right\|_{L^2}^2 - \left\|N^{-}(\cdot, t)\right\|_{L^2}^2 - 2\int_0^t \left\|\nabla N^{-}(\cdot, s)\right\|_{L^2}^2 ds \geq 0.$$

Since $\left\|N_0^{-}\right\|_{L^2}^2 = 0$, we have $N^{-} = 0$ *a.e.* in Ω_T. ☐

The next Lemma states mass (or charge) conservation.

Lemma 3.3.3. (Mass Conservation) *The $L^\infty(0, T; L^1(\Omega))$-norm of a weak solution $n^{\pm} : \Omega_T \to \mathbb{R}$ is conserved, i.e.,*

$$\left\|n^{\pm}(\cdot, t)\right\|_{L^1(\Omega)} = \int_\Omega n^{\pm}(\cdot, t)dx = \int_\Omega n_0^{\pm}dx = \left\|n_0^{\pm}\right\|_{L^1},$$

for every $t \in [0, T)$.

Proof. This is a simple consequence of (3.2.16) and given boundary conditions. ☐

The following two lemmas present energy inequalities, which we obtain by using special test functions.

Lemma 3.3.4. (Energy Inequality I) *The weak solution $(\mathbf{u}, n^{+}, n^{-}, \Psi_0)$ of (3.2.1) – (3.2.9) satisfies the Energy Inequality I, i.e., (3.2.27).*

Proof. We test equation (3.2.1) with admissible $\mathbf{u}$, equations (3.2.4) and (3.2.6) with $\pm\Psi_0$ and then integrate over Ω. ☐

Lemma 3.3.5. (Energy Inequality II) *Suppose that* $(\mathbf{u}, n^+, n^-, \Psi_0)$ *is a weak solution, then (3.2.28) is valid.*

Proof. We test the n^--equation of (3.2.6) with the admissible test function $(\log(n^- + \delta) - \Psi)$ for a small $\delta > 0$. Since $\frac{\partial}{\partial t}[n(\ln n - 1)] = n_t \ln n$, we have

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left((n^- + \delta), \left(\log(n^- + \delta) - 1\right)\right) - \left(n_t^-, \Psi\right) \\
&\quad - \left(\left((n^- + \delta)\nabla\Psi - \nabla n^- + \mathbf{u}\left(n^- + \delta\right)\right), \nabla\left(\log\left(n^- + \delta\right) - \Psi\right)\right) = 0.
\end{aligned} \tag{3.3.2}
$$

First we compute the second line in (3.3.2), i.e.,

$$
\begin{aligned}
&\int_\Omega \Big\{ -(n^- + \delta)\nabla\Psi\nabla\log\left(n^- + \delta\right) + \nabla n^-\nabla\log\left(n^- + \delta\right) + (n^- + \delta)\left|\nabla\Psi\right|^2 - \nabla n^-\nabla\Psi \Big\}\, \mathrm{d}x \\
&\qquad - \left(\mathbf{u}\left(n^- + \delta\right), \nabla\left(\log\left(n^- + \delta\right) - \Psi\right)\right) =: I_1^-(\delta) + I_2^-(\mathbf{u}),
\end{aligned} \tag{3.3.3}
$$

where I_1^- represents the integral term in (3.3.3) and $I_2^-(\mathbf{u})$ the term depending on $\mathbf{u}$. To rewrite I_1^- we need the following two conversions

$$
\nabla n^-\nabla\Psi = \frac{n^- + \delta}{n^- + \delta}\nabla\left(n^- + \delta\right)\nabla\Psi = \left(n^- + \delta\right)\nabla\log\left(n^- + \delta\right)\nabla\Psi
$$

and

$$
\begin{aligned}
\nabla n^-\nabla\log\left(n^- + \delta\right) &= \frac{(n^- + \delta)}{(n^- + \delta)}\nabla\left(n^- + \delta\right)\nabla\log\left(n^- + \delta\right) \\
&= \left(n^- + \delta\right)\left|\nabla\log\left(n^- + \delta\right)\right|^2.
\end{aligned}
$$

Therefore

$$
\begin{aligned}
I_1^-(\delta) = &\int_\Omega \left(n^- + \frac{\delta}{2}\right)\left[\nabla\left(\log\left(n^- + \delta\right) - \Psi\right)\right]^2 dx \\
&+ \frac{\delta}{2}\int_\Omega \left|\nabla\log\left(n^- + \delta\right)\right|^2 dx - \frac{\delta}{2}\int_\Omega \left|\nabla\Psi\right|^2 dx
\end{aligned} \tag{3.3.4}
$$

and since $\mathbf{u}$ is divergence free

$$
I_2^-(\mathbf{u}) \quad = \quad -\left(\mathbf{u}\left(n^- + \delta\right), \nabla\Psi\right).
$$

Now we repeat the same calculations for the equation (3.2.4). Hence we test with $(\log(n^+ + \delta) + \Psi)$ to obtain

$$
\begin{aligned}
I_1^+(\delta) := &\int_\Omega \left(n^+ + \frac{\delta}{2}\right)\left[\nabla\left(\log\left(n^+ + \delta\right) + \Psi\right)\right]^2 dx \\
&+ \frac{\delta}{2}\int_\Omega \left|\nabla\log\left(n^+ + \delta\right)\right|^2 dx - \frac{\delta}{2}\int_\Omega \left|\nabla\Psi\right|^2 dx
\end{aligned} \tag{3.3.5}
$$

and

$$
I_2^+(\mathbf{u}) := \left(\mathbf{u}\left(n^+ + \delta\right), \nabla\Psi\right).
$$

Adding up the equations (3.2.4) and (3.2.6) tested with $(\log(n^\pm + \delta) \pm \Psi)$ and using $-\Delta\Psi_0 = n^+ - n^-$, delivers

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left((n^+ + \delta), \left(\log\left(n^+ + \delta\right) - 1\right)\right) + \frac{\mathrm{d}}{\mathrm{d}t}\left((n^- + \delta), \left(\log\left(n^+ + \delta\right) - 1\right)\right) \\
&\quad + \frac{\mathrm{d}}{\mathrm{d}t}\left\|\nabla\Psi_0(\cdot, t)\right\|_{L^2}^2 = -I_1^+(\delta) - I_1^-(\delta) - I_2^+(\mathbf{u}) - I_2^-(\mathbf{u}) - L_1,
\end{aligned} \tag{3.3.6}
$$

where $L_1 = \Big(\nabla\big(\Psi_0(\cdot,t)\big)_t, \nabla\Psi_1(\cdot,t)\Big)$. The Navier-Stokes equation (3.2.1) we test with $\mathbf{u}$, i.e.,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_{L^2}^2 + \|\nabla\mathbf{u}\|_{L^2}^2 = \left(-\left(n^+ - n^-\right)\nabla\Psi, \mathbf{u}\right). \tag{3.3.7}$$

Now we add up the equations (3.3.6) and (3.3.7) to obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\left(n^+ + \delta\right), \left(\log\left(n^+ + \delta\right) - 1\right)\right) + \frac{\mathrm{d}}{\mathrm{d}t}\left(\left(n^- + \delta\right), \left(\log\left(n^+ + \delta\right) - 1\right)\right) + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\|\nabla\Psi_0\|_{L^2}^2\right)\\ + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_{L^2}^2 + \|\nabla\mathbf{u}\|_{L^2}^2 = -I_1^+(\delta) - I_1^-(\delta) - L_1.\end{aligned} \tag{3.3.8}$$

For a constant C_δ the definition

$$\begin{aligned}W_\delta(t) \quad := \quad & \int_\Omega \left(n^+ + \delta\right)\left(\log\left(n^+ + \delta\right) - 1\right) + \left(n^- + \delta\right)\left(\log\left(n^- + \delta\right) - 1\right)\\ & + \frac{1}{2}\left|\nabla\Psi_0\right|^2 + \frac{1}{2}\left|\mathbf{u}\right|^2 \,\mathrm{d}x + \int_0^t\int_\Omega \left|\nabla\mathbf{u}\right|^2 \,\mathrm{d}x\,ds + C_\delta.\end{aligned}$$

enables to write (3.3.8) as

$$\frac{\mathrm{d}}{\mathrm{d}t}W_\delta(t) = -I_1^+(\delta) - I_1^-(\delta) - L_1. \tag{3.3.9}$$

Moreover, with (3.3.9) $W_0(t)$ is a Lyapunov function if we choose Ψ_1 and the boundary conditions such that

$$I_1^+(0) + I_1^-(0) - L_1 \leq 0, \qquad \text{for all } t \in [0,T). \tag{3.3.10}$$

Then for ($\delta \to 0$) and assumption (3.3.10) we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}W_0(t) \quad = \quad & -\int_\Omega n^+\left|\nabla\left(\log\left(n^+\right) + \Psi\right)\right|^2 dx\\ & -\int_\Omega n^-\left|\nabla\left(\log\left(n^-\right) - \Psi\right)\right|^2 dx - L_1 \leq 0.\end{aligned}$$

It is only left to guarantee that $W_0(t) \geq 0$ for all $t \geq 0$. The problematic case occurs when $n^\pm = 1$. Therefore we choose $C_0 = 2\mu(\Omega)$. □

We are able to verify L^∞-boundedness of the solutions to the Nernst-Planck equations in the following way.

Lemma 3.3.6. ($L^\infty(\Omega_T)$-Bound) *The weak solutions $n^\pm$ of the concentration equations (3.2.4) and (3.2.6) satisfy*

$$n^\pm \in L^\infty(\Omega_T).$$

Proof. The main idea is to adapt a method introduced by Moser [55] to our problem. Let us formally multiply equation (3.2.4) by $\left(n^+\right)^{2^k-1}$. Integration over Ω, integration by parts and taking into account of $\operatorname{div}\mathbf{u} = 0$ *a.e.* in Ω_T result in

$$\begin{aligned}\frac{1}{2^k}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left(n^+\right)^{2^k} dx + \left(2^k - 1\right)\int_\Omega \frac{1}{2^k}\nabla\left(n^+\right)^{2^k}\nabla\Psi\,\mathrm{d}x\\ + \left(2^k - 1\right)\int_\Omega \left(n^+\right)^{2^k-2}\left(\nabla n^+\right)^2 dx = 0.\end{aligned}$$

Note that $\left((n^+)^{2^{k-1}-1}(\nabla n^+)\right)^2 = \left(\frac{1}{2^{k-1}}\nabla(n^+)^{2^{k-1}}\right)^2$. After integration by parts we obtain, in consideration of $-\Delta\Psi_0 = n^+ - n^-$, Hölder's inequality for the exponents $\alpha = \frac{p_k+1}{p_k}$ and $\beta := p_k + 1$ and using the definitions $\nu_k := \frac{2^k-1}{2^k}$, $\mu_k := \frac{2^k-1}{2^{2k-2}}$ and $p_k := 2^k$, the inequality

$$
\begin{aligned}
\frac{1}{p_k}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left(n^+\right)^{p_k} dx \leq & -\frac{\nu_k}{p_k+1}\int_\Omega \left(n^+\right)^{p_k+1} dx + \frac{\nu_k}{p_k+1}\int_\Omega \left(n^-\right)^{p_k+1} dx \\
& - \mu_k \int_\Omega \left|\nabla \left(n^+\right)^{p_{k-1}}\right|^2 \mathrm{d}x + \nu_k \int_\Omega \left(n^+\right)^{p_k} \left(-\Delta\Psi_1\right) \mathrm{d}x.
\end{aligned} \tag{3.3.11}
$$

Repeating the same steps for the equation (3.2.6) implies

$$
\begin{aligned}
\frac{1}{p_k}\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_\Omega \left(n^-\right)^{p_k} dx\right) \leq & -\frac{\nu_k}{p_k+1}\int_\Omega \left(n^-\right)^{p_k+1} dx + \frac{\nu_k}{p_k+1}\int_\Omega \left(n^+\right)^{p_k+1} dx \\
& - \mu_k \int_\Omega \left|\nabla (n^-)^{p_{k-1}}\right|^2 dx + \nu_k \int_\Omega \left(n^-\right)^{p_k} \left(-\Delta\Psi_1\right) \mathrm{d}x.
\end{aligned} \tag{3.3.12}
$$

Hence adding up (3.3.11) and (3.3.12) provides after applying Hölder's ($p = 1, q = \infty$) and Gronwall's inequality

$$
\|n^+\|_{L^{p_k}}^{p_k} + \|n^-\|_{L^{p_k}}^{p_k} \leq \left(\|n_0^+\|_{L^\infty(\Omega_T)}^{p_k} + \|n_0^-\|_{L^\infty(\Omega_T)}^{p_k}\right) T\mu\left(\Omega\right) \exp\{\nu_k T \|\Delta\Psi_1\|_{L^\infty}\} < \infty, \tag{3.3.13}
$$

for all $k \in \mathbb{N}$, since $n_0^+ \in L^\infty(\Omega)$. Now take the estimate (3.3.13) to the power of $1/p_k$ and use for $a, b \geq 0$ and $l \in \mathbb{N}$ the inequality

$$
\left(a^l + b^l\right)^{\frac{1}{l}} \leq a + b, \tag{3.3.14}
$$

to obtain

(3.3.15)

$$
\begin{aligned}
\|n^+\|_{L^{p_k}} + \|n^-\|_{L^{p_k}} &\leq \left(\|n_0^+\|_{L^\infty(\Omega_T)} + \|n_0^-\|_{L^\infty(\Omega_T)}\right)\left(T\mu(\Omega)\right)^{\frac{1}{p_k}} \exp\left\{\frac{\nu_k}{p_k} T \|\Delta\Psi_1\|_{L^\infty}\right\} \\
&=: C_{n_0^+}^{p_k} + C_{n_0^-}^{p_k}.
\end{aligned}
$$

Therefore $n^\pm \in L^p(\Omega_T)$ for all $p \in \mathbb{N}$, and in the limit $k \to \infty$ we find

$$
\|n^+\|_{L^\infty} + \|n^-\|_{L^\infty} \leq \left(\|n_0^+\|_{L^\infty(\Omega_T)} + \|n_0^-\|_{L^\infty(\Omega_T)}\right) =: C_{n_0^+}^\infty + C_{n_0^-}^\infty. \tag{3.3.16}
$$

□

Remark 3.3.7. A further property, which strongly uses the coupled character of the Nernst-Planck-Poisson system, is, that constants $c = p = n \geq 0$ are special solutions for n^+ and n^-. Via initial conditions we immediately obtain uniqueness of these solutions. In the presence of only one concentration, either n^+ or n^-, constants cannot survive any more as solutions.

3.3.2 STEP A) (2): A Priori Estimates

Here we remind necessary lemmas that allow to apply Aubin-Lions' Compactness result [48].

Lemma 3.3.8. *For dimension $N = 2$ put $p = 2$, and for $N = 3$ put $p = \frac{4}{3}$. Then the weak solution of (3.2.1) satisfies $\mathbf{u} \in W^{1,p}(0, T; V^{-1,2}(\Omega, \mathbb{R}^N))$.*

Proof. In view of the regularity of weak solutions we can immediately verify that the last three terms of (3.2.1) are in $L^2(0,T;V^{-1,2}(\Omega))$. Finally testing $(\mathbf{u}\cdot\nabla)\mathbf{u}$ with $\mathbf{v}\in L^2(0,T;V^{1,2}(\Omega))$ we obtain by applying for dimension $N=3$ the inequality

$$\|\mathbf{u}\|_{L^4} \le c\|\mathbf{u}\|_{L^2}^{1/4}\|\nabla\mathbf{u}\|_{L^2}^{3/4} \tag{3.3.17}$$

the estimate

$$\int_0^T \|(\mathbf{u}\cdot\nabla)\,\mathbf{u}\|_{V^{-1,2}}^{\frac{4}{3}}\,dt \le c\,\|\mathbf{u}\|_{L^\infty(0,T;L^2(\Omega))}^{\frac{2}{3}}\,\|\nabla\mathbf{u}\|_{L^2(0,T;L^2(\Omega))}^2 < \infty,$$

thanks to (3.2.20). For dimension $N=2$, the same estimate is valid with exponent 2 instead of $\frac{4}{3}$ since in this case the inequality (3.3.17) is

$$\|\mathbf{u}\|_{L^4} \le c\|\mathbf{u}\|_{L^2}^{1/2}\|\nabla\mathbf{u}\|_{L^2}^{1/2}. \tag{3.3.18}$$

□

Lemma 3.3.9. *Weak solutions of (3.2.4) and (3.2.6) satisfy* $n^\pm \in W^{1,\frac{6}{5}}(0,T;(H^1(\Omega))^*)$ *for dimension* $N=2$ *and* 3.

Proof. We test the equations (3.2.4) respectively (3.2.6) with $\phi\in H^1(\Omega)$. Using Hölder's inequality with exponents 2, 4 and 4, known interpolation results as $\|\cdot\|_{L^4}\le c\|\cdot\|_{L^2}^{\frac{1}{4}}\|\nabla\cdot\|_{L^2}^{\frac{3}{4}}$ in $N=3$ and Young's inequality with exponents $p=2, q=2$ and $p=10, q=\frac{10}{9}$ provides

$$\|n_t^\pm\|_{(W^{1,2})^*}^{\frac{6}{5}} \le c\Big(\|\mathbf{u}\|_{L^2}^6 + \|n^\pm\|_{L^2}^6 + \|\nabla\Psi\|_{L^2}^6 + \|\nabla\mathbf{u}\|_{L^2}^2 + \|\nabla n^\pm\|_{L^2}^2 + \|\Delta\Psi\|_{L^2}^2\Big). \tag{3.3.19}$$

The proof can be done in the same way for $N=2$. □

Remark 3.3.10. The vanishing Neumann boundary data avoid the occurrence of boundary terms on the right hand side of (3.3.19). Further the $L^\infty(\Omega_T)$-bound allows to improve the result to $n_t^\pm \in W^{1,2}(0,T;(H^1(\Omega))^*)$.

3.3.3 STEP A) (3): Local Existence of $(\mathbf{u}, n^+, n^-, \Psi_0)$

i) We define a Fixed Point Map $F: Y\to Y$, $\overline{\mathbf{y}} := (\overline{n}^+,\overline{n}^-)\mapsto \mathbf{y} := (n^+,n^-)$, where $\mathbf{y}$ is a solution of the system

$$(I)\qquad \begin{aligned} -\Delta\overline{\Psi}_0 &= \overline{n}^+ - \overline{n}^- && \text{in } \Omega_T\\ \langle\nabla\overline{\Psi}_0,\mathbf{n}\rangle &= 0 && \text{on } \partial\Omega\times(0,T)\end{aligned}$$

$$(II)\qquad \begin{aligned} \overline{\mathbf{u}}_t + (\overline{\mathbf{u}}\cdot\nabla)\,\overline{\mathbf{u}} - \Delta\overline{\mathbf{u}} + \nabla p &= -\left(\overline{n}^+ - \overline{n}^-\right)\nabla\overline{\Psi}_0 && \text{in } \Omega_T\\ \operatorname{div}\overline{\mathbf{u}} &= 0 && \text{on } \partial\Omega\times(0,T)\\ \overline{\mathbf{u}} &= 0 && \text{on } \partial\Omega\times(0,T)\end{aligned}$$

$$(III)\qquad \begin{aligned} n_t^\pm \mp \operatorname{div}\left(n^\pm\nabla\overline{\Psi}_0\right) - \Delta n^\pm + (\overline{\mathbf{u}}\cdot\nabla)\,n^\pm &= \pm\operatorname{div}\left(n^\pm\nabla\Psi_1\right) && \text{in } \Omega_T\\ \langle J_{n^\pm},\mathbf{n}\rangle &= 0 && \text{on } \partial\Omega\times(0,T)\end{aligned}$$

for the given data $\overline{\mathbf{y}}$. Further we set

$$Y := \left\{ \mathbf{y} := (n^+, n^-)\,; n^+, n^- \in L^4(0,T;L^2(\Omega)) \right\}$$

and we equip this space with the norm

$$\left\| (n^+, n^-) \right\|_Y := \left\| n^+ \right\|_{L^4(0,T;L^2)} + \left\| n^- \right\|_{L^4(0,T;L^2)} .$$

We define the subset $B_R \subset Y$ as follows,

$$B_R := \{ \mathbf{y} \in Y; \|\mathbf{y}\|_Y \le R < \infty \} ,$$

where $R, T_0 > 0$ will be fixed later on.

The system $(I) - (III)$ allows to apply standard parabolic and elliptic existence results [47]. Note that in (I) we have a right hand side in L^2 that provides a unique $\overline{\Psi}_0 \in L^4(0,T;H^2)$. Also in (II), the right hand side is in $L^2(\Omega_T)$ what provides the unique standard weak solution $\mathbf{u} \in L^\infty(0,T;L^2) \cap L^2(0,T;H^1)$. For (III), we obtain well-posedness for coefficients $\overline{b}^j_\pm$ and $\overline{c}^\pm$, introduced in Remark 3.2.1, at least in $L^2(0,T;L^2)$, i.e., we get a unique $n^\pm \in L^\infty(0,T;L^2) \cap L^2(0,T;H^1)$.

These observations immediately imply that F is well defined.

ii) To apply Schauder's Fixed Point Theorem, we verify next that

1) $B_R \subset Y$ is closed and convex,

2) $F : B_R \to B_R$ is continuous,

3) FB_R is precompact, i.e., the closure $\mathrm{cl}(FB_R)$ is compact in Y.

1) is an immediate consequence of the definition of B_R.

2) To obtain the self-mapping property, we test (3.2.4) and (3.2.6) in dimension $N = 3$ with $n^\pm$, i.e.,

(3.3.20)
$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|n^\pm\|^2_{L^2} + \|\nabla n^\pm\|^2_{L^2} \le c\Big(\|\overline{n}^+\|^4_{L^2} + \|\overline{n}^-\|^4_{L^2} + \|\Psi_1\|^4_{H^2}\Big)\|n^\pm\|^2_{L^2} + \frac{1}{2}\|\nabla n^\pm\|^2_{L^2},$$

Now for $\overline{C}(t) := \|\overline{n}^+\|^4_{L^2} + \|\overline{n}^-\|^4_{L^2} + \|\Psi_1\|^4_{H^2}$ we apply Gronwall's inequality to (3.3.20), i.e.,

$$\|n^\pm(T,\cdot)\|^2_{L^2} \le \exp\left\{ \int_0^T \overline{C}(t)dt \right\} \|n_0^\pm\|^2_{L^2} =: C < \infty. \tag{3.3.21}$$

We can proceed in the same way for dimension $N \le 2$. Hence the ball B_R is invariant under F for $R > 0$ large enough and $T > 0$ small enough, since

$$\|n^\pm\|_{L^4(0,T;L^2(\Omega))} = \left(\int_0^T \left(\int_\Omega |n^\pm|^2 dx \right)^2 dt \right)^{\frac{1}{4}} \le T^{\frac{1}{4}} C^{\frac{1}{2}}_{\overline{n}^\pm}(T, n_0^\pm, \Psi_1) \le \frac{1}{2}R. \tag{3.3.22}$$

To prove the continuity of F, we define (n_1^+, n_1^-), respectively (n_2^+, n_2^-), as the images of $F(\overline{n}_1^+, \overline{n}_1^-)$, respectively $F(\overline{n}_2^+, \overline{n}_2^-)$. Our aim is now to control $\|n_1^+ - n_2^+\|^4_{L^2}$ via $\|\overline{n}_1^+ - \overline{n}_2^+\|^4_{L^2}$

and the same for $\|n_1^- - n_2^-\|_{L^2}^4$. In the following we differ $(\overline{\psi})_1$ from the external potential ψ_1. The equation (3.2.4) reads in such a difference form as

(3.3.23)
$$(n_1^+ - n_2^+)_t - \operatorname{div}\big((n_1^+ - n_2^+)\nabla(\overline{\psi})_1\big) - \operatorname{div}\big(n_2^+\nabla\big((\overline{\psi})_1 - (\overline{\psi})_2\big)\big) - \Delta(n_1^+ - n_2^+) \\ + ((\overline{\mathbf{u}}_1 - \overline{\mathbf{u}}_2)\cdot\nabla)n_1^+ + (\overline{\mathbf{u}}_2\cdot\nabla)(n_1^+ - n_2^+) = 0,$$

and after testing with $n_1^+ - n_2^+$ and in consideration of $\big((\mathbf{u}_2\cdot\nabla)(n_1^+ - n_2^+), (n_1^+ - n_2^+)\big) = 0$, thanks to $\operatorname{div}\mathbf{u}_i = 0$, for $i = 1, 2$, and with the control $\nabla n_{1,2}^+ \in L^2$ provided by (3.3.20) and (3.3.21), we obtain in dimension $N = 3$ (and similarly for $N = 2$)

(3.3.24)
$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|n_1^+ - n_2^+\|_{L^2}^2 + \|\nabla(n_1^+ - n_2^+)\|_{L^2}^2 \le c\Big(\|\overline{n}_1^+ - \overline{n}_1^-\|_{L^2}^4 + \|\Delta\psi_1\|_{L^2}^4\Big)\|n_1^+ - n_2^+\|_{L^2}^2 \\ + \frac{3}{4}\|\nabla\big(n_1^+ - n_2^+\big)\|_{L^2}^2 + c\|\nabla n_1^+\|_{L^2}^2\|\overline{\mathbf{u}}_1 - \overline{\mathbf{u}}_2\|_{L^2}^{\frac{2}{3}} \\ + c\|\nabla n_2^+\|_{L^2}\|n_2^+\|_{L^2}\big(\|\overline{n}_1^+ - \overline{n}_2^+\|_{L^2}^2 + \|\overline{n}_1^- - \overline{n}_2^-\|_{L^2}^2\big) \\ + c\|n_1^+\|_{L^2}^{\frac{2}{3}}\|\nabla(\overline{\mathbf{u}}_1 - \overline{\mathbf{u}}_2)\|_{L^2}^2.$$

In (3.3.24) no boundary terms occur, since we avoid integration by parts and use the convexity of the domain. Let us define $\alpha(t) := \frac{1}{2}c_{L^4}C(\epsilon)\Big(\|\overline{n}_1^+ - \overline{n}_1^-\|_{L^2}^4 + \|\Delta\psi_1\|_{L^2}^4\Big) + c\|\nabla n_1^+\|_{L^2}^2\|\overline{\mathbf{u}}_1 - \overline{\mathbf{u}}_2\|_{L^2}^{\frac{2}{3}} + c\|n_1^+\|_{L^2}^{\frac{2}{3}}\|\nabla(\overline{\mathbf{u}}_1 - \overline{\mathbf{u}}_2)\|_{L^2}^2$, and $\beta(t) := c_S(c_S + 1)^{\frac{1}{2}}c_{L^3}\|\nabla n_2^+\|_{L^2}$. After multiplication of (3.3.24) with $\exp\Big(-\int_0^t \alpha(s)\,ds\Big)$ and via the estimates (3.3.20) and (3.3.21) we now obtain

(3.3.25)
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\exp\Big(-\int_0^t \alpha(s)\,ds\Big)\|n_1^+ - n_2^+\|_{L^2}^2\right) \\ \le \exp\Big(-\int_0^t \alpha(s)\,ds\Big)\beta(t)\|n_2^+\|_{L^2}\big(\|\overline{n}_1^+ - \overline{n}_2^+\|_{L^2}^2 + \|\overline{n}_1^- - \overline{n}_2^-\|_{L^2}^2\big).$$

Integration over t yields to

(3.3.26)
$$\exp\Big(-\int_0^t \alpha(s)\,ds\Big)\|n_1^+ - n_2^+\|_{L^2}^2 \\ \le c\int_0^t \exp\Big(-\int_0^s \alpha(r)\,dr\Big)\beta\|n_2^+\|_{L^2}\big(\|\overline{n}_1^+ - \overline{n}_2^+\|_{L^2}^2 + \|\overline{n}_1^- - \overline{n}_2^-\|_{L^2}^2\big)\,ds \\ \le c\|n_2^+\|_{L^\infty(0,T;L^2(\Omega))}\left(\int_0^t \exp\Big(-\int_0^s \alpha(r)\,dr\Big)\beta(s)^2\,ds\right)^{\frac{1}{2}} \\ \left(\left(c\int_0^t \exp\Big(-\int_0^s \alpha(r)\,dr\Big)\big(\|\overline{n}_1^+ - \overline{n}_2^+\|_{L^2}^4\,ds\right)^{\frac{1}{2}}\right. \\ \left. + \left(c\int_0^t \exp\Big(-\int_0^s \alpha(r)\,dr\Big)\big(\|\overline{n}_1^- - \overline{n}_2^-\|_{L^2}^4\big)\,ds\right)^{\frac{1}{2}}\right),$$

where α and β is controlled via estimates (3.3.20) and (3.3.21). Now we repeat the same as for (3.3.23) for $n_1^- - n_2^-$. By using the analogous definitions $\tilde{\alpha}(t)$, $\tilde{\beta}(t)$ and adding up the estimates provides smallness of $\|n_1^+ - n_2^+\|_{L^2} + \|n_1^- - n_2^-\|_{L^2}$ controllable with the smallness of $\|\overline{n}_1^+ - \overline{n}_2^+\|_{L^2} + \|\overline{n}_1^- - \overline{n}_2^-\|_{L^2}$.

3) is a consequence of Aubin-Lions' compactness result. The estimate (3.3.20) provides $n^\pm \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))$; by Lemma 3.3.9, we obtain additional regularity of solutions $n_t^\pm$ in time. Therefore, $cl(FB_R)$ is compact in the $\|\cdot\|_{L^2(0,T;L^2(\Omega))}$-norm by Aubin-Lions, and the compactness in Y follows from its local boundedness in the $L^\infty(0,T;L^2(\Omega))$-norm.

STEP B) (1): Global Existence of Weak Solutions

To achieve global existence by repeatedly applying the established local existence result we have to derive uniform bounds. Therefore we test the Navier-Stokes equation (3.2.1) with $\mathbf{u}$ and use the Lemma 3.3.6 to obtain

$$\begin{aligned}(3.3.27)\qquad &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_{L^2}^2 + \|\nabla\mathbf{u}\|_{L^2}^2 \\ &\leq \|\nabla\Psi\|_{L^2(\Omega)}\left(\|n^+\|_{L^\infty(\Omega_T)} + \|n^-\|_{L^\infty(\Omega_T)}\right)\|\mathbf{u}\|_{L^2} \\ &\leq c\left(\|n^+\|_{L^\infty(\Omega_T)} + \|n^-\|_{L^\infty(\Omega_T)}\right)^2\left(\mu(\Omega)\right)^{1/2}\|\nabla\mathbf{u}\|_{L^2},\end{aligned}$$

which we rewrite as

$$\begin{aligned}(3.3.28)\qquad &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_{L^2}^2 + \frac{1}{2}\|\nabla\mathbf{u}\|_{L^2}^2 \\ &\leq c_S\Big(\|n^+\|_{L^\infty(\Omega_T)} + \|n^-\|_{L^\infty(\Omega_T)}\Big)^4\left(\mu(\Omega)\right) =: C(\Omega,n^\pm) < \infty.\end{aligned}$$

If we do the same procedure for the Nernst-Planck equations (3.2.4)-(3.2.6) we directly obtain, under consideration of $\left((\mathbf{u}\cdot\nabla)n^\pm, n^\pm\right) = 0$ and the convexity of the domain, that

$$\begin{aligned}(3.3.29)\qquad &\frac{1}{2}\|n^\pm(\cdot,T)\|_{L^2}^2 + \frac{1}{2}\int_0^T \|\nabla n^\pm(\cdot,t)\|_{L^2}^2\,\mathrm{d}t \\ &\leq cT(C_{n_0^\pm}^\infty)^2\big(C_{n_0^+}^\infty + C_{n_0^-}^\infty\big)^2 + \frac{1}{2}\|n_0^\pm\|_{L^2}^2 =: C(\Omega,T,n_0^+,n_0^-) < \infty.\end{aligned}$$

For the definition of $C_{n_0^\pm}^\infty$ see (3.3.15) respectively (3.3.16). Therefore the local existence result can be extended to a global existence result by its repeated application in view of the uniform bounds (3.3.28) and (3.3.29), which guarantee that the right end T_l of the time interval $(0,T_l)$ obtained from the local existence result can be used to define the new initial data $\mathbf{u}(\cdot,T_l), n^\pm(\cdot,T_l)$, which again allow to apply the local existence result.

Remark 3.3.11. Lemma 3.3.8 already implies $\mathbf{u} \in C(0,T;L^2) \cap L^2(0,T;H^1)$. But already in dimension $N = 3$ we do not have continuity in time any more. Further the convective term $(\mathbf{u}\cdot\nabla)n^\pm$ in (3.2.4)-(3.2.6) enables only $n_t^\pm \in L^q(0,T;(H^1(\Omega))^*)$ for $q < 2$ without using the L^∞-bound. This lack of in time continuity is the reason why we do not obtain energy identities at the moment, i.e., we have only weak convergence in time and therefore lower semicontinuity of the norm what ends in energy inequalities.

3.3.4 Proof of Theorem 3.2.3

We use a Gronwall type argument. Therefore we introduce the following variables

$$\begin{aligned} \eta^{\pm} &:= n_1^{\pm} - n_2^{\pm}, \qquad \mathbf{v} := \mathbf{u}_1 - \mathbf{u}_2, \\ \varphi &:= (\Psi)_1 - (\Psi)_2\,, \end{aligned} \tag{3.3.30}$$

where $n_i^{\pm}, (\Psi)_i$, and $\mathbf{u}_i$ are the assumed non-unique solutions. Further we distinguish Ψ_i from $(\Psi)_i$, since $\Psi = \Psi_0 + \Psi_1$. The equations (3.2.1)-(3.2.9) look in these new variables like

$$\partial_t \mathbf{v} + (\mathbf{v}\cdot\nabla)\,\mathbf{u}_1 + (\mathbf{u}_2\cdot\nabla)\,\mathbf{v} - \Delta\mathbf{v} = -\left(\eta^+ - \eta^-\right)\nabla(\Psi)_1 - \left(n_2^+ - n_2^-\right)\nabla\varphi, \tag{3.3.31}$$

$$\partial_t \eta^{\pm} \mp \operatorname{div}\left(\eta^{\pm}\nabla(\Psi)_1 \mp n_2^{\pm}\nabla\varphi\right) - \Delta\eta^{\pm} + (\mathbf{v}\cdot\nabla)n_1^{\pm} + (\mathbf{u}_2\cdot\nabla)\eta^{\pm} \;=\; 0. \tag{3.3.32}$$

$$-\Delta\left(\Psi_0\right) = \eta^+ - \eta^-. \tag{3.3.33}$$

In the following we multiply (3.3.31) with $\mathbf{v}$ and equations (3.3.32) with $n^{\pm}$, integrate them over Ω and add them up to

$$\begin{aligned} &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|\mathbf{v}\|_{L^2}^2 + \|\eta^+\|_{L^2}^2 + \|\eta^-\|_{L^2}^2\right) + \left(\|\nabla\mathbf{v}\|_{L^2}^2 + \|\nabla\eta^+\|_{L^2}^2 + \|\nabla\eta^-\|_{L^2}^2\right) \\ &\quad \le C_1(N)\|\mathbf{v}\|_{L^2}^2 + C_2\left(\|\eta^+\|_{L^2}^2 + \|\eta^-\|_{L^2}^2\right) \\ &\qquad + \frac{1}{4}\|\nabla\mathbf{v}\|_{L^2}^2 + \frac{3}{4}\left(\|\nabla\eta^+\|_{L^2}^2 + \|\nabla\eta^-\|_{L^2}^2\right), \end{aligned} \tag{3.3.34}$$

what is a consequence of estimates using standard Hölder and Young inequalities. The associated constants to (3.3.34) are

$$\begin{aligned} C_1(N) :=& \frac{1}{2}\|\Delta(\Psi)_1\|_{L^\infty(\Omega)} + \|n_2^+\|_{L^\infty(\Omega)}^2 + \|n_2^-\|_{L^\infty(\Omega)}^2 \\ &+ C_N\|\nabla\mathbf{u}_1\|_{L^2}^2 + C\left(\|n_1^+\|_{L^2}^2 + \|n_1^-\|_{L^2}^2\right) \end{aligned} \tag{3.3.35}$$

$$C_2 := \left[C\|\Delta(\Psi)_1\|_{L^\infty(\Omega)}^2 + C\right], \tag{3.3.36}$$

where N is the dimension and $C_1(2) = C$ corresponds to the case $N = 2$ and $C_1(3) = 0$ to the case $N = 3$ (neglection of the convective term $(\mathbf{u}\cdot\nabla)\mathbf{u}$). Using Young's inequality with $\epsilon = \frac{1}{4}$-depending constants and defining $C_3 := \max\{C_1,\, C_2\}$ provide with Gronwall's inequality

$$\left(\|\mathbf{v}\|_{L2}^2 + \|\eta^+\|_{L^2}^2 + \|\eta^-\|_{L^2}^2\right) \le \left(\|\mathbf{v}_0\|_{L2}^2 + \|\eta_0^+\|_{L^2}^2 + \|\eta_0^-\|_{L^2}^2\right)\exp\Big(\int_0^{\mathrm{t}} \mathrm{C}_3\,\mathrm{ds}\Big) = 0, \tag{3.3.37}$$

since $\left(\|\mathbf{v}_0\|_{L2}^2 + \|\eta_0^+\|_{L^2}^2 + \|\eta_0^-\|_{L^2}^2\right) = 0$, i.e., $\mathbf{v}_0 = 0$ and $\eta_0^{\pm} = 0$.

3.3.5 Proof of Theorem 3.2.4

In order to obtain existence of strong solutions, we first state a standard regularity result in the Navier-Stokes theory which later on allows to improve the regularity of the weak solutions $n^{\pm}$. The following theorem uses the fact that $\mathbf{f} \in L^\infty(0,T;V^{0,2}(\Omega,\mathbb{R}^d))$ which is stated here for the convenience of the reader.

Theorem 3.3.12. *For given* $\mathbf{f}$ *and* $\mathbf{u}_0$ *satisfying*

$$\mathbf{f} \in L^2(0,T;V^{0,2}(\Omega,\mathbb{R}^d)), \quad \mathbf{u}_0 \in V^{1,2}(\Omega,\mathbb{R}^d), \tag{3.3.38}$$

there exists a unique strong solution to the Navier-Stokes equations satisfying

$$\mathbf{u} \in L^2(0,T;V_0^{1,2} \cap V^{2,2}) \cap C([0,T];V^{1,2}) \cap W^{1,2}(0,T;L^2), \tag{3.3.39}$$

where in $d=3$ *the time* $T = T(\mathbf{u}_0)$ *is finite.*

The existence of the pressure $p \in L^2(0,T;H^1/\mathbb{R})$ we obtain as usual via De Rham's theorem (see [**?**]). Now, we are able to improve the result of Lemma 3.3.9 by using Lemma 3.3.6 and Theorem 3.3.12 which implies $\mathbf{u} \in L^\infty(0,T;V^{1,2})$ as the key to

Lemma 3.3.13. *The weak solutions of (3.2.4) and (3.2.6) satisfy* $n^\pm \in W^{1,2}(0,T;L^2(\Omega)) \cap L^2(0,T;H^2(\Omega))$.

Proof. First in a just formal way we establish $\Delta n^\pm \in L^2(\Omega_T)$. Therefore we multiply (3.2.4) and (3.2.6) with $-\Delta n^\pm$ and integrate in space,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla n^\pm\|_{L^2}^2 + \|\Delta n^\pm\|_{L^2}^2 \le \big|(\nabla n^\pm \nabla\Psi, \Delta n^\pm)\big| + \big|(n^\pm\Delta\Psi, \Delta n^\pm)\big| + \big|((\mathbf{u}\cdot\nabla)n^\pm, \Delta n^\pm)\big|, \tag{3.3.40}$$

where we use the vanishing Neumann boundary conditions in Definition 3.2.7 iii). The first term on the right hand side becomes with Hölder's and Young's inequalities

$$\big|(\nabla n^\pm \nabla\Psi, \Delta n^\pm)\big| \le c\|\nabla\Psi\|_{L^\infty}\|\nabla n^\pm\|_{L^2}^2 + \frac{1}{8}\|\Delta n^\pm\|_{L^2}^2,$$

and the second term

$$\big|(n^\pm\Delta\Psi, \Delta n^\pm)\big| \le c\|n^\pm\|_{L^\infty}^2\|\Delta\Psi\|_{L^2}^2 + \frac{1}{8}\|\Delta n^\pm\|_{L^2}^2.$$

The last term is controlled in dimension $d=3$ using (3.3.17) by

$$\begin{aligned} \Big|\Big((\mathbf{u}\cdot\nabla)n^\pm, \Delta n^\pm\Big)\Big| &\le \|\mathbf{u}\|_{L^4}\|\nabla n^\pm\|_{L^4}\|\Delta n^\pm\|_{L^2} \\ &\le c\|\mathbf{u}\|_{L^2}^{\frac{1}{4}}\|\nabla\mathbf{u}\|_{L^2}^{\frac{3}{4}}\|\nabla n^\pm\|^{\frac{1}{4}}\|\Delta n^\pm\|_{L^2}^{\frac{7}{4}} \\ &\le c\|\mathbf{u}\|_{L^2}^2\|\nabla\mathbf{u}\|_{L^2}^6\|\nabla n^\pm\|_{L^2}^2 + \frac{1}{4}\|\Delta n^\pm\|_{L^2}^2\,, \end{aligned} \tag{3.3.41}$$

where $\|\nabla\mathbf{u}\|_{L^2}^6$ is under control by Theorem 3.3.12. Putting things together leads to

$$\begin{aligned} &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla n^\pm\|_{L^2}^2 + \frac{1}{2}\|\Delta n^\pm\|_{L^2}^2 \\ &\le c\Big(\|\mathbf{u}\|_{L^2}^2\|\nabla\mathbf{u}\|_{L^2}^6 + \|\nabla\Psi\|_{L^\infty}^2\Big)\|\nabla n^\pm\|_{L^2}^2 + c\|n^\pm\|_{L^\infty}^2\Big(\|n^+ - n^-\|_{L^2}^2 + \|\Psi_e\|_{L^2}^2\Big). \end{aligned} \tag{3.3.42}$$

Now we are able to establish the claimed result by testing (3.2.4) and (3.2.6) with $n_t^\pm$ and using Young's inequality to arrive at

$$\frac{1}{4}\|n_t^\pm\|_{L^2}^2 + \frac{\mathrm{d}}{\mathrm{d}t}\|\nabla n^\pm\|_{L^2}^2 \le c\|\mathrm{div}(n^\pm\nabla\Psi)\|_{L^2}^2 + c\|\Delta n^\pm\|_{L^2}^2\|\mathbf{u}\|_{L^2}^{\frac{2}{3}} + c\|\nabla n^\pm\|_{L^2}^{\frac{2}{3}}\|\nabla\mathbf{u}\|_{L^2}^2. \tag{3.3.43}$$

It is left to control $\|\mathrm{div}(n^\pm\nabla\Psi)\|_{L^2}^2$. Since $\Psi \in H^3(\Omega)$, we estimate using Sobolev's embedding

$$\|\mathrm{div}(\mathrm{n}^\pm\nabla\Psi)\|_{L^2}^2 \le \|\nabla n^\pm\nabla\Psi\|_{L^2}^2 + \|n^\pm\Delta\Psi\|_{L^2}^2 \le \|\nabla n^\pm\|_{L^2}^2\|\nabla\Psi\|_{L^\infty}^2 + \|n^\pm\|_{L^\infty}^2\|\Delta\Psi\|_{L^2}^2, \tag{3.3.44}$$

since via $(A2)$ we have

$$\|\Delta\Psi_i\|_{L^2}^2 = \big(\Delta\Psi_i, \Delta\Psi_i\big) = \big((n^+ - n^-), \Delta\Psi_i\big) \le \big(\|n^+\|_{L^2} + \|n^-\|_{L^2}\big)\|\Delta\Psi_i\|_{L^2} \tag{3.3.45}$$

and hence $\|\Delta\Psi\|_{L^2} \le \big(\|n^+\|_\infty + \|n^-\|_{L^\infty}\big)\big(\mu(\Omega)\big)^{\frac{1}{2}} + \|\Psi_e\|_{L^2}$. □

Global ($d = 2$) and local ($d = 3$) existence of strong solutions follows from the regularity improvements in Lemma 3.3.13 and Theorem 3.3.12. Then a consequence of the two results $n^{\pm} \in L^2(0,T;H^2)$, $n_t^{\pm} \in L^2(0,T;L^2)$ is by interpolation, see ([49]), that $n^{\pm} \in C([0,T];H^1)$.

Chapter 4

Convergent Discretizations for the Nernst-Planck-Poisson System

4.1 Introduction

Let $\Omega \subset \mathbb{R}^d$, for $d = 2, 3$ be a bounded Lipschitz domain. The classical drift-diffusion system describes evolution of positively, and negatively charged particles $p, n : (0, T] \times \Omega \to \mathbb{R}_0^+$, and the electric potential $\psi : (0, T] \times \Omega \to \mathbb{R}$,

$$p_t = \operatorname{div}\big(\nabla p + p\nabla\psi\big) \quad \text{in } \Omega_T := (0, T] \times \Omega\,, \tag{4.1.1}$$
$$n_t = \operatorname{div}\big(\nabla n - n\nabla\psi\big) \quad \text{in } \Omega_T\,, \tag{4.1.2}$$
$$-\Delta\psi = p - n \quad \text{in } \Omega_T\,. \tag{4.1.3}$$

This system was formulated by W. Nernst and M. Planck to describe the potential difference in a galvanic cell (e.g., rechargeable batteries, or biological cells). System (4.1.1)–(4.1.3) has applications in electrochemistry, analytical chemistry ([67, 71]; construction of separation devices or sensors [Lambda sensor]), and in biology (where cell membranes separate regions of different ionic concentrations, or neuronal behaviour). In addition, these equations also appear in areas like plasma physics, and semiconductor device modelling, where they are known as van Roosbroeck equations.

We supplement the above problem by the following initial and boundary conditions,

$$p(0, \cdot) = p_0\,, \quad n(0, \cdot) = n_0 \qquad \text{in } \Omega\,, \tag{4.1.4}$$
$$\partial_{\mathbf{n}} p = \partial_{\mathbf{n}} n = \partial_{\mathbf{n}} \psi = 0 \qquad \text{on } \partial\Omega_T := (0, T] \times \partial\Omega\,. \tag{4.1.5}$$

It is well-known that non-negativity of p_0, n_0 is conserved in Ω_T, and that masses

$$\begin{aligned} M_p &= \int_\Omega p_0(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_\Omega p(t, \mathbf{x})\,\mathrm{d}\mathbf{x}\,, \\ M_n &= \int_\Omega n_0(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_\Omega n(t, \mathbf{x})\,\mathrm{d}\mathbf{x}\,, \end{aligned} \tag{4.1.6}$$

stay invariant for all $t \in [0, T]$; moreover, because of (4.1.5), the electroneutrality condition

$$M_p = M_n \tag{4.1.7}$$

is required as well to obtain existence of solutions to (4.1.1)–(4.1.5).

We propose and analyze two Schemes A and B of convergent finite element discretizations of (4.1.1)–(4.1.5). The first energy based approach enjoys a discrete energy equality as motivated in [71] by choosing corresponding admissible test functions in the discrete setting; cf. Section 4.3. We verify further properties for iterates of this scheme, including the conservation of mass, non-negativity, discrete maximum principle, and a perturbed, discrete version of an entropy law which is obtained in the discrete setting by applying interpolation techniques to the derivation of the entropy law in [14, 71]. In order to validate these properties analytically, and also to numerically solve the implicit Scheme A, we introduce the fixed point Algorithm A_1, and establish M-matrix property of the system matrix on strongly acute meshes: non-negativity, and L^∞-boundedness of iterates will then be concluded, as well as a contraction principle, which allows to construct unique solutions to Scheme A. Moreover, a stopping criterion in Algorithm A_1 is provided, which accounts for increments of computed potentials, and overall convergence to solutions of Scheme A for the threshold parameter tending to zero is verified. Finally, convergence of iterates from Algorithm A_1, resp. Scheme A to weak solutions of (4.1.1)–(4.1.5) is established in Section 4.3.2.

To validate a discrete *perturbed* entropy law for iterates of Algorithm A_1 and Scheme A requires stronger regularity assumptions for initial data, as well as a mesh-constraint to hold; cf. Lemma 2, and Theorem 2, ii). In order to have a discrete entropy law for iterates under less requirements on the initial data, we propose Scheme B in Section 4.4. The construction of such a scheme adapts ideas from [36, 6] and transfers the ideas concerning the entropy law of the continuous context [71] more naturally to the discrete setting. Existence of iterates which solve this nonlinear scheme is shown by Brouwer's fixed point theorem, and further characterizations are provided in Theorem 4; convergence to weak solutions of (4.1.1)–(4.1.5) for vanishing discretization and regularization parameters is shown. Finally, the application of fully implicit schemes is motivated by the aim that the discretizations should be able to reproduce such physically relevant behaviors as the energy and entropy principle. To overcome the implicit character in practice, we choose a suitable fixed point algorithm which is shown to converge to the implicit scheme applying Banach's fixed point theorem, for a suitable stopping criterion accounting for increments of charge densities.

We verify convergence for all, threshold, discretization, and regularization parameters tending to zero.

For the analysis of the schemes below, we consider the different sets of data:

- Regularity of the domain: The bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, for $d = 2, 3$, either has $C^{1,1}$ boundary, or is convex polygonal (resp. polyhedral, for $d = 3$).

- Regularity of the initial data:

  (I1) $p(0, \cdot) = p_0$ and $n(0, \cdot) = n_0$ are in $L^\infty(\Omega)$, and non-negative.

  (I2) $p(0, \cdot) = p_0$ and $n(0, \cdot) = n_0$ are in $W^{1,2}(\Omega)$, and non-negative.

In the following, we need some restrictions regarding possible triangulations $\mathcal{T}_h$ of $\Omega \subset \mathbb{R}^d$, and depending on which properties of the continuum problem we wish to conserve:

- Regularity of the mesh:

  (T1) $\mathcal{T}_h$ is quasi-uniform and strongly acute.

  (T2) $\mathcal{T}_h$ is quasi-uniform and right-angled.

We recall the meaning of strongly acute meshes and right-angled meshes in Section 2.2. In the literature, there are different numerical approximations available for the steady state Nernst-Planck-Poisson equations, see e.g. [17, 3, 39, 53, 54]. The most related works in spirit to the present one are [17, 20, 21]: in [21], existence as well as uniqueness of iterates of a finite volume based discretization for the extended model (4.1.8)–(4.1.12) with positive initial data is shown by Brouwer's fixed point theorem; asymptotic convergence ($t \to \infty$) towards solutions of a discretization of the steady-state problem is established in [20].

In the present work, we propose and compare two different finite element discretizations, which are motivated by two Lyapunov structures inherent to the problem, and which are therefore referred to as energy-based vs. entropy based discretization. Next to establishing convergence of iterates of fully practical schemes to solutions of (4.1.1)–(4.1.5), our main focus is to recover characteristic properties of the limiting schemes at finite discretization scales, and to identify necessary analytical and numerical requirements needed to establish these properties for Schemes A and B, as well as Algorithms A_1 and B_1; see Figure 4.1.1.

Most of the obtained results remain valid for an extended version of (4.1.1)–(4.1.5), where (4.1.1)–(4.1.3) are replaced by

$$p_t = \operatorname{div}\big(\nabla r(p) + p\nabla\psi\big) \quad \text{in } \Omega_T\,, \tag{4.1.8}$$
$$n_t = \operatorname{div}\big(\nabla r(n) - n\nabla\psi\big) \quad \text{in } \Omega_T\,, \tag{4.1.9}$$
$$-\Delta\psi = p - n + c\,, \tag{4.1.10}$$

for a given doping profile $c \in L^\infty(\Omega)$, and $r(s) = s^\alpha$, for $\alpha > 1$; we refer to [41, 21, 20] for a more detailed discussion of this model and references. Moreover, instead of (4.1.5) we may allow for Dirichlet-Neumann boundary conditions which do not change in time,

$$p = p_D\,, \quad n = n_D\,, \quad \psi = \psi_D \qquad \text{on } (0,T] \times \Gamma_D\,, \tag{4.1.11}$$
$$\partial_{\mathbf{n}} r(p) = \partial_{\mathbf{n}} r(n) = \partial_{\mathbf{n}}\psi = 0 \qquad \text{on } (0,T] \times \Gamma_N\,. \tag{4.1.12}$$

The remainder of this work starts with Section 4.2, where necessary material and notation are collected. Energy based discretizations (i.e., Schemes A_i, for $i = 1, 2, 3$) are studied in Section 4.3; entropy based discretizations are introduced and analyzed in Section 4.4. In Section 4.5, we highlight necessary modifications of the arguments to validate most of the results in Sections 4.3 and 4.4 for (4.1.8)–(4.1.12). Comparative computational results are reported in Section 4.6.

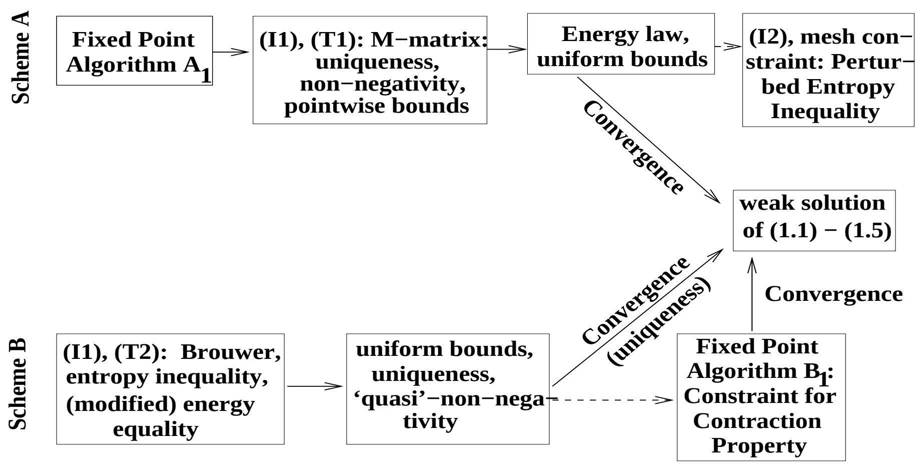


Figure 4.1.1: Outline: Study of energy based (Scheme A) and entropy based (Scheme B) discretizations of (4.1.1)–(4.1.5).

4.2 Preliminaries

The standard Sobolev space notation is used in this paper; see [1] for details. In particular, let $(\cdot,\cdot)$ denote the standard $L^2(\Omega)$-inner product. The generic constant $C>0$ is independent of p,n,ψ, the mesh parameters $k,h>0$, and $T\equiv t_J>0$.

4.2.1 Solvability of the Nernst-Planck-Poisson System.

We recall the concept of weak solutions to (4.1.1)–(4.1.7).

Definition 1. *Suppose (I1), and let $T>0$. The triple $(p,n,\psi):\Omega_T\to\mathbb{R}^3$ is called a weak solution of (4.1.1)–(4.1.7) if*

(1) $p,n\in L^2(0,T;W^{1,2}(\Omega))\cap C([0,T];L^2(\Omega))$

(2) initial data are attained, i.e., for $t\to 0$,

$$p(t,\cdot)\to p_0\,,\qquad n(t,\cdot)\to n_0\qquad \text{in } L^2(\Omega)\,.$$

(3) (4.1.1)–(4.1.3) *hold in the weak sense, i.e., for all $(\phi_1,\phi_2,\phi_3)\in\big[W^{1,2}(\Omega_T)\big]^3$ with $\phi_1(T)=0=\phi_2(T)$, there holds*

$$\int_0^T\Big[-\big(p,(\phi_1)_t\big)+\big(\nabla p,\nabla\phi_1\big)+\big(p\nabla\psi,\nabla\phi_1\big)\Big]\,\mathrm{d}s=\big(p_0,\phi_1(0,\cdot)\big)\,,$$
$$\int_0^T\Big[-\big(n,(\phi_2)_t\big)+\big(\nabla n,\nabla\phi_2\big)-\big(n\nabla\psi,\nabla\phi_2\big)\Big]\mathrm{d}s=\big(n_0,\phi_2(0,\cdot)\big)\,,$$
$$\int_0^T\Big[\big(\nabla\psi,\nabla\phi_3\big)-\big(p-n,\phi_3\big)\Big]\mathrm{d}s=0\,.$$

A weak solution of (4.1.1)–(4.1.7) enjoys the two additional characterizations [32, 71]:

(P1) p, n show mass conservation (see (4.1.6)), and satisfy the following energy law for a.e. $t\in[0,T]$,

$$\frac{1}{2}\|\nabla\psi(t,\cdot)\|_{L^2}^2+\int_0^t\Big(\|p-n\|_{L^2}^2+\Big\|\sqrt{p+n}\nabla\psi\Big\|_{L^2}^2\Big)\,\mathrm{d}s=\frac{1}{2}\|\nabla\psi(0,\cdot)\|_{L^2}^2\,.$$

(P2) The weak solutions p and n satisfy the entropy law for a.e. $t\in[0,T]$,

$$W(t)+\int_0^t\big[I^+(s)+I^-(s)\big]\,\mathrm{d}s\le W(0)\,,$$

where

$$W(t)=\int_\Omega\Big[p(t,\cdot)\big(\ln p(t,\cdot)-1\big)+1+n(t,\cdot)\big(\ln n(t,\cdot)-1\big)+1+\frac{1}{2}|\nabla\psi(t,\cdot)|^2\Big]\,\mathrm{d}\mathbf{x}\,,$$
$$I^+=\int_\Omega p\big|\nabla(\ln p-\psi)\big|^2\,\mathrm{d}\mathbf{x}\qquad\text{and}\qquad I^-=\int_\Omega n\big|\nabla\big(\ln n-\psi\big)\big|^2\mathrm{d}\mathbf{x}\,.$$

In the following, we write $E(\psi) := \frac{1}{2}\|\nabla\psi\|_{L^2}^2$ for the electric energy density. The term $\|\sqrt{p+n}\nabla\psi\|_{L^2}^2$ stands for the total electric energy. Moreover the difference $p-n$ corresponds to the physical term charge density. Finally the mapping $t \mapsto W(t)$ is referred to as the entropy.

Existence of a unique weak solution in the sense of Definition 1 is shown in [32]. Asymptotic convergence of solutions of (4.1.1)–(4.1.5) to steady states [14] with exponential rate is shown in [5, 13]. For the energy property (P1) we refer to [71] and the entropy characterization (P2) can be found in [32] or in a more general context also in [71].

Further results for the drift-diffusion model regarding existence and asymptotic studies in the case of different boundary conditions may be found in [29, 30, 31, 32].

4.2.2 Finite element spaces

We denote a triangulation of a bounded polygonal or polyhedral domain $\Omega \subset \mathbb{R}^d$ with $\mathcal{T}_h$ for $d = 2, 3$. Moreover, let $\mathcal{T}_h$ be a quasi-uniform triangulation of Ω into triangles or tetrahedrons of maximal diameter $h > 0$, see [16]. Let $\mathcal{N}_h = \{\mathbf{x}_\ell\}_{\ell\in L}$ denote the set of all nodes of $\mathcal{T}_h$. We define the finite element space

$$V_h = \left\{\Phi \in C(\overline{\Omega}) : \Phi\big|_K \in P_1(K)\right\},$$

and the nodal interpolation operator $\mathcal{I}_h : C(\overline{\Omega}) \to V_h$, such that $\mathcal{I}_h\psi = \sum_{\mathbf{z}\in\mathcal{N}_h} \psi(\mathbf{z})\varphi_{\mathbf{z}}$; here, $\{\varphi_{\mathbf{z}} : \mathbf{z} \in \mathcal{N}_h\} \subset V_h$ denotes the nodal basis for V_h, and $\psi \in C(\overline{\Omega})$. For functions $\phi, \psi \in C(\overline{\Omega})$, a discrete inner product is defined by

$$\big(\phi,\psi\big)_h := \int_\Omega \mathcal{I}_h[\phi\,\psi]\,\mathrm{d}\mathbf{x} = \sum_{\mathbf{z}\in\mathcal{N}_h} \beta_{\mathbf{z}}\phi(\mathbf{z})\psi(\mathbf{z}),$$

where $\beta_{\mathbf{z}} = \int_\Omega \varphi_z\,\mathrm{d}\mathbf{x}$ for all $\mathbf{z} \in \mathcal{N}_h$; we define $||\psi||_h^2 := (\psi,\psi)_h$. Recall that for all $\Phi, \Psi \in V_h$,

$$||\Psi||_{L^2} \le ||\Psi||_h \le (d+2)^{1/2}||\Psi||_{L^2} \qquad \forall\,\Psi \in V_h\,, \tag{4.2.1}$$

$$\big|(\Phi,\Psi)_h - (\Phi,\Psi)\big| \le Ch||\Phi||_{L^2}\,||\Psi||_{W^{1,2}} \qquad \forall\,\Phi,\Psi \in V_h\,. \tag{4.2.2}$$

Set $[\cdot,\cdot]_1 = (\cdot,\cdot)$, $[\cdot,\cdot]_2 = (\cdot,\cdot)_h$ and let $\|\cdot\|_i$ be their induced norms. Further we define the discrete Laplace operators $\mathcal{L}_h^i : W^{1,2}(\Omega) \to V_h$ for $i = 1, 2$ by

$$\Big[\mathcal{L}_h^i\Psi,\Phi\Big]_i = (\nabla\Psi,\nabla\Phi) \qquad \forall\,\Phi \in V_h\,.$$

The following discrete Sobolev interpolation inequality for $i = 1, 2$ follows from the arguments in [38, Lemma 4.4],

$$\|\nabla\Phi\|_{L^6} \le C\big(\|\mathcal{L}_h^i\Phi\|_{L^2} + \|\Phi\|_{W^{1,2}}\big) \qquad \forall\,\Phi \in V_h\,. \tag{4.2.3}$$

Special properties of quasi-uniform triangulations $\mathcal{T}_h$ are required in below.

Definition 2. *1. We say that the triangulation $\mathcal{T}_h$ of Ω is weakly acute if for all $z \in \mathcal{N}_h \setminus \partial\Omega$ and all $y \in \mathcal{N}_h \setminus \{z\}$ we have $(\nabla\varphi_z, \nabla\varphi_y) \le 0$.*
2. If we require moreover that $(\nabla\varphi_z, \nabla\varphi_y) < 0$ is satisfied for a certain triangulation $\mathcal{T}_h$, then we call such a triangulation strongly acute.

It is known that a triangulation $\mathcal{T}_h$ of $\Omega \subset \mathbb{R}^d$ satisfies property 2. if the sum of opposite angles to each common side/face of adjacent triangles is $\le \pi - \theta$, with $\theta > 0$ independent of $h > 0$, see [46, 58]. A triangulation $T \in \mathcal{T}_h$ is called right-angled for $d = 3$, if all tetrahedrons have one vertex with exactly one right angle, one vertex with exactly two right angles, and all other angles are strictly acute; see Section 4 for more details. We note that a cube is easily partitioned into such tetrahedrons. Sufficient for our analysis is to assume that each element has d mutually perpendicular edges; the case that a tetrahedron has a vertex with three right angles is unrealistic in practice and therefore, for ease of exposition, excluded.

4.2.3 Discrete time-derivatives and interpolations

Given a time-step size $k > 0$, and a sequence $\{\varphi^j\}$ in some Banach space X, we set $d_t\varphi^j := k^{-1}\{\varphi^j - \varphi^{j-1}\}$ for $j \geq 1$. Note that $(d_t\varphi^j, \varphi^j) = \frac{1}{2}d_t\|\varphi^j\|^2 + \frac{k}{2}\|d_t\varphi^j\|^2$, if X is a Hilbert space. Piecewise constant interpolations of $\{\varphi^j\}$ are defined for $t \in [t_j, t_{j+1})$, and $0 \leq j \leq J$ by

$$\underline{\varphi}(t) := \varphi^j \quad \text{and} \quad \overline{\varphi}(t) := \varphi^{j+1}\,,$$

and a piecewise affine interpolation on $[t_j, t_{j+1})$ is defined by

$$\varphi(t) := \frac{t - t_j}{k}\varphi^{j+1} + \frac{t_{j+1} - t}{k}\varphi^j\,.$$

Note that there holds $\|\underline{\Phi} - \Phi\|_X + \|\overline{\Phi} - \Phi\|_X \leq 2k\|d_t\Phi\|_X$.

4.3 Energy based Schemes: Stability and Convergence

4.3.1 Existence and Stability

We consider an implicit discretization of (4.1.1)–(4.1.5).

Scheme A. Let $(P^0, N^0) \in [V_h]^2$, such that $(P^0 - N^0, 1) = 0$. For every $j \geq 1$, find iterates $(P^j, N^j, \Psi^j) \in [V_h]^3$, where $(\Psi^j, 1) = 0$, such that for all $(\Phi_1, \Phi_2, \Phi_3) \in [V_h]^3$ and for $i = 1$, 2 holds

$$[d_tP^j, \Phi_1]_i + \Big(P^j\nabla\Psi^j, \nabla\Phi_1\Big) + (\nabla P^j, \nabla\Phi_1) = 0\,, \tag{4.3.1}$$

$$[d_tN^j, \Phi_2]_i - \Big(N^j\nabla\Psi^j, \nabla\Phi_2\Big) + (\nabla N^j, \nabla\Phi_2) = 0\,, \tag{4.3.2}$$

$$(\nabla\Psi^j, \nabla\Phi_3) = [P^j - N^j, \Phi_3]_i\,. \tag{4.3.3}$$

The main result in this section is given in the following

Theorem 1. *Let (I1), (T1) be valid, let $i = 2$, $k > 0$ and $h > 0$ sufficiently small, and $T \equiv t_J > 0$. Suppose that $0 \leq P^0, N^0 \leq 1$. For every $j \geq 1$, there exists a unique $(P^j, N^j, \Psi^j) \in [V_h]^3$, such that* (4.3.1)–(4.3.3) *hold. Moreover,*

$$0 \leq P^j, N^j \leq 1 \qquad (1 \leq j \leq J)\,, \tag{4.3.4}$$

and there exists $C \equiv C(\Omega) > 0$ such that

i)
$$E(\Psi^J) + \frac{k^2}{2}\sum_{j=1}^J \|\nabla d_t\Psi^j\|_{L^2}^2 + k\sum_{j=1}^J\Big(P^j + N^j, |\nabla\Psi^j|^2\Big) + k\sum_{j=1}^J \big\|\Delta_h\Psi^j\big\|_i^2 = E(\Psi^0)\,,$$

ii)
$$\frac{1}{2}\Big(\|P^J\|_i^2 + \|N^J\|_i^2\Big) + \frac{k^2}{2}\sum_{j=1}^J\Big(\|d_tP^j\|_i^2 + \|d_tN^j\|_i^2\Big) + \frac{k}{2}\sum_{j=1}^J\Big(\|\nabla P^j\|_{L^2}^2 + \|\nabla N^j\|_{L^2}^2\Big) \leq \frac{1}{2}\Big(\|P^0\|_i^2 + \|N^0\|_i^2\Big) + 2E(\Psi^0)\,,$$

iii)
$$k\sum_{j=1}^J\Big[\|d_tP^j\|^2_{(W^{1,2})^*} + \|d_tN^j\|^2_{(W^{1,2})^*}\Big] \leq C\Big[\|P^0\|_i^2 + \|N^0\|_i^2 + E(\Psi^0)\Big]\,,$$

Assertion i) is a discrete version of the energy equality for (4.1.1)–(4.1.3); see property (P1).

The main difficulty in the proof comes from the nonlinear terms in (4.3.1)–(4.3.2), whose effective treatment requires non-negativity, and L^∞-bounds for iterates $\big(P^j, N^j\big)$. For this purpose, we introduce an implementable Algorithm A_1, which is a simple fixed-point scheme, together with a suitable stopping criterion, which includes a threshold parameter $\theta > 0$, which will be specified below.

Algorithm $\mathbf{A_1}$. 1. Let $(P^0, N^0) \in \big[V_h\big]^2$, such that $\big(P^0 - N^0, 1\big) = 0$. For $j \geq 1$, set $(P^{j,0}, N^{j,0}) := (P^{j-1}, N^{j-1})$, and $\ell := 0$.

2. For $\ell \geq 1$, compute $\big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big) \in \big[V_h\big]^3$, where $\big(\Psi^{j,\ell}, 1\big) = 0$, such that for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$ and for $i = 1, 2$,

$$\frac{2}{k}\big[P^{j,\ell}, \Phi_1\big]_i + \Big(P^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi_1\Big) + \Big(\nabla P^{j,\ell}, \nabla\Phi_1\Big) = \frac{1}{k}\Big[P^{j-1} + P^{j,\ell-1}, \Phi_1\Big]_i, \tag{4.3.5}$$

$$\frac{2}{k}\big[N^{j,\ell}, \Phi_2\big]_i - \Big(N^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi_2\Big) + \Big(\nabla N^{j,\ell}, \nabla\Phi_2\Big) = \frac{1}{k}\Big[N^{j-1} + N^{j,\ell-1}, \Phi_2\Big]_i, \tag{4.3.6}$$

$$\Big(\nabla\Psi^{j,\ell}, \nabla\Phi_3\Big) = \Big[P^{j,\ell} - N^{j,\ell}, \Phi_3\Big]_i. \tag{4.3.7}$$

3. For fixed $\theta > 0$, stop if

$$\|\nabla\{\Psi^{j,\ell} - \Psi^{j,\ell-1}\}\|_{L^2} + \frac{1}{k}\Big[\|P^{j,\ell} - P^{j,\ell-1}\|_i + \|N^{j,\ell} - N^{j,\ell-1}\|_i\Big] \leq \theta\,, \tag{4.3.8}$$

set $\big(P^j, N^j, \Psi^j\big) := \big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big)$, and go to 4.; otherwise, set $\ell \leftarrow \ell + 1$ and continue with 2.

4. Stop if $j + 1 = J$; set $j \leftarrow j + 1$ and go to 1. otherwise.

The subsequent proof of Theorem 3.1 uses existing iterates of Algorithm A_1 to construct those of Scheme A; crucial steps are to show non-negativity and L^∞-bounds of iterates of *both* numerical schemes in Steps 1 to 4 of the proof below which then allows to verify the properties of iterates of Scheme A in Step 5 as given in Theorem 3.1.

Proof. (of Theorem 3.1) We first establish by induction the existence of $0 \leq P^{1,\ell}, N^{1,\ell} \leq 1$, and the uniqueness of solutions $\big\{\big(P^{1,\ell}, N^{1,\ell}\big)\big\}_{\ell\geq 1}$ via Banach's fixed point theorem. This requires to validate the contraction property for iterates to identify

$$\big(P^1, N^1\big) := \Big(\lim_{\ell\to\infty} P^{1,\ell}, \lim_{\ell\to\infty} N^{1,\ell}\Big) \in \big[V_h\big]^2$$

as unique solution of Scheme A, for $j = 1$. The results are extended to $0 \leq P^{j,\ell}, P^{j,\ell} \leq 1$ $(j, \ell \geq 1)$ afterwards.

Step 1: L^p-bound for $\nabla\Psi^{1,\ell-1}$. Let $0 \leq P^{1,\ell-1}, N^{1,\ell-1} \leq 1$, such that $\big(P^{1,\ell-1} - N^{1,\ell-1}, 1\big) = 0$. The solution $\Psi^{1,\ell-1} \in V_h$ of (4.3.7) may be interpreted as the Ritz projection of $\psi^{1,\ell-1} \in W^{1,2}(\Omega)/\mathbb{R}$, i.e., $\Psi^{1,\ell-1} = P_1\psi^{1,\ell-1}$, such that $\big(\Psi^{1,\ell-1}, 1\big) = 0$, and

$$\big(\nabla\psi^{1,\ell-1}, \nabla\phi_3\big) = \big[P^{1,\ell-1} - N^{1,\ell-1}, \phi_3\big]_i \qquad \forall\, \phi_3 \in W^{1,2}(\Omega) \cap C(\overline{\Omega})\,,$$

where by assumption $\big(P^{1,\ell-1} - N^{1,\ell-1}, 1\big) = 0$. By $W^{1,p}(\Omega)$-stability of P_1, cf. [16, Theorem 8.5.3], there holds $\|\Psi^{1,\ell-1}\|_{W^{1,p}} \leq C\|\psi^{1,\ell-1}\|_{W^{1,p}}$. By Sobolev embedding, the right-hand side is bounded by $C\|P^{1,\ell-1} - N^{1,\ell-1}\|_{L^p}$, for $1 \leq p < \frac{2d}{d-2}$, for $d = 2$, and $1 \leq p \leq \frac{2d}{d-2}$ in the case $d = 3$.

Existence of a unique solution $\big(P^{1,\ell}, N^{1,\ell}\big) \in \big[V_h\big]^2$ follows from Lax-Milgram lemma for $k = k(\Omega) > 0$ sufficiently small. Setting $\Phi_1 = \Phi_2 = 1$ in (4.3.5), (4.3.6) then yields conservation of mass for iterates $\big(P^{1,\ell}, N^{1,\ell}\big)$.

Step 2: M-matrix property for system matrix of (4.3.5)–(4.3.7)*; non-negativity of* $\big(P^{1,\ell}, N^{1,\ell}\big)$. Let $\{\varphi_{\mathbf{x}_\beta}\}_{\beta=1}^L$ be the canonical basis of V_h. We employ vectors $\mathbf{x}^{1,\ell} = (x_\beta^{1,\ell})_{\beta=1}^L$, and $\mathbf{y}^{1,\ell} = (y_\beta^{1,\ell})_{\beta=1}^L$, with

$$P^{1,\ell} = \sum_{\beta=1}^L x_\beta^{1,\ell}\varphi_{\mathbf{x}_\beta} \quad \text{and} \quad N^{1,\ell} = \sum_{\beta=1}^L y_\beta^{1,\ell}\varphi_{\mathbf{x}_\beta}$$

to restate (4.3.5)–(4.3.6) as follows: For every $\ell \geq 1$, find $[\mathbf{x}^{1,\ell}, \mathbf{y}^{1,\ell}]^\top \in \mathbb{R}^{2L}$, such that $\boldsymbol{\mathcal{A}}[\mathbf{x}^{1,\ell}, \mathbf{y}^{1,\ell}]^\top = \mathbf{f}^{1,\ell}$. Here,

$$\boldsymbol{\mathcal{A}} := \begin{pmatrix} \frac{2}{k}M + C\big(\Psi^{1,\ell-1}\big) + K & \mathbf{0} \\ \mathbf{0} & \frac{2}{k}M - C\big(\Psi^{1,\ell-1}\big) + K \end{pmatrix} \in \mathbb{R}^{2L\times 2L},$$

where $M := \big\{m_{\beta\beta'}\big\}_{\beta,\beta'=1}^L$, $K := \big\{k_{\beta\beta'}\big\}_{\beta,\beta'=1}^L$, and $\tilde{C}\big(\Psi^{1,\ell-1}\big) := \big\{c_{\beta\beta'}(\Psi^{1,\ell-1})\big\}_{\beta,\beta'=1}^L$, such that

$$\begin{aligned} m_{\beta\beta'} &:= \Big(\varphi_{\mathbf{x}_\beta}, \varphi_{\mathbf{x}_{\beta'}}\Big)_h, \\ k_{\beta\beta'} &:= \Big(\nabla\varphi_{\mathbf{x}_\beta}, \nabla\varphi_{\mathbf{x}_{\beta'}}\Big), \\ c_{\beta\beta'}\big(\Psi^{1,\ell-1}\big) &:= \Big(\varphi_{\mathbf{x}_\beta}\nabla\Psi^{1,\ell-1}, \nabla\varphi_{\mathbf{x}_{\beta'}}\Big). \end{aligned} \tag{4.3.9}$$

For the right-hand side, $f_\beta^{1,\ell} := \frac{1}{k}\big(P^0 + P^{1,\ell-1}, \varphi_{\mathbf{x}_\beta}\big)$, and $f_{L+\beta}^{1,\ell} := \frac{1}{k}\big(N^0 + N^{1,\ell-1}, \varphi_{\mathbf{x}_\beta}\big)$, for $1 \leq \beta \leq L$.

We verify that $\boldsymbol{\mathcal{A}} := \big\{a_{\beta\beta'}\big\}_{\beta,\beta'=1}^{2L}$ is an M-matrix:

a) Non-positivity of off-diagonal entries of $\boldsymbol{\mathcal{A}}$. Since $\mathcal{T}_h$ is strongly acute, there exists $C_{\theta_0} > 0$, such that $k_{\beta\beta'} \leq -C_{\theta_0}h^{d-2} < 0$ uniformly in $h > 0$, for any pair of adjacent nodes. Moreover, $m_{\beta\beta'} = 0$ in this case. The remaining entries are bounded as follows,

$$\big|c_{\beta\beta'}\big(\Psi^{1,\ell-1}\big)\big| \leq \|\nabla\Psi^{1,\ell-1}\|_{L^{\gamma'}}\|\varphi_{\mathbf{x}_\beta}\nabla\varphi_{\mathbf{x}_{\beta'}}\|_{L^\gamma}, \tag{4.3.10}$$

for values $\frac{d}{d-1} > \gamma \geq 1$, and $\gamma^{-1} + \big(\gamma'\big)^{-1} = 1$. In order to conclude non-positivity of $c_{\beta\beta'}(\Psi^{1,\ell-1}) + k_{\beta\beta'}$ for sufficiently small $h > 0$, a dimensionality argument leads to $d-2 < \frac{d}{\gamma} - 1$, and hence $\frac{2d}{d+2} < \gamma < \frac{d}{d-1}$. In turn, this bound allows to apply the result from Step 1, i.e., for $d = 2, 3$ there exist $d < \gamma' < \frac{2d}{d-2}$ such that $\|\nabla\Psi^{1,\ell-1}\|_{L^{\gamma'}} \leq C$. This verifies non-positivity of off-diagonal entries of $\boldsymbol{\mathcal{A}}$ for $h < h_0(\Omega)$ sufficiently small.

b) Strict positivity of diagonal entries of $\boldsymbol{\mathcal{A}}$. By evidence, $\frac{2}{k}m_{\beta\beta} \geq c_{\theta_0}h^d$, and $k_{\beta\beta} \geq c_{\theta_0}h^{d-2}$, for some $c_{\theta_0} > 0$. Similar to a), in order to make sure that $c_{\beta\beta}\big(\Psi^{1,\ell-1}\big) + \frac{2}{k}m_{\beta\beta} + k_{\beta\beta} > 0$, a dimensionality argument leads to $d - 2 < \frac{d}{\gamma} - 1$, and we may conclude as above.

c) $\boldsymbol{\mathcal{A}}$ *is strictly diagonal dominant.* We again use the fact that the number of neighboring nodes $\mathbf{x}_{\beta'} \in \mathcal{N}_h$ for each $\mathbf{x}_\beta$ is bounded independently of $h > 0$. Hence, there exists a constant $\overline{C} \equiv \overline{C}\big(\#\{\beta' : k_{\beta\beta'} \neq 0\}\big) > 0$, such that for sufficiently small k, $h > 0$

$$\begin{aligned} a_{\beta\beta} &\geq \frac{1}{k}Ch^d + Ch^{d-2} - Ch^{\frac{d}{\gamma}-1} > \overline{C}\max_{\beta\neq\beta'}|a_{\beta\beta'}| \\ &= \overline{C}\Big(C_{\theta_0}h^{d-2} + Ch^{\frac{d}{\gamma}-1}\Big) \geq \sum_{\beta\neq\beta'}|a_{\beta\beta'}|, \end{aligned} \tag{4.3.11}$$

where $C_{\theta_0} > 0$ is as in a). Thanks to $1 \leq \gamma < \frac{d}{d-1}$, we conclude $\sum_{\beta'\neq\beta}|a_{\beta\beta'}| < a_{\beta\beta}$ for all $1 \leq \beta \leq 2L$.

Hence, from a)–c) we may conclude that $\boldsymbol{\mathcal{A}}$ is an M-matrix, which then implies non-negativity of $\big(P^{1,\ell}, N^{1,\ell}\big)$.

Step 3: Boundedness of $0 \leq P^{1,\ell}, N^{1,\ell} \leq 1$. Non-negativity of iterates follows from M-matrix property for the system matrix $\boldsymbol{\mathcal{A}}$, and non-negativity of each term on the right-hand side of (4.3.5), (4.3.6). Let $\overline{P}^{1,r} := P^{1,r} - 1$, for $r = \ell-1, \ell$, and $\overline{P}^0 = P^0 - 1$. We assume $\overline{P}^{1,\ell-1}, \overline{P}^0 < 0$, and for every $\Phi_1 \in V_h$,

$$\frac{2}{k}\big[\overline{P}^{1,\ell}, \Phi_1\big]_i + \Big(\big\{\overline{P}^{1,\ell} + 1\big\}\nabla\Psi^{1,\ell-1}, \nabla\Phi_1\Big) + \big(\nabla\overline{P}^{1,\ell}, \nabla\Phi_1\big) = \frac{1}{k}\big[\overline{P}^{1,\ell-1} + \overline{P}^0, \Phi_1\big]_i . \tag{4.3.12}$$

Let $[\Phi_1]^+ := \mathcal{I}_h\big(\max\{0,\Phi_1\}\big)$, and $[\Phi_1]^- := \mathcal{I}_h\big(\min\{0,\Phi_1\}\big)$ for $\Phi_1 \in V_h$. Then

$$\begin{aligned}\frac{2}{k}\big\|[\Phi_1]^+\big\|_i^2 + \big\|\nabla[\Phi_1]^+\big\|_{L^2}^2 \;&\leq\; \frac{2}{k}\big[[\Phi_1]^+, \Phi_1\big]_i + \big(\nabla[\Phi_1]^+, \nabla\Phi_1\big) \\ &\quad + \Big([\Phi_1]^-\nabla\Psi^{1,\ell-1}, \nabla[\Phi_1]^+\Big) \qquad \forall\, \Phi_1 \in V_h .\end{aligned} \tag{4.3.13}$$

This result follows from $\boldsymbol{\mathcal{A}}$ being an M-matrix, for $h > 0$ sufficiently small,

$$\begin{aligned}&\frac{2}{k}\Big[\Phi_1 - [\Phi_1]^+, [\Phi_1]^+\Big]_i + \Big([\Phi_1]^-\nabla\Psi^{1,\ell-1}, \nabla[\Phi_1]^+\Big) + \Big(\nabla\big\{\Phi_1 - [\Phi_1]^+\big\}, \nabla[\Phi_1]^+\Big) \\ &\quad \geq \frac{2}{k}\big[[\Phi_1]^-, [\Phi_1]^+\big]_i + \Big([\Phi_1]^-\nabla\Psi^{1,\ell-1}, \nabla[\Phi_1]^+\Big) + \big(\nabla[\Phi_1]^-, \nabla[\Phi_1]^+\big) \\ &\quad \geq \sum_{\beta,\beta'} a_{\beta\beta'}[\Phi_1]^+(\mathbf{x}_\beta)[\Phi_1]^-(\mathbf{x}_{\beta'}) \geq 0 .\end{aligned}$$

We may also verify (4.3.13), with negative sign in front of the last term.

Now, putting $\Phi_1 = [\overline{P}^{1,\ell}]^+$ in (4.3.12), and noting that $\overline{P}^{1,\ell} = [\overline{P}^{1,\ell}]^+ + [\overline{P}^{1,\ell}]^-$, , as well as $\big(\nabla\Psi^{1,\ell-1}, \nabla[\overline{P}^{1,\ell}]^+\big) = \big[\overline{P}^{1,\ell-1} - \overline{N}^{1,\ell-1}, [\overline{P}^{1,\ell}]^+\big]_i$, and the following bound, which for $d \leq 3$ uses interpolation of $L^3(\Omega)$ between $L^2(\Omega)$ and $W^{1,2}(\Omega)$,

$$\begin{aligned}\Big([\overline{P}^{1,\ell}]^-\nabla\Psi^{1,\ell-1}, \nabla[\overline{P}^{1,\ell}]^+\Big) \;&\leq\; \big\|[\overline{P}^{1,\ell}]^-\big\|_{L^3}\big\|\nabla\Psi^{1,\ell-1}\big\|_{L^6}\big\|\nabla[\overline{P}^{1,\ell}]^+\big\|_{L^2} \\ &\leq\; C\|[\overline{P}^{1,\ell}]^-\|_{L^2}^2\|\nabla\Psi^{1,\ell-1}\|_{L^6}^4 + \frac{1}{2}\|\nabla[\overline{P}^{1,\ell}]^+\|_{L^2}^2 ,\end{aligned}$$

with positive $C \equiv C(\Omega)$, we find

$$\begin{aligned}&\frac{2}{k}\Big[1 - Ck\|\nabla\Psi^{1,\ell-1}\|_{L^6}^4\Big]\|[\overline{P}^{1,\ell}]^+\|_i^2 + \Big[1 - \frac{1}{2}\Big]\|\nabla[\overline{P}^{1,\ell}]^+\|_{L^2}^2 \\ &\qquad \leq \Big[\frac{1}{k} - 1\Big]\Big(\overline{P}^{1,\ell-1}, [\overline{P}^{1,\ell}]^+\Big) + \Big(\overline{N}^{1,\ell-1}, [\overline{P}^{1,\ell}]^+\Big) + \frac{1}{k}\Big[\overline{P}^0, [\overline{P}^{1,\ell}]^+\Big]_i \leq 0 .\end{aligned} \tag{4.3.14}$$

We proceed similarly with $\overline{N}^{1,\ell} \in V_h$, and arrive at

$$\begin{aligned}&\frac{2}{k}\Big[1 - Ck\|\nabla\Psi^{1,\ell-1}\|_{L^6}^4\Big]\|[\overline{N}^{1,\ell}]^+\|_i^2 + \Big[1 - \frac{1}{2}\Big]\|\nabla[\overline{N}^{1,\ell}]^+\|_{L^2}^2 \\ &\qquad \leq \Big[\frac{1}{k} - 1\Big]\Big(\overline{N}^{1,\ell-1}, [\overline{N}^{1,\ell}]^+\Big) + \Big(\overline{P}^{1,\ell-1}, [\overline{N}^{1,\ell}]^+\Big) + \frac{1}{k}\Big[\overline{N}^0, [\overline{N}^{1,\ell}]^+\Big]_i \leq 0 .\end{aligned} \tag{4.3.15}$$

By Step 1, we have $\|\nabla\Psi^{1,\ell-1}\|_{L^6} \leq C$, for $d \leq 3$, such that for $k \equiv k(\Omega) > 0$ small enough, (4.3.14), (4.3.15) imply that $0 \leq P^{1,\ell}, N^{1,\ell} \leq 1$.

Step 4. Contraction property. We show that for $k \equiv k(\Omega) > 0$ sufficiently small, there exists $0 < q < 1$ such that for every $\ell \geq 1$,

$$\Big\{\big\|P^{1,\ell+1} - P^{1,\ell}\big\|_i + \big\|N^{1,\ell+1} - N^{1,\ell}\big\|_i\Big\} \leq q\Big\{\big\|P^{1,\ell} - P^{1,\ell-1}\big\|_i + \big\|N^{1,\ell} - N^{1,\ell-1}\big\|_i\Big\} . \tag{4.3.16}$$

Let $e^\ell_\Phi := \Phi^{1,\ell} - \Phi^{1,\ell-1} \in V_h$, for letters $\Phi = P, N, \Psi$. Subtraction of two subsequent equations in (4.3.5)–(4.3.7) ($j = 0$) implies for every $\ell \geq 2$ and $i = 1, 2$, and all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$,

$$\frac{2}{k}\big[e^\ell_P, \Phi_1\big]_i + \big(\nabla e^\ell_P, \nabla\Phi_1\big) + \Big(e^\ell_P \nabla\Psi^{1,\ell-1} + P^{1,\ell-1}\nabla e^{1,\ell-1}_\Psi, \nabla\Phi_1\Big) = \frac{1}{k}\big(e^{\ell-1}_P, \Phi_1\big)\,, \tag{4.3.17}$$

$$\frac{2}{k}\big[e^\ell_N, \Phi_2\big]_i + \big(\nabla e^\ell_N, \nabla\Phi_2\big) - \Big(e^\ell_N \nabla\Psi^{1,\ell-1} + N^{1,\ell-1}\nabla e^{1,\ell-1}_\Psi, \nabla\Phi_2\Big) = \frac{1}{k}\big(e^{\ell-1}_N, \Phi_2\big)\,, \tag{4.3.18}$$

$$\Big(\nabla e^\ell_\Psi, \nabla\Phi_3\Big) = \Big[e^\ell_P - e^\ell_N, \Phi_3\Big]_i\,. \tag{4.3.19}$$

Choose $\big(\Phi_1, \Phi_2, \Phi_3\big) = \big(e^\ell_P, e^\ell_N, e^\ell_\Psi\big)$. For $d \leq 3$ and uniformly in $\ell \geq 1$, by the previous step and (4.3.7), $\big\|\nabla\Psi^{1,\ell}\big\|_{L^6} \leq C$, for some $C \equiv C(\Omega)$. Therefore, by interpolation of $L^3(\Omega)$ between $L^2(\Omega)$ and $L^6(\Omega)$, for example,

$$\begin{aligned}&\Big|\Big(e^\ell_P \nabla\Psi^{1,\ell-1} + P^{1,\ell-1}\nabla e^{1,\ell-1}_\Psi, \nabla e^\ell_P\Big)\Big| \\ &\leq \frac{1}{2}\Big[\|e^{\ell-1}_P\|^2_i + \|e^{\ell-1}_N\|^2_i\Big] + C\Big[\|\nabla\Psi^{1,\ell-1}\|^4_{L^6} + \frac{1}{2}\Big]\|e^\ell_P\|^2_i + \frac{1}{2}\|\nabla e^\ell_P\|^2_{L^2}\,,\end{aligned} \tag{4.3.20}$$

where we used Step 3, and (4.3.19). By rearranging terms, and using Step 1, we arrive at

$$\Big[2 - \frac{1}{2} - Ck\Big]\Big[\|e^\ell_P\|^2_i + \|e^\ell_N\|^2_i\Big] + \frac{k}{2}\Big[\|\nabla e^\ell_P\|^2_{L^2} + \|\nabla e^\ell_N\|^2_{L^2}\Big] \leq \big[\frac{1}{2} + \frac{k}{2}\big]\Big[\|e^{\ell-1}_P\|^2_i + \|e^{\ell-1}_N\|^2_i\Big]\,. \tag{4.3.21}$$

Hence, (4.3.16) is valid; by Banach fixed point theorem, $V_h \ni \Phi^1 = \lim_{\ell\to\infty}\Phi^{1,\ell}$, for letters $\Phi = P, N, \Psi$, where $\big(P^1, N^1, \Psi^1\big) \in \big[V_h\big]^3$ solves (4.3.1)–(4.3.3), for $j = 1$. Moreover, $0 \leq P^1, N^1 \leq 1$, and $(P^1 - N^1, 1) = 0$. The above argument and results may now be extended to all $j \geq 1$.

Uniqueness of solutions to Scheme A now follows easily from $0 \leq P^j, N^j \leq 1$.

Step 5: Verification of assertions i)–iii). Assertion i) follows from choosing $\big(\Phi_1, \Phi_2, \Phi_3\big) = \big(\Psi^j, -\Psi^j, P^j - N^j\big)$ in (4.3.1)–(4.3.3), adding (4.3.1)–(4.3.2), and finally summing over indices $1 \leq j \leq J$.

In order to show ii), choose $\big(\Phi_1, \Phi_2\big) = \big(P^j, N^j\big)$, and employ Young's inequality, together with $0 \leq P^j, N^j \leq 1$.

To verify assertion iii), we use approximation properties of the $L^2(\Omega)$-projection $P_0 : L^2(\Omega) \to V_h$, such that $\big(\varphi - P_0\varphi, \Phi\big) = 0$ for all $\Phi \in V_h$. By $W^{1,2}(\Omega)$-stability of P_0 [25], and (4.2.2), as well as (4.3.1) we get

$$\begin{aligned}\|d_t P^j\|_{(W^{1,2})^*} &\leq \sup_{\varphi\in W^{1,2}}\frac{(d_t P^j, P_0\varphi)_h}{\|\varphi\|_{W^{1,2}}} + \sup_{\varphi\in W^{1,2}}\frac{\big|\big(d_t P^j, P_0\varphi\big) - \big(d_t P^j, P_0\varphi\big)_h\big|}{\|\varphi\|_{W^{1,2}}} \\ &\leq C\Big[\|\nabla\Psi^j\|_{L^2} + \|\nabla P^j\|_{L^2} + Ch\|d_t P^j\|_{L^2}\Big]\,.\end{aligned} \tag{4.3.22}$$

In order to bound the last term, we observe (4.2.1), and again use (4.3.1) with $\Phi_1 = d_t P^j$, to conclude

$$\|d_t P^j\|^2_h \leq \Big[\|\nabla\Psi^j\|_{L^2} + \|\nabla P^j\|_{L^2}\Big]\|\nabla d_t P^j\|_{L^2}\,.$$

By inverse estimate, we then obtain from Theorem 1, i) and ii) that $k\sum_{j=1}^J \|d_t P^j\|^2_{(W^{1,2})^*} \leq CE(\Psi^0)$.

Thanks to $0 \leq P^j, N^j \leq 1$ uniformly for $j \geq 1$, this now implies assertions ii), iii) for general $t_J > 0$. □

Remark 1. *The 'shifted' fixed point scheme (Algorithm A_1) is needed in* (4.3.14) *and* (4.3.15) *to efficiently deal with the second term in* (4.3.12) *in Step 3.*

In the next step, we validate a discrete entropy principle which holds for solutions of Scheme A, in the case of strictly positive initial data. For $F(s) := s\big(\ln s - 1\big) + 1$, we introduce the discrete entropy functional

$$j \mapsto W^j := \int_\Omega \mathcal{I}_h\Big[F(P^j) + F(N^j)\Big] + \frac{1}{2}|\nabla \Psi^j|^2 \,\mathrm{d}\mathbf{x} \qquad (\, 0 \leq j \leq J\,).$$

First, we need the following technical

Lemma 1. *Suppose (I2), (T1), that* $k \leq Ch^2$, *and* $0 \leq P^0, N^0 \leq 1$, *and choose* $[\cdot,\cdot]_2 = (\cdot,\cdot)_h$. *For every* $T \equiv t_J > 0$, *the solution* $\big\{(\,P^j, N^j, \Psi^j\,)\big\}_{j=1}^J$ *of Scheme A satisfies*

$$\text{i)} \qquad \frac{1}{2}\max_{1\leq j\leq J}\Big(1 - \frac{k}{Ch^2}\Big)\Big[\|\nabla P^j\|^2_{L^2} + \|\nabla N^j\|^2_{L^2}\Big] + \frac{k^2}{2}\sum_{j=1}^J\Big[\|\nabla d_t P^j\|^2_{L^2} + \|\nabla d_t N^j\|^2_{L^2}\Big]$$
$$+k\sum_{j=1}^J\Big[\|\mathcal{L}_h^1 P^j\|^2_{L^2} + \|\mathcal{L}_h^1 N^j\|^2_{L^2}\Big] \leq C\Big\{E(\Psi^0) + \|\nabla P^0\|^2_{L^2} + \|\nabla N^0\|^2_{L^2}\Big\},$$

$$\text{ii)} \qquad k\sum_{j=1}^J\Big[\|d_t P^j\|^2_{L^2} + \|d_t N^j\|^2_{L^2}\Big] \leq C\Big\{E(\Psi^0) + \|\nabla P^0\|^2_{L^2} + \|\nabla N^0\|^2_{L^2}\Big\}.$$

Proof. To validate assertion i), choose $\Phi_1 = -\mathcal{L}_h^1 P^j \in V_h$ in (4.3.1) to find

$$\frac{1}{2}d_t\|\nabla P^j\|^2_{L^2} + \frac{k}{2}\|\nabla d_t P^j\|^2_{L^2} + \|\mathcal{L}_h^1 P^j\|^2_{L^2} \leq \Big|\Big([P^j\nabla\Psi^j, \nabla\mathcal{L}_h^1 P^j\Big)\Big|. \tag{4.3.23}$$

Let $\overline{\Psi}^j \in W^{1,2}(\Omega)/\mathbb{R}$ be the weak solution to $-\Delta\overline{\Psi}^j = P^j - N^j$ in Ω, with $\partial_{\mathbf{n}}\overline{\Psi}^j = 0$ on $\partial\Omega$. Then, by standard regularity and error analysis, and successively using (4.2.2), we obtain

$$\begin{aligned} \|\nabla\{\overline{\Psi}^j - \Psi^j\}\|_{L^2} &\leq Ch\Big(\|D^2\overline{\Psi}^j\|_{L^2} + \|P^j - N^j\|_{L^2}\Big) \\ &\leq Ch\|P^j - N^j\|_{L^2}\,. \end{aligned} \tag{4.3.24}$$

We may now use (4.3.24) to bound the last term in (4.3.23), an inverse inequality, integration by parts, interpolation of $L^3(\Omega)$ between $L^2(\Omega)$ and $L^6(\Omega)$, and (4.2.3),

$$\begin{aligned} &\Big|\Big(P^j\nabla\big[(\Psi^j - \overline{\Psi}^j) + \overline{\Psi}^j\big], \nabla\mathcal{L}_h^1 P^j\Big)\Big| \\ &\leq \|\nabla\{\Psi^j - \overline{\Psi}^j\}\|_{L^2}Ch^{-1}\|\mathcal{L}_h^1 P^j\|_{L^2} + \\ &\quad +C\Big(\|\nabla P^j\|_{L^3}\|\nabla\overline{\Psi}^j\|_{L^6} + \|\Delta\overline{\Psi}^j\|_{L^2}\Big)\|\mathcal{L}_h^1 P^j\|_{L^2} \\ &\leq C\Big[\|P^j - N^j\|_{L^2} + \big(\|\mathcal{L}_h^1 P^j\|_{L^2} + \|\nabla P^j\|_{L^2}\big)^{1/2}\|\nabla P^j\|^{1/2}_{L^2}\Big]\|\mathcal{L}_h^1 P^j\|_{L^2} \\ &\leq C\Big[\|P^j - N^j\|^2_{L^2} + \|\nabla P^j\|^4_{L^2}\Big] + \frac{1}{2}\|\mathcal{L}_h^1 P^j\|^2_{L^2}\,. \end{aligned} \tag{4.3.25}$$

We insert this upper bound into (4.3.23), and repeat the steps for (4.3.2) correspondingly. After adding both inequalities, and summing over all iteration steps, we employ an inverse estimate, together with the implicit version of the discrete Gronwall lemma,

$$
\begin{aligned}
&\Big(1-\frac{k}{Ch^2}\|P^J\|_{L^2}^2\Big)\|\nabla P^J\|_{L^2}^2+\Big(1-\frac{k}{Ch^2}\|N^J\|_{L^2}^2\Big)\|\nabla N^J\|_{L^2}^2\\
&\quad+\frac{k^2}{2}\sum_{j=1}^{J}\Big[\|\nabla d_tP^j\|_{L^2}^2+\|\nabla d_tN^j\|_{L^2}^2\Big]+k\sum_{j=1}^{J}\Big[\|\mathcal{L}_h^iP^j\|_h^2+\|\mathcal{L}_h^iN^j\|_h^2\Big]\\
&\quad+k\sum_{j=1}^{J}\Big[\|d_tP^j\|_{L^2}^2+\|d_tN^j\|_{L^2}^2\Big]\leq E(\Psi^0)+\sum_{j=1}^{J-1}k\|\nabla P^j\|_{L^2}^2\|\nabla P^j\|_{L^2}^2\\
&\quad+\sum_{j=1}^{J-1}k\|\nabla P^j\|_{L^2}^2\|\nabla P^j\|_{L^2}^2+\frac{1}{2}\Big\{\|\nabla P^0\|_{L^2}^2+\|\nabla N^0\|_{L^2}^2\Big\}\\
&\quad\leq C\exp\Big[\sum_{j=1}^{J-1}k\big(\|\nabla P^j\|^2+\|\nabla N^j\|^2\big)\Big]\Big\{E(\Psi^0)+\|\nabla P^0\|_{L^2}^2+\|\nabla N^0\|_{L^2}^2\Big\}\,.
\end{aligned}
$$

Together with Theorem 1, ii), this verifies the assertion. To verify assertion ii), we choose $\Phi_1=d_tP^j$ in (4.3.1) to obtain

$$
\|d_tP^j\|_{L^2}^2+\frac{1}{2}d_t\|\nabla P^j\|_{L^2}^2+\frac{k}{2}\|\nabla d_tP^j\|_{L^2}^2\leq\Big|\Big(P^j\nabla\Psi^j,\nabla d_tP^j\Big)\Big|. \tag{4.3.26}
$$

We may now proceed with (4.3.26) as with the term on the right-hand side of (4.3.23), using integration by parts. This settles the proof. □

The proof shows that a coupling of temporal and spatial discretization parameters is needed to efficiently handle the convective terms; in fact, this restrictive coupling $k\leq Ch^2$ is a main motivation to construct and study the entropy-based discretization (Scheme B) in Section 4.

We are now ready to verify a perturbed discrete entropy law for iterates of Scheme A with the help of mass lumping. In contrast to the entropy law in the continuous context [71], we are in the finite element context not able to remove the regularizing parameter $\delta>0$ for the logarithm by taking the limit $\delta\to 0$.

Lemma 2. *Let (I2), (T1), and $k\leq Ch^2$, be valid, for some $T\equiv t_J>0$. Suppose that $\delta\leq P^0,N^0\leq 1$, for some $0<\delta<1$, and let $\big\{\big(P^j,N^j,\Psi^j\big)\big\}_{j=1}^J$ solve Scheme A, for $[\cdot,\cdot]_2=(\cdot,\cdot)_h$. Then, for all $0\leq j<j'\leq J$,*

$$
\begin{aligned}
&W^{j'}-W^j+\frac{k^2}{2}\sum_{\ell=j+1}^{j'}\|\nabla d_t\Psi^\ell\|_{L^2}^2+k\sum_{\ell=j+1}^{j'}\Big[\Big(P^\ell,\Big|\nabla\big\{\Psi^\ell+\mathcal{I}_h\big[F'(P^\ell)\big]\big\}\Big|^2\Big)\\
&+\Big(N^\ell,\Big|\nabla\big\{\Psi^\ell-\mathcal{I}_h\big[F'(N^\ell)\big]\big\}\Big|^2\Big)\Big]\leq Ch\delta^{-4}\Big[E(\Psi^0)+\|\nabla P^0\|_{L^2}^2+\|\nabla N^0\|_{L^2}^2\Big]^2.
\end{aligned}
\tag{4.3.27}
$$

Proof. Since $P^j,N^j\geq\delta$, for $j\geq 0$, we may choose $\Phi_1=\mathcal{I}_h\big[F'(P^j)\big]+\Psi^j$ in (4.3.1),

$$
\begin{aligned}
&\Big(d_tP^j,F'(P^j)\Big)_h+\big(d_tP^j,\Psi^j\big)_h\\
&\quad=-\Big(P^j\nabla\Psi^j,\nabla\big\{\mathcal{I}_h\big[F'(P^j)\big]+\Psi^j\big\}\Big)-\Big(\nabla P^j,\nabla\big\{\mathcal{I}_h\big[F'(P^j)\big]+\Psi^j\big\}\Big)\,.
\end{aligned}
\tag{4.3.28}
$$

We use the identity $P^j\nabla F'(P^j) = \nabla P^j$ to estimate the right hand side of (4.3.28)

$$\begin{aligned} &= -\Big(P^j\nabla\big\{F'(P^j)+\Psi^j\big\},\nabla\big\{\mathcal{I}_h\big[F'(P^j)\big]+\Psi^j\big\}\Big)\\ &\leq -\Big(P^j,\big|\nabla\big\{\mathcal{I}_h\big[F'(P^j)\big]+\Psi^j\big\}\big|^2\Big)+\\ &\quad +\|\nabla\big\{\mathcal{I}_h\big[F'(P^j)\big]+\Psi^j\big\}\|_{L^2}\Big[\|\nabla\big\{F'(P^j)-\mathcal{I}_h\big[F'(P^j)\big]\big\}\|_{L^2}\Big]\,. \end{aligned}$$

We employ $W^{1,2}$-stability of the interpolation operator to bound the first factor of the last term by $2\big[E(\Psi^0)+\delta^{-2}\|\nabla P^j\|^2_{L^2}\big]$. For the second factor, we use standard interpolation estimates for each element $K\in\mathcal{T}_h$, and $D^2P^j\big|_K=0$ for all $K\in\mathcal{T}_h$,

$$\begin{aligned} \Big(\sum_{K\in\mathcal{T}_h}\|\nabla\big\{F'(P^j)-\mathcal{I}_h\big[F'(P^j)\big]\big\}\|^2_{L^2(K)}\Big)^{1/2} &\leq Ch\Big(\sum_{K\in\mathcal{T}_h}\|D^2F'(P^j)\|^2_{L^2(K)}\Big)^{1/2}\\ &\leq Ch\delta^{-2}\|\nabla P^j\|^2_{L^4}\,. \end{aligned}$$

We put things together in (4.3.28), proceed correspondingly with (4.3.2), where

$$\Phi_2 = \mathcal{I}_h\big[F'(N^j)\big]-\Psi^j\,,$$

and add both results. On using convexity of F, we arrive at

$$\begin{aligned} &d_tW^j+\frac{k}{2}\|\nabla d_t\Psi^j\|^2_{L^2}+\Big(P^j,\big|\nabla\big\{\Psi^j+\mathcal{I}_h\big[F'(P^j)\big]\big\}\big|^2\Big)+\Big(N^j,\big|\nabla\big\{\Psi^j-\mathcal{I}_h\big[F'(N^j)\big]\big\}\big|^2\Big)\\ &\leq C\Big[E(\Psi^0)+\delta^{-2}\big(\|\nabla P^j\|^2_{L^2}+\|\nabla N^j\|^2_{L^2}\big)\Big]h\delta^{-2}\big(\|\nabla P^j\|^2_{L^4}+\|\nabla N^j\|^2_{L^4}\big)\,. \end{aligned}$$

After summation over indices, and employing (4.2.3), and Lemma 1 this yields to the assertion. □

Lemma 2 motivates choices $h=o(\delta^4)$ to make sure that the perturbations in the entropy inequality asymptotically vanish. In the above, we use Algorithm A_1 as a tool to construct solutions to Scheme A. Of course, it is of practical value as well, and is already shown to terminate (cf. contraction property of the scheme). In below, we show that the given stopping criterion is appropriate for convergence.

Theorem 2. *i) Suppose (I1), (T1), fix $T=t_J>0$, and let $k,h>0$ be sufficiently small. For every $0\leq j$, there exists a unique solution $\big(P^{j,\overline{\ell}},N^{j,\overline{\ell}},\Psi^{j,\overline{\ell}}\big)\in\big[V_h\big]^3$ of Algorithm A_1, such that $0\leq P^{j,\ell},N^{j,\ell}\leq 1$. Let $[\cdot,\cdot]_1=(\cdot,\cdot)$, then $\big\{P^{j,\overline{\ell}},N^{j,\overline{\ell}},\Psi^{j,\overline{\ell}}\big\}_{1\leq j\leq J}$ satisfies assertions i)–iii) of Theorem 1, as well as (4.3.27), where each right-hand sides are increased by $C\theta^2t_J$. Moreover, $\big(P^{j,\ell},N^{j,\ell},\Psi^{j,\ell}\big)\to\big(P^j,N^j,\Psi^j\big)$ $(\theta\to 0)$ for every $j\geq 1$, which solves Scheme A.*

ii) Suppose that additionally (I2), and $k\leq Ch^2$ are valid. Then, assertions i)–iii) of Theorem 1 hold also for $[\cdot,\cdot]_2=(\cdot,\cdot)_h$.

In order to verify the corresponding versions i)–iii) of Theorem 1, we restate Algorithm A_1 as a perturbed version of Scheme A.

Proof. Step 1: Assertion i). Fix $j\geq 1$. Suppose that for some $\overline{\ell}\geq 0$ the stopping criterion is met, then $\big(P^{j,\overline{\ell}}, N^{j,\overline{\ell}}, \Psi^{j,\overline{\ell}}\big) = \big(P^j, N^j, \Psi^j\big)$. We may restate (4.3.5)–(4.3.7) as follows,

$$\begin{aligned}
&\text{(4.3.29)} && \Big(d_t P^j, \Phi_1\Big) + \Big(P^j \nabla \Psi^j, \nabla \Phi_1\Big) + \Big(\nabla P^j, \nabla \Phi_1\Big) \\
&&& \quad = \Big(P^j \nabla\big\{\Psi^j - \Psi^{j,\overline{\ell}-1}\big\}, \nabla \Phi_1\Big) + \frac{1}{k}\Big(P^{j,\overline{\ell}-1} - P^{j,\overline{\ell}}, \Phi_1\Big), \\
&\text{(4.3.30)} && \Big(d_t N^j, \Phi_2\Big) + \Big(N^j \nabla \Psi^j, \nabla \Phi_2\Big) + \Big(\nabla N^j, \nabla \Phi_2\Big) \\
&&& \quad = \Big(N^j \nabla\big\{\Psi^j - \Psi^{j,\overline{\ell}-1}\big\}, \nabla \Phi_2\Big) + \frac{1}{k}\Big(N^{j,\overline{\ell}-1} - N^{j,\overline{\ell}}, \Phi_2\Big), \\
&\text{(4.3.31)} && \Big(\nabla \Psi^j, \nabla \Phi_3\Big) = \Big(P^j - N^j, \Phi_3\Big).
\end{aligned}$$

Thanks to $0 \leq P^j, N^j \leq 1$, we have for example,

$$\begin{aligned}
\Big|\Big(P^j \nabla\big\{\Psi^j - \Psi^{j,\overline{\ell}-1}\big\}, \nabla \Phi_1\Big)\Big| &\leq \|\nabla\big\{\Psi^j - \Psi^{j,\overline{\ell}-1}\big\}\|_{L^2(\Omega)} \|\nabla \Phi_1\|_{L^2(\Omega)}, \\
\frac{1}{k}\Big|\Big(P^{j,\overline{\ell}-1} - P^{j,\overline{\ell}}, \Phi_1\Big)\Big| &\leq \frac{1}{k}\big\|P^{j,\overline{\ell}-1} - P^{j,\overline{\ell}}\big\|_{L^2} \|\Phi_1\|_{L^2}.
\end{aligned}$$

We may now follow the argumentation in the proof of Theorem 1 (Step 5) to validate the modified versions of i)–iii) in Theorem 1.

Step 2: Assertion ii). For used mass-lumping, we apply estimate (4.2.2) to the perturbation term $(d_t P^j, \Phi_1) - (d_t P^j, \Phi_1)_h$, which occurs additionally in this situation on the right-hand side of (4.3.29)–(4.3.30). □

4.3.2 Convergence.

For fixed $(k, h) > 0$, and fixed $T \equiv t_J > 0$, consider interpolations of solutions to Scheme A, as introduced in Subsection 4.2.3 such that $(\mathcal{P}_{k,h}, \mathcal{N}_{k,h}, \mathbf{\Psi}_{k,h}) : \Omega_T \to \big[\mathbb{R}^+\big]^2 \times \mathbb{R}$.

Thanks to the a priori bounds in Theorem 1, for every $T > 0$, and $(k, h) \to 0$, there exist a subsequence $\big\{(\mathcal{P}_{k,h}, \mathcal{N}_{k,h}, \mathbf{\Psi}_{k,h})\big\}_{k,h}$, and $(\hat{p}, \hat{n}, \hat{\psi}) \in \big[L^2(0, T; W^{1,2}(\Omega))\big]^3$, such that

$$\begin{aligned}
&\mathcal{P}_{k,h} \rightharpoonup \hat{p}, \quad \mathcal{N}_{k,h} \rightharpoonup \hat{n} && \text{in } L^2\Big(0, T; W^{1,2}(\Omega)\Big) \cap W^{1,2}\Big(0, T; \big(W^{1,2}(\Omega)\big)^*\Big), \\
\text{(4.3.32)} \quad &\mathcal{P}_{k,h} \overset{*}{\rightharpoonup} \hat{p}, \quad \mathcal{N}_{k,h} \overset{*}{\rightharpoonup} \hat{n} && \text{in } L^\infty(\Omega_T), \\
&\overline{\mathcal{P}}_{k,h},\, \mathcal{P}_{k,h} \to \hat{p}, \quad \overline{\mathcal{N}}_{k,h},\, \mathcal{N}_{k,h} \to \hat{n} && \text{in } L^2(\Omega_T), \\
&\nabla \overline{\mathbf{\Psi}}_{k,h},\, \nabla \mathbf{\Psi}_{k,h} \overset{*}{\rightharpoonup} \nabla \hat{\psi} && \text{in } L^\infty\Big(0, T; L^2(\Omega)\Big),
\end{aligned}$$

where $(4.3.32)_3$ follows from Aubin-Lions lemma. Note also that $(4.3.32)_1$ implies $\hat{p}, \hat{n} \in C\big([0, T]; L^2(\Omega)\big)$. We conclude in the following, that the sequences $\overline{\mathcal{P}}_{k,h}$, $\mathcal{P}_{k,h}$, $\overline{\mathcal{N}}_{k,h}$, $\mathcal{N}_{k,h}$ and $\nabla \overline{\mathbf{\Psi}}_{k,h}$, $\nabla \mathbf{\Psi}_{k,h}$ converge to the same limit as $h, k \to 0$. Hence, the identity

$$\|\mathcal{P}_{k,h} - \overline{\mathcal{P}}_{k,h}\|^2_{L^2(0,T;L^2)} = \sum_{j=1}^{J} \|P^j - P^{j-1}\|^2_{L^2} \int_{t_{j-1}}^{t_j} \Big(\frac{s - t_j}{k}\Big)^2 ds = \frac{k^3}{3} \sum_{j=1}^{J} \|d_t P^j\|^2_{L^2}$$

tends to zero for $k \to 0$. In the same way this works for the remaining overlined interpolations. Equations (4.3.1)–(4.3.3) may be restated as follows for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \Big[W^{1,2}\big(0, T; V_h\big)\Big]^3$, for $[\cdot,\cdot]_1 = (\cdot,\cdot)$,

$$\int_0^t \Big[\big((\mathcal{P}_{k,h})_t,\Phi_1\big) + \big(\overline{\mathcal{P}}_{k,h}\nabla\overline{\mathbf{\Psi}}_{k,h},\nabla\Phi_1\big) + \big(\nabla\overline{\mathcal{P}}_{k,h},\nabla\Phi_1\big)\Big]\mathrm{d}s = 0\,, \tag{4.3.33}$$

$$\int_0^t \Big[\big((\mathcal{N}_{k,h})_t,\Phi_2\big) + \big(\overline{\mathcal{N}}_{k,h}\nabla\overline{\mathbf{\Psi}}_{k,h},\nabla\Phi_2\big) + \big(\nabla\overline{\mathcal{N}}_{k,h},\nabla\Phi_2\big)\Big]\mathrm{d}s = 0\,, \tag{4.3.34}$$

$$\int_0^t \Big[\big(\nabla\overline{\mathbf{\Psi}}_{k,h},\nabla\Phi_3\big) - \big(\overline{\mathcal{P}}_{k,h} - \overline{\mathcal{N}}_{k,h},\Phi_3\big)\Big]\mathrm{d}s = 0\,. \tag{4.3.35}$$

For $[\cdot,\cdot]_2 = (\cdot,\cdot)_h$, additional error terms arise on the right-hand sides of (4.3.33), (4.3.34), for example $\int_0^t\Big[\big((\mathcal{P}_{k,h})_t,\Phi_1\big) - \big((\mathcal{P}_{k,h})_t,\Phi_1\big)_h\Big]\mathrm{d}s$, and in (4.3.35) correspondingly. We use integration by parts to obtain

$$\begin{aligned}
&\Big|\int_0^t\Big[\big((\mathcal{P}_{k,h})_t,\Phi_1\big) - \big((\mathcal{P}_{k,h})_t,\Phi_1\big)_h\Big]\mathrm{d}s\Big| \le \Big|\int_0^t\Big[\big(\mathcal{P}_{k,h},(\Phi_1)_t\big) - \big(\mathcal{P}_{k,h},(\Phi_1)_t\big)_h\Big]\mathrm{d}s\Big| \\
&+ \Big|\Big[\big(\mathcal{P}_{k,h}(t,\cdot),\Phi_1(t,\cdot)\big) - \big(\mathcal{P}_{k,h}(t,\cdot),\Phi_1(t,\cdot)\big)_h\Big]\Big| \\
&+ \Big|\Big[\big(\mathcal{P}_{k,h}(0,\cdot),\Phi_1(0,\cdot)\big) - \big(\mathcal{P}_{k,h}(0,\cdot),\Phi_1(0,\cdot)\big)_h\Big]\Big| \\
&\le Ch\Big[\|\mathcal{P}_{k,h}\|_{L^2(\Omega_T)}\|(\Phi_1)_t\|_{L^2(0,T;W^{1,2}(\Omega))} + \|\mathcal{P}_{k,h}\|_{L^\infty(0,T;L^2(\Omega))}\|\Phi_1\|_{C([0,T]:W^{1,2}(\Omega))}\Big]\,.
\end{aligned} \tag{4.3.36}$$

Next, we integrate by parts in time in the leading terms of (4.3.33), (4.3.34), and choose $\Phi_i = \mathcal{I}_h\phi_i$ for all $\phi_i \in C^\infty(\overline{\Omega_T})$ $(i=1,2,3)$. Recall that $\mathcal{I}_h\phi_i \to \phi_i$ in $W^{1,\infty}(\Omega_T)$ $(h\to 0)$. Note, that the right-hand side of (4.3.36) vanishes for $h \to 0$. Hence, we conclude from (4.3.32) for $(k,h) \to 0$ that for all $(\phi_1,\phi_2,\phi_3) \in \big[C^\infty(\overline{\Omega_T})\big]^3$, and almost every $t\in[0,T]$,

$$\Big(\hat p(t,\cdot),\phi_1(t,\cdot)\Big) + \int_0^t\Big[-\Big(\hat p,(\phi_1)_t\Big) + \big(\hat p\nabla\hat\psi,\nabla\phi_1\big) + \big(\nabla\hat p,\nabla\phi_1\big)\Big]\mathrm{d}s = \Big(p_0,\phi_1(0,\cdot)\Big)\,, \tag{4.3.37}$$

$$\Big(\hat n(t,\cdot),\phi_2(t,\cdot)\Big) + \int_0^t\Big[-\Big(\hat n,(\phi_2)_t\Big) + \big(\hat n\nabla\hat\psi,\nabla\phi_2\big) + \big(\nabla\hat n,\nabla\phi_2\big)\Big]\mathrm{d}s = \Big(n_0,\phi_2(0,\cdot)\Big)\,, \tag{4.3.38}$$

$$\int_0^t\Big[\big(\nabla\hat\psi,\nabla\phi_3\big) - \big(\hat p - \hat n,\phi_3\big)\Big]\mathrm{d}s = 0\,. \tag{4.3.39}$$

By continuity, (4.3.37)–(4.3.39) holds for all

$$(\phi_1,\phi_2,\phi_3) \in \Big[L^2\big(0,T;W^{1,2}(\Omega)\big) \cap W^{1,2}\Big(0,T;\big(W^{1,2}(\Omega)\big)^*\Big)\Big]^3\,.$$

Property (1) of Definition 1 now follows from (4.3.4), by convexity of $[0,1]$. Because of $\hat p,\hat n \in L^\infty(\Omega_T)$, a simple calculation implies uniqueness of solutions $\big(\hat p,\hat n,\hat\psi\big)$. Point (3) of Definition 1 is a consequence of $\hat p,\hat n \in C\big([0,T];L^2(\Omega)\big)$; property (5) of it follows from testing (4.3.37)–(4.3.39) with the admissible $(\phi_1,\phi_2,\phi_3) = (\hat\psi,\hat\psi,\hat p - \hat n)$.

The entropy inequality follows from convexity of W and Lemma 2 (which requires (I2), (T1), and $k \le Ch^2$), or may alternatively be recovered from [32, Section 5] (which requires only (I1)). — We collect the results of this section in the following

Theorem 3. *Suppose (I1), (T1), and $T \equiv t_J > 0$. Let $0 \le P^0, N^0 \le 1$, $\big(p_0,n_0\big) \in \big[L^\infty(\Omega,[0,1])\big]^2$, and $P^0 \to p_0$, $N^0 \to n_0$ in $L^2(\Omega)$. Let $\big(\mathcal{P},\mathcal{N},\mathbf{\Psi}\big) : \Omega_T \to [0,1]^2\times\mathbb{R}$ be constructed from the unique solution $\big\{\big(P^j,N^j,\Psi^j\big)\big\}_{j=1}^J \in \big[V_h\big]^3$ of Scheme A by continuous interpolation. For $\big(k,h\big)\to 0$, the limit of every convergent sequence $\big\{\big(\mathcal{P}_{k,h},\mathcal{N}_{k,h},\mathbf{\Psi}_{k,h}\big)\big\}_{k,h}$ is the weak solution of* (4.1.1)–(4.1.5).

The following result is an immediate consequence of Lemma 2.

Corollary 1. *The results of Theorem 3 apply to Algorithm A_1, for $\big(k, h, \theta\big) \to 0$.*

4.4 Entropy based schemes: Stability and Convergence

We study an entropy based discretization of (4.1.1)–(4.1.3), by adapting ideas from [36, 6]. So far, we consider $F : \mathbb{R}^+ \to \mathbb{R}^+$, such that $F(x) := x\big(\ln x - 1\big) + 1 \geq 0$; for given $0 < \varepsilon \leq \frac{1}{2}$, consider the regularization $F_\varepsilon : \mathbb{R} \to \mathbb{R}^+$, such that

$$F_\varepsilon(x) := \begin{cases} \frac{x^2-\varepsilon^2}{2\varepsilon} + x\big(\ln\varepsilon - 1\big) + 1\,, & x \leq \varepsilon\,, \\ x\big(\ln x - 1\big) + 1\,, & \varepsilon \leq x \leq 2\,, \\ \frac{x^2-\varepsilon^2}{4} + x\big(\ln 2 - 1\big) + 1\,, & 2 \leq x\,. \end{cases} \tag{4.4.1}$$

In below, we use its derivatives,

$$F'_\varepsilon(x) = \begin{cases} x\varepsilon^{-1} + \ln\varepsilon - 1\,, & x \leq \varepsilon\,, \\ \ln x\,, & \varepsilon \leq x \leq 2\,, \\ \frac{x}{2} + \ln 2 - 1\,, & 2 \leq x\,, \end{cases} \qquad F''_\varepsilon(x) = \begin{cases} \varepsilon^{-1}\,, & x \leq \varepsilon\,, \\ x^{-1}\,, & \varepsilon \leq x \leq 2\,, \\ \frac{1}{2}\,, & 2 \leq x\,. \end{cases}$$

Let $s_\varepsilon(x) := \big[F''_\varepsilon(x)\big]^{-1}$. The following results can be found in [6],

$$\begin{aligned} F_\varepsilon(x) \geq \frac{\varepsilon}{2}x^2 - 2 \quad \forall\, 2 \geq x \geq 0 \quad \text{and} \quad F_\varepsilon(x) \geq \frac{x^2}{2\varepsilon} \qquad & \forall\, x \leq 0\,, \\ \max\Big\{s_\varepsilon(x), xF'_\varepsilon(x)\Big\} \leq 2F_\varepsilon(x) + 1 \qquad & \forall\, x \in \mathbb{R}\,, \\ s_\varepsilon(x)F'_\varepsilon(x) \geq x - 1 \qquad & \forall\, x \in \mathbb{R}\,. \end{aligned} \tag{4.4.2}$$

We introduce the following regularization of (4.1.1)–(4.1.3),

$$p^\varepsilon_t = \operatorname{div}\Big(\nabla p^\varepsilon - s_\varepsilon(p^\varepsilon)\nabla\psi^\varepsilon\Big) \quad \text{in } \Omega_T\,, \tag{4.4.3}$$

$$n^\varepsilon_t = \operatorname{div}\Big(\nabla n^\varepsilon + s_\varepsilon(n^\varepsilon)\nabla\psi^\varepsilon\Big) \quad \text{in } \Omega_T\,, \tag{4.4.4}$$

$$-\Delta\psi^\varepsilon = p^\varepsilon - n^\varepsilon \quad \text{in } \Omega_T\,. \tag{4.4.5}$$

This approach is related to the one in [32], where truncation of concentrations is used in the nonlinear terms to establish existence of weak solutions. In the following, we study a fully discrete version of (4.4.3)–(4.4.5); in order to validate a discrete entropy law, we need a proper discretization of the nonlinearities, which meets the following compatibility condition; cf. [36, 6].

Definition 3. *For any $\varepsilon \in (0, 1)$, and $\varepsilon \geq 1$ sufficiently large, we call $\boldsymbol{\mathcal{S}}_\varepsilon : V_h \to \big[L^\infty(\Omega)\big]^{d\times d}$ an entropy-provider if for all $\Phi \in V_h$*

i) $\boldsymbol{\mathcal{S}}_\varepsilon(\Phi)$ *is symmetric and positive definite*,

ii) $\boldsymbol{\mathcal{S}}_\varepsilon(\Phi)\nabla\mathcal{I}_h\big[F'_\varepsilon(\Phi)\big] = \nabla\Phi$.

We briefly recall the construction of $\boldsymbol{\mathcal{S}}_\varepsilon$ for $d = 1$. For basis functions $\{\varphi_z\} \subset V_h$, simplizes $K \subset \mathcal{T}_h$ of uniform mesh-size $h > 0$, and representations $\Phi = \sum_{z\in\mathcal{N}_h}\Phi(z)\varphi_z$, we may write for neighboring z, z', such that $K_0 := (z, z') \in \mathcal{T}_h$: $\Phi = \Phi(z-h)\varphi_{z-h} + \Phi_z\varphi_z$ on K_0. Moreover, we compute

$$\nabla\Phi = \Phi(z-h)\nabla\varphi_{z-h} + \Phi(z)\nabla\varphi_z = \frac{-\Phi(z-h) + \Phi(z)}{h} = \frac{\Phi(z) - \Phi(z-h)}{z - (z-h)}\,,$$

$$\nabla\mathcal{I}_h\big[F'_\varepsilon(\Phi)\big] = F'_\varepsilon\big(\Phi(z-h)\big)\nabla\varphi_{z-h} + F'_\varepsilon\big(\Phi(z)\big)\nabla\varphi_z = \frac{F'_\varepsilon\big(\Phi(z)\big) - F'_\varepsilon\big(\Phi(z-h)\big)}{z - (z-h)}\,.$$

Hence, item ii) of Definition 3 leads for $\Phi(z-h) \leq \xi \leq \Phi(z)$ to

$$\boldsymbol{\mathcal{S}}_\varepsilon(\Phi) = \frac{\nabla\Phi}{\nabla\mathcal{I}_h\big[F_\varepsilon'(\Phi)\big]} = \begin{cases} \frac{\Phi(z-h)-\Phi(z)}{F_\varepsilon'\big(\Phi(z-h)\big)-F_\varepsilon'\big(\Phi(z)\big)} = \frac{1}{F_\varepsilon''(\xi)}\,, & \Phi(z-h) \neq \Phi(z)\,, \\ \frac{1}{F''\big(\Phi(z)\big)}\,, & \Phi(z-h) = \Phi(z)\,. \end{cases}$$

The extension to $d > 1$ has been considered in [36], and motivates to validate the following result, which adapts [6, Lemma 2.1] to our case.

Lemma 3. *Assume (T2), and $0 < \varepsilon < 1$. For every $\Phi \in V_h$,*

$$\begin{array}{ll} \text{i)} & \varepsilon\boldsymbol{\xi}^\top\boldsymbol{\xi} \leq \boldsymbol{\xi}^\top\boldsymbol{\mathcal{S}}_\varepsilon(\Phi)\boldsymbol{\xi} \leq 2\boldsymbol{\xi}^\top\boldsymbol{\xi} \qquad \forall\boldsymbol{\xi} \in \mathbb{R}^d\,, \\ \text{ii)} & \max_{\mathbf{x}\in K}\Big|\Big|\Big|\big(\boldsymbol{\mathcal{S}}_\varepsilon(\Phi) - s_\varepsilon(\Phi)\mathbb{I}\big)(\mathbf{x})\Big|\Big|\Big|_2 \leq h_K\big|\nabla\Phi\big| \quad \forall K \in \mathcal{T}_h\,. \end{array}$$

Moreover, for all $\Phi_1, \Phi_2 \in V_h$, and $K \in \mathcal{T}_h$ there holds

$$\text{iii)} \quad \Big|\Big|\Big|\Big(\boldsymbol{\mathcal{S}}_\varepsilon(\Phi_1) - \boldsymbol{\mathcal{S}}_\varepsilon(\Phi_2)\Big)\Big|_K\Big|\Big|\Big|_2 \leq \frac{2}{\varepsilon}\max_{K\in\mathcal{T}_h}\Big\{\max_{1\leq\ell\leq d}\Big[\big|\Phi_1(\mathbf{z}_{K_\ell})-\Phi_2(\mathbf{z}_{K_\ell})\big| + \big|\Phi_1(\mathbf{z}_{K_0})-\Phi_2(\mathbf{z}_{K_0})\big|\Big]\Big\}\,.$$

Here, $\mathbb{I} \in \mathbb{R}^{d\times d}$ denotes the identity matrix, $|||\cdot|||_2$ the spectral norm, and $\mathbf{z}_{K_0}$ is the node of $K \in \mathcal{T}_h$ where the connecting edges to the other nodes $\mathbf{z}_{K_\ell}$, $\ell = 1, .., d$ form a right angle.

We are now ready to propose the following

Scheme B. Fix $0 < \varepsilon < 1$, and let $\big(P^0, N^0\big) \in \big[V_h\big]^2$, such that $\big(P^0 - N^0, 1\big) = 0$. For every $j \geq 1$, find iterates $\big(P^j, N^j, \Psi^j\big) \in \big[V_h\big]^3$, where $(\Psi^j, 1) = 0$ such that for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$ holds

$$\big(d_tP^j, \Phi_1\big)_h + \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_\varepsilon(P^j)\nabla\Phi_1\Big) + \big(\nabla P^j, \nabla\Phi_1\big) = 0\,, \tag{4.4.6}$$

$$\big(d_tN^j, \Phi_2\big)_h - \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_\varepsilon(N^j)\nabla\Phi_2\Big) + \big(\nabla N^j, \nabla\Phi_2\big) = 0\,, \tag{4.4.7}$$

$$\big(\nabla\Psi^j, \nabla\Phi_3\big) = \big(P^j - N^j, \Phi_3\big)_h\,. \tag{4.4.8}$$

The entropy provider $\boldsymbol{\mathcal{S}}_\varepsilon$ enables that the system (4.4.6)–(4.4.8) allows for the same cancellation effects as in the continuous proof of the entropy law [71] and requires therefore less regularity on the initial data and not the mesh-constraint $k < Ch^2$ as for Scheme A; cf. Lemma 2 respectively Theorem 4. The main results of this section are given in the following

Theorem 4. *Fix $T \equiv t_J > 0$, let (I1), (T2) be valid, and $k > 0$ be sufficiently small. For every $j \geq 1$, there exists a unique solution $\big(P^j, N^j, \Psi^j\big) \in \big[V_h\big]^3$ that solves Scheme B. Moreover,* *iterates satisfy*

$$\text{i)}\qquad E\big(\Psi^J\big) + \frac{k^2}{2}\sum_{j=1}^{J}\|\nabla d_t\Psi^j\|_{L^2}^2 + k\sum_{j=1}^{J}\Big(\nabla\Psi^j, \big[\boldsymbol{\mathcal{S}}_\varepsilon(P^j) + \boldsymbol{\mathcal{S}}_\varepsilon(N^j)\big]\nabla\Psi^j\Big)$$
$$+k\sum_{j=1}^{J}\|P^j - N^j\|_h^2 = E\big(\Psi^0\big)\,,$$

$$\text{ii)}\qquad W^J + \frac{k^2}{2}\sum_{\ell=1}^{J}\|\nabla d_t\Psi^\ell\|_{L^2}^2 + 2k\sum_{j=1}^{J}\|P^j - N^j\|_h^2 + k\sum_{j=1}^{J}\Big(\nabla\Psi^j, [\boldsymbol{\mathcal{S}}_\varepsilon(P^j) + \boldsymbol{\mathcal{S}}_\varepsilon(N^j)]\nabla\Psi^j\Big)$$
$$+k\sum_{j=1}^{J}\Big[\Big(\boldsymbol{\mathcal{S}}_\varepsilon(P^j)\nabla\mathcal{I}_h\big[F_\varepsilon'(P^j)\big], \nabla\mathcal{I}_h\big[F_\varepsilon'(P^j)\big]\Big)$$
$$+\Big(\boldsymbol{\mathcal{S}}_\varepsilon(N^j)\nabla\mathcal{I}_h\big[F_\varepsilon'(N^j)\big], \nabla\mathcal{I}_h\big[F_\varepsilon'(N^j)\big]\Big)\Big] \le W^0\,,$$

$$\text{iii)}\qquad \frac{1}{2}\Big(\|P^J\|_h^2 + \|N^J\|_h^2\Big) + \frac{k^2}{2}\sum_{j=1}^{J}\Big(\|d_tP^j\|_h^2 + \|d_tP^j\|_h^2\Big) + k\sum_{j=1}^{J}\Big(\|\nabla P^j\|_{L^2}^2 + \|\nabla N^j\|_{L^2}^2\Big)$$
$$\le \frac{1}{2}\Big(\|P^0\|_h^2 + \|N^0\|_h^2\Big) + 8E(\Psi^0)\,,$$

$$\text{iv)}\qquad k\sum_{j=1}^{J}\Big[\|d_tP^j\|_{(W^{1,2})^*} + \|d_tN^j\|_{(W^{1,2})^*}\Big] \le C\Big[\|P^0\|_h^2 + \|N^0\|_h^2 + E(\Psi^0)\Big]\,.$$

Proof. Step 1: Existence. Fix $j \ge 1$, and define the following continuous mapping $\mathcal{F}^j : \big[V_h\big]^2 \to \big[V_h\big]^2$ as

$$\text{(4.4.9)}\qquad \Big(\mathcal{F}^j[\mathcal{P},\mathcal{N}], [\Phi_1,\Phi_2]\Big) := \Big(\big(\mathcal{F}_1^j[\mathcal{P}],\Phi_1\big), \big(\mathcal{F}_2^j[\mathcal{N}],\Phi_2\big)\Big) = 0\,,$$

where for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$ it holds

$$\begin{aligned}
\Big(\mathcal{F}_1^j[\mathcal{P}],\Phi_1\Big) := \frac{1}{k}\Big(\mathcal{P} - P^{j-1},\Phi_1\Big)_h + \Big(\nabla\Psi, \boldsymbol{\mathcal{S}}_\varepsilon(\mathcal{P})\nabla\Phi_1\Big) + \Big(\nabla\mathcal{P},\nabla\Phi_1\Big) &= 0\,,\\
\Big(\mathcal{F}_2^j[\mathcal{N}],\Phi_2\Big) := \frac{1}{k}\Big(\mathcal{N} - N^{j-1},\Phi_2\Big)_h - \Big(\nabla\Psi, \boldsymbol{\mathcal{S}}_\varepsilon(\mathcal{N})\nabla\Phi_2\Big) + \Big(\nabla\mathcal{N},\nabla\Phi_2\Big) &= 0\,,\\
\Big(\nabla\Psi_j,\nabla\Phi_3\Big) - \Big(\mathcal{P}-\mathcal{N},\Phi_3\Big)_h &= 0 \qquad \forall\,\Phi_3 \in V_h\,,
\end{aligned}$$

and for $(\Psi,1) = 0$. We employ the bound $\|\nabla\Psi\|_{L^2} \le C\|\mathcal{P}-\mathcal{N}\|_{L^2}$, and Lemma 3, i) to estimate

$$\begin{aligned}
\Big(\mathcal{F}^j[\mathcal{P},\mathcal{N}],[\mathcal{P},\mathcal{N}]\Big) &\ge \frac{1}{k}\|\mathcal{P}\|_h\Big[\big(1-2\frac{k}{2}\big) - \|P^{j-1}\|_h\Big]\|\mathcal{P}\|_h\\
&\quad + \frac{1}{k}\|\mathcal{N}\|_h\Big[\big(1-2\frac{k}{2}\big) - \|N^{j-1}\|_h\Big]\|\mathcal{N}\|_h + \frac{1}{2}\Big[\|\nabla\mathcal{P}\|_{L^2}^2 + \|\nabla\mathcal{N}\|_{L^2}^2\Big]\\
&\ge 0\,,
\end{aligned}$$

which holds for all $\mathcal{P}$, $\mathcal{N} \in V_h$ with

$$\|\mathcal{P}\| \ge C\|P^{j-1}\| \quad \text{and} \quad \|\mathcal{N}\| \ge C\|N^{j-1}\| \quad \text{and } k < 1\,.$$

Hence by a corollary of Brouwer's fixed point theorem [72, p. 37], this implies existence of $\big(P^j, N^j\big) \in \big[V_h\big]^2$, such that (4.4.9) is valid.

Step 2: Discrete energy equality i), discrete entropy inequality ii), and bounds iii), iv). Assertion i) follows from choosing $\Phi_1 = -\Phi_2 = \Psi^j$ in (4.4.6), (4.4.7), adding both equations, as well as (4.4.8), for $\Phi_3 = \Psi^j$, and $\Phi_3 = P^j - N^j$.

For ii), we choose $\Phi_1 = \mathcal{I}_h\big[F'_\varepsilon(P^j)\big] + \Psi^j$, and $\Phi_2 = \mathcal{I}_h\big[F'_\varepsilon(N^j)\big] - \Psi^j$. We proceed separately.

$$\Big(d_t P^j, \mathcal{I}_h\big[F'_\varepsilon(P^j)\big] + \Psi^j\Big)_h + \Big(d_t N^j, \mathcal{I}_h\big[F'_\varepsilon(N^j)\big] - \Psi^j\Big)_h \\ \leq \Big(d_t[F_\varepsilon(P^j) + F_\varepsilon(N^j)], 1\Big)_h + \big(d_t[P^j - N^j], \Psi_j\big)_h .$$

We employ Definition 3, ii) to conclude

$$\Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_{\boldsymbol{\varepsilon}}(P^j)\nabla\Big[\mathcal{I}_h\big[F'_{\boldsymbol{\varepsilon}}(P^j)\big] + \Psi^j\Big]\Big) - \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_{\boldsymbol{\varepsilon}}(N^j)\nabla\Big[\mathcal{I}_h\big[F'_{\boldsymbol{\varepsilon}}(N^j)\big] - \Psi^j\Big]\Big) \\ = \Big(\nabla\Psi^j, \nabla[P^j - N^j]\Big) + \Big(\nabla\Psi^j, [\boldsymbol{\mathcal{S}}_{\boldsymbol{\varepsilon}}(P^j) + \boldsymbol{\mathcal{S}}_{\boldsymbol{\varepsilon}}(N^j)]\nabla\Psi^j\Big) .$$

Similarly,

$$\Big(\nabla P^j, \nabla\mathcal{I}_h\big[F'_\varepsilon(P^j) + \Psi\big]\Big) + \Big(\nabla N^j, \nabla\mathcal{I}_h\big[F'_\varepsilon(N^j) - \Psi\big]\Big) \\ = \Big(\boldsymbol{\mathcal{S}}_{\boldsymbol{\varepsilon}}(P^j)\nabla\mathcal{I}_h\big[F'_\varepsilon(P^j)\big], \nabla\mathcal{I}_h\big[F'_\varepsilon(P^j)\big]\Big) + \Big(\boldsymbol{\mathcal{S}}_{\boldsymbol{\varepsilon}}(N^j)\nabla\mathcal{I}_h\big[F'_\varepsilon(N^j)\big], \nabla\mathcal{I}_h\big[F'_\varepsilon(N^j)\big]\Big) \\ + \Big(\nabla[P^j - N^j], \nabla\Psi^j\Big) .$$

Putting things together yields to assertion ii).

In order to show estimate iii), choose $\big(\Phi_1, \Phi_2\big) = \big(P^j, N^j\big)$ in (4.4.6)–(4.4.7); then, Lemma 3, i), together with the bound $k\sum_{j=1}^J \|\nabla\Psi^j\|_{L^2}^2 \leq k\sum_{j=1}^J \|P^j - N^j\|_h^2$ validate assertion iii).

To verify iv), we proceed as in Step 5 in the proof of Theorem 1, and again employ Lemma 3, i).

Uniqueness of $\big\{\big(P^j, N^j, \Psi^j\big)\big\}_{j=1}^J \subset [V_h]^3$ now easily follows from iii). □

In below, we denote $P_{\mathbf{z}_p} := \min_{\mathbf{z}\in\mathcal{N}_h} P(\mathbf{z})$, $N_{\mathbf{z}_p} := \min_{\mathbf{z}\in\mathcal{N}_h} N(\mathbf{z})$, and $H^j(P,N) := \big(F_\varepsilon(P^j) + F_\varepsilon(N^j), 1\big)_h$. We now verify 'quasi-non-negativity' of iterates of Scheme B in the following lemma, by following corresponding strategies in [36].

Lemma 4. *Fix $T \equiv t_J > 0$, let (I1), (T2) be valid, and $\varepsilon \leq P^0, N^0 \leq 1$. For arbitrary $0 < \sigma \equiv \sigma(\varepsilon) := -\frac{C[H^0(P,N)+E(\Psi^0)]+\varepsilon}{\ln\varepsilon - 1} \ll 1$, we can choose $\varepsilon > 0$ such that P^j, $N^j \geq -\sigma$.*

Proof. Recall the discrete entropy inequality in Theorem 4, ii), which can be written as

$$H^j(P,N) \leq H^0(P,N) + E(\Psi^0) - E(\Psi^j) \qquad \forall\, j \geq 0 . \tag{4.4.10}$$

The regularity of the triangulation implies $Ch^d \geq \beta_{\mathbf{z}} \geq ch^d$, and we conclude

$$H^0(P,N) + E(\Psi^0) - E(\Psi^j) \geq H^j(P,N) = \sum_{\mathbf{z}\in\mathcal{N}_h} \beta_{\mathbf{z}}\Big\{F_\varepsilon(P^j(\mathbf{z})) + F_\varepsilon(N^j(\mathbf{z}))\Big\} \\ \geq ch^d \sum_{\mathbf{z}\in\mathcal{N}_h}\Big\{\big[\frac{-\varepsilon}{2} + P^j(\mathbf{z})(\ln\varepsilon - 1)\big] + \big[\frac{-\varepsilon}{2} + N^j(\mathbf{z})(\ln\varepsilon - 1)\big]\Big\} \\ \geq c\Big\{-\varepsilon + (\ln\varepsilon - 1)(P_{\mathbf{z}_p} + N_{\mathbf{z}_n})\Big\} .$$

The uniform bound for $H^0(P,N)+E(\Psi^0)$ then leads to

$$-\sigma = \frac{C[H^0(P,N)+E(\Psi^0)]+\varepsilon}{\ln\varepsilon - 1} \leq P_{\mathbf{z}_p} + N_{\mathbf{z}_p}\,. \tag{4.4.11}$$

□

Theorem 4 provides upper bounds for iterates of Scheme B which are uniform in $\big(\varepsilon,k,h\big)\in(0,1)^3$, and we may now proceed like in Section 4.3.2: For fixed $T\equiv t_J>0$, consider interpolations $(\mathcal{P}_{\varepsilon,k,h},\mathcal{N}_{\varepsilon,k,h},\mathbf{\Psi}_{\varepsilon,k,h}):\Omega_T\to\big[\mathbb{R}\big]^3$ of iterates from Scheme B, with the following properties for $\big(\varepsilon,k,h\big)\to 0$,

$$\begin{aligned}
\mathcal{P}_{\varepsilon,k,h}\rightharpoonup \hat p,\quad \mathcal{N}_{\varepsilon,k,h}\rightharpoonup \hat n \quad &\text{in } L^2\Big(0,T;W^{1,2}(\Omega)\Big)\cap W^{1,2}\Big(0,T;\big(W^{1,2}(\Omega)\big)^*\Big)\,,\\
\overline{\mathcal{P}}_{\varepsilon,k,h},\,\mathcal{P}_{\varepsilon,k,h}\to\hat p,\quad &\text{in } L^2(\Omega_T)\,,\\
\overline{\mathcal{N}}_{\varepsilon,k,h},\,\mathcal{N}_{\varepsilon,k,h}\to\hat n\quad &\text{in } L^2(\Omega_T)\,,\\
\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h},\,\nabla\mathbf{\Psi}_{\varepsilon,k,h}\overset{*}{\rightharpoonup}\nabla\hat\psi\quad &\text{in } L^\infty\Big(0,T;L^2(\Omega)\Big)\,,
\end{aligned} \tag{4.4.12}$$

for some $\big(\hat p,\hat n,\hat\psi\big)\in\big[L^2\big(0,T;W^{1,2}(\Omega)\big)\big]^3$; assertion $(4.4.12)_2$ follows from Aubin-Lions lemma. Again, we drop indices in (4.4.12). That $\overline{\mathcal{P}}_{\varepsilon,k,h}$, $\overline{\mathcal{N}}_{\varepsilon,k,h}$ and $\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h}$ converge to the same limit for $\varepsilon,h,k\to 0$ is verified as in Section 3.2.

We wish to identify the above limits; for this purpose, equations (4.3.1)–(4.3.3) are restated for all $\big(\Phi_1,\Phi_2,\Phi_3\big)\in\Big[W^{1,2}\big(0,T;V_h\big)\Big]^3$, and $t\equiv t_j\in[0,T]$,

$$\begin{aligned}
\int_0^t\Big[\big((\mathcal{P}_{\varepsilon,k,h})_t,\Phi_1\big)_h+\Big(\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h},\boldsymbol{\mathcal{S}}_\varepsilon(\overline{\mathcal{P}}_{\varepsilon,k,h})\nabla\Phi_1\Big)+\big(\nabla\overline{\mathcal{P}}_{\varepsilon,k,h},\nabla\Phi_1\big)\Big]\mathrm{d}s &= 0\,,\\
\int_0^t\Big[\big((\mathcal{N}_{\varepsilon,k,h})_t,\Phi_2\big)_h-\Big(\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h},\boldsymbol{\mathcal{S}}_\varepsilon(\overline{\mathcal{N}}_{\varepsilon,k,h})\nabla\Phi_2\Big)+\big(\nabla\overline{\mathcal{N}}_{\varepsilon,k,h},\nabla\Phi_2\big)\Big]\mathrm{d}s &= 0\,,\\
\int_0^t\Big[\big(\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h},\nabla\Phi_3\big)-\big(\overline{\mathcal{P}}_{\varepsilon,k,h}-\overline{\mathcal{N}}_{\varepsilon,k,h},\nabla\Phi_3\big)_h\Big]\mathrm{d}s &= 0\,.
\end{aligned} \tag{4.4.13}$$

For the leading and last terms in $(4.4.13)_1$–$(4.4.13)_2$, we may follow the arguments in Section 4.3.2 below (4.3.35). For the middle term in (4.3.33), we use Lemma 3, ii), and Theorem 4, i) to conclude

$$\begin{aligned}
&\Big|\Big(\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h},\Big[\big\{\boldsymbol{\mathcal{S}}_\varepsilon(\overline{\mathcal{P}}_{\varepsilon,k,h})-s_\varepsilon(\overline{\mathcal{P}}_{\varepsilon,k,h})\mathbb{I}\big\}+\big\{s_\varepsilon(\overline{\mathcal{P}}_{\varepsilon,k,h})-[\overline{\mathcal{P}}_{\varepsilon,k,h}]_2^+\big\}\mathbb{I}\Big]\nabla\Phi_1\Big)\Big|\\
&\qquad\leq h\|\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h}\|_{L^2}\|\nabla\overline{\mathcal{P}}_{\varepsilon,k,h}\|_{L^2}\|\nabla\Phi_1\|_{L^\infty}+C\varepsilon\|\nabla\overline{\mathbf{\Psi}}_{\varepsilon,k,h}\|_{L^2}\|\nabla\Phi_1\|_{L^2}\,,
\end{aligned}$$

where $\Phi_1=\mathcal{I}_h\phi_1$, for all $\phi_1\in C^\infty(\overline{\Omega_T})$, and $[\cdot]_2^+:=\min\big\{2,\max\{0,\cdot\}\big\}$. Hence, passing to the limit $\big(\varepsilon,k,h\big)\to 0$ leads to

$$\big(\hat p(t),\phi_1(t)\big)+\int_0^t\Big[-\big(\hat p,(\phi_1)_t\big)+\Big([\hat p]_2^+\nabla\hat\psi,\nabla\phi_1\Big)+\big(\nabla\hat p,\nabla\phi_1\big)\Big]\,\mathrm{d}s=\Big(p_0,\phi_1(0)\Big)\,, \tag{4.4.14}$$

$$\big(\hat n(t),\phi_2(t)\big)-\int_0^t\Big[\big(\hat n,(\phi_2)_t\big)+\Big([\hat n]_2^+\nabla\hat\psi,\nabla\phi_2\Big)+\big(\nabla\hat n,\nabla\phi_2\big)\Big]\,\mathrm{d}s=\Big(n_0,\phi_2(0)\Big)\,, \tag{4.4.15}$$

$$\int_0^t\Big[\big(\nabla\hat\psi,\nabla\phi_3\big)-\big(\hat p-\hat n,\phi_3\big)\Big]\mathrm{d}s=0\,. \tag{4.4.16}$$

Again, we may extend (4.4.14)–(4.4.16) to all

$$\big(\phi_1,\phi_2,\phi_3\big)\in\Big[L^2\Big(0,T;W^{1,2}(\Omega)\Big)\cap W^{1,2}\Big(0,T;\big(W^{1,2}(\Omega)\big)^*\Big)\Big]^3\,.$$

To verify uniqueness of solutions $\big(\hat{p}, \hat{n}\big)$ we first define $e_{\hat{p}} := \hat{p}_1 - \hat{n}_2$, $e_{\hat{n}} := \hat{n}_1 - \hat{n}_2$ and $e_{\hat{\psi}} := \hat{\psi}_1 - \hat{\psi}_2$. On choosing $\big(\phi_1, \phi_2, \phi_3\big) = \big(e_{\hat{p}}, e_{\hat{n}}, e_{\hat{\psi}}\big)$, we estimate via Theorem 4, iii)

$$\begin{aligned}\Big|\Big(\big\{[\hat{p}_1]_2^+ - \hat{p}_1]_2^+\big\}\nabla\hat{\psi}_1 + \big[\hat{p}_2\big]_2^+\nabla e_{\hat{\psi}}, \nabla e_{\hat{p}}\Big)\Big| &\leq \|e_{\hat{p}}\|_{L^3}\|\nabla\hat{\psi}_2\|_{L^6}\|\nabla e_{\hat{p}}\|_{L^2} + C\|\nabla e_{\hat{\psi}}\|_{L^2}\|\nabla e_{\hat{p}}\|_{L^2} \\ &\leq C\Big(1+T\Big)^2\|e_{\hat{p}}\|_{L^2}^2 + C\Big[\|e_{\hat{p}}\|_{L^2}^2 + \|e_{\hat{n}}\|_{L^2}^2\Big] + \frac{1}{2}\|\nabla e_{\hat{p}}\|_{L^2}^2\,.\end{aligned}$$

We repeat the argument for $e_{\hat{n}}$, and afterwards sum both inequalities. Then, for all $t \in [0, T]$,

$$\begin{aligned}&\frac{1}{2}\Big[\|e_{\hat{p}}(t)\|^2 + \|e_{\hat{n}}(t)\|^2\Big] + \int_0^t \frac{1}{2}\Big[\|\nabla e_{\hat{p}}\|^2 + \|\nabla e_{\hat{n}}\|^2\Big]\mathrm{d}s \\ &\qquad\leq \frac{1}{2}\Big[\|e_{\hat{p_0}}\|^2 + \|e_{\hat{n_0}}\|^2\Big] + C(1+T)^2\int_0^t \Big[\|e_{\hat{p}}\|^2 + \|e_{\hat{n}}\|^2\Big]\mathrm{d}s\,,\end{aligned}$$

and Gronwall's inequality implies uniqueness of solutions $\big(\hat{p}, \hat{n}\big)$ to (4.4.14)–(4.4.16).

Now, the weak solution to (4.1.1)–(4.1.5) which is constructed in [32] satisfies (4.4.14)–(4.4.16), and hence coincides with the above $\big(\hat{p}, \hat{n}\big)$. We collect the results of this section in the following

Theorem 5. *Suppose (I1), (T2), and let* $T \equiv t_J > 0$. *Let* $0 \leq P^0, N^0 \leq 1$, $\big(p_0, n_0\big) \in \big[L^\infty(\Omega, [0,1])\big]^2$, *and* $P^0 \to p_0$, $N^0 \to n_0$ *in* $L^2(\Omega)$. *Let* $\big(\mathcal{P}_{\varepsilon,k,h}, \mathcal{N}_{\varepsilon,k,h}, \mathbf{\Psi}_{\varepsilon,k,h}\big) : \Omega_T \to \mathbb{R}^3$ *be constructed from the unique solution* $\big\{\big(P^j, N^j, \Psi^j\big)\big\}_{j=1}^J \in \big[V_h\big]^3$ *of Scheme B by continuous interpolation. For* $\big(\varepsilon,\, k, h\big) \to 0$, *the limit of every convergent sequence* $\big\{\big(\mathcal{P}_{\varepsilon,k,h}, \mathcal{N}_{\varepsilon,k,h}, \mathbf{\Psi}_{\varepsilon,k,h}\big)\big\}_{(\varepsilon,k,h)}$ *is the unique weak solution of* (4.1.1)–(4.1.5).

We employ a fixed point algorithm to solve the nonlinear scheme; for practical purposes, we add a stopping criterion, and later show overall convergence to (4.1.1)–(4.1.5) for all, discretization and threshold parameters tending to zero.

Algorithm B$_1$. 1. For $j \geq 1$, set $\big(P^{j,0}, N^{j,0}\big) = \big(P^{j-1}, N^{j-1}\big)$, and $\ell := 0$.
2. For $\ell \geq 1$, compute $\big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big) \in \big[V_h\big]^3$, where $\big(\Psi^{j,\ell}, 1\big) = 0$, such that for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$,

$$\frac{1}{k}\big(P^{j,\ell}, \Phi_1\big)_h + \Big(\nabla\Psi^{j,\ell}, \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\ell-1})\nabla\Phi_1\Big) + \big(\nabla P^{j,\ell}, \nabla\Phi_1\big) = \frac{1}{k}\big(P^{j-1}, \Phi_1\big)_h\,, \tag{4.4.17}$$

$$\frac{1}{k}\big(N^{j,\ell}, \Phi_2\big)_h - \Big(\nabla\Psi^{j,\ell}, \boldsymbol{\mathcal{S}}_\varepsilon(N^{j,\ell-1})\nabla\Phi_2\Big) + \big(\nabla N^{j,\ell}, \nabla\Phi_2\big) = \frac{1}{k}\big(N^{j-1}, \Phi_2\big)_h\,, \tag{4.4.18}$$

$$\big(\nabla\Psi^{j,\ell}, \nabla\Phi_3\big) = \big(P^{j,\ell} - N^{j,\ell}, \Phi_3\big)_h\,. \tag{4.4.19}$$

3. For fixed $\theta > 0$, stop if

$$\max_{\varphi=P,N}\|\boldsymbol{\mathcal{S}}_\varepsilon(\varphi^{j,\ell}) - \boldsymbol{\mathcal{S}}_\varepsilon(\varphi^{j,\ell-1})\|_{L^\infty} \leq \theta\,, \tag{4.4.20}$$

set $\big(P^j, N^j, \Psi^j\big) := \big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big)$, and go to 1.; otherwise, set $\ell \leftarrow \ell + 1$ and continue with 2.
4. Stop if $j + 1 = J$; set $j \leftarrow j + 1$ and go to 1. otherwise.

Unique solvability of (4.4.17)–(4.4.19) follows from Lax-Milgram theorem. The following bounds can be easily verified. We collect some useful a priori bounds in the following

Lemma 5. *Suppose (I1), (T2), and let $T \equiv t_J > 0$. Let $\big(P^{j-1}, N^{j-1}\big) \in [V_h]^2$ be uniformly bounded in $[L^2(\Omega)]^2$, and $k > 0$ sufficiently small. For every $0 \le j, \ell$, there exist functions $\big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big) \in [V_h]^3$, which satisfy Algorithm B_1, and satisfy*

$$\text{i)} \qquad \frac{1}{2}\|\nabla\Psi^{j,\ell}\|_{L^2}^2 + k\|P^{j,\ell} - N^{j,\ell}\|_h^2 \le C\|P^{j-1} - N^{j-1}\|_h^2\,,$$

$$\text{ii)} \qquad \frac{1}{2}\Big[\|P^{j,\ell}\|_h^2 + \|N^{j,\ell}\|_h^2\Big] + \frac{k}{2}\Big[\|\nabla P^{j,\ell}\|^2 + \|\nabla N^{j,\ell}\|^2\Big] \le C\Big[\|P^{j-1}\|_h^2 + \|N^{j-1}\|_h^2\Big]\,.$$

Proof. To verify assertion i), we employ $\Phi_i = \Psi^{j,\ell}$ $(i = 1,2)$ and subtract (4.4.18) from (4.4.17). Thanks to (4.4.19), and Lemma 3, i), we obtain

$$\Big[\frac{1}{k} + \varepsilon\Big]\|\nabla\Psi^{j,\ell}\|_{L^2}^2 + \|P^{j,\ell} - N^{j,\ell}\|_h^2 \le \frac{C}{2k}\|P^{j-1} - N^{j-1}\|_h^2 + \frac{1}{2k}\|\nabla\Psi^{j,\ell}\|_{L^2}^2\,.$$

Next, we choose $\big(\Phi_1, \Phi_2, \Phi_3\big) = \big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big)$ in (4.4.17)–(4.4.19). Thanks to Lemma 3, i), and assertion i), we obtain assertion ii).

Unique solvability of (4.4.17)–(4.4.19) follows similarly from Lax-Milgram theorem, for $k < \frac{1}{8}$. □

The following theorem states that Algorithm B_1 terminates, and that iterates converge to weak solutions of Definition 1, provided that $k \le C\varepsilon^4$ holds, and all $(k, h, \varepsilon) \to 0$.

Theorem 6. *Suppose (I1), (T2). Fix $T \equiv t_J > 0$, for $0 \le P^0, N^0 \le 1$, and $k \le \tilde{C}\varepsilon^4$, for $\tilde{C} > 0$ sufficiently small. Then iterates $\big\{\big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big)\big\}_{j,\ell\ge 0}$ of Algorithm B_1 converge to a weak solution of (4.1.1)–(4.1.5) for $(k, h, \varepsilon, \theta) \to 0$. Moreover, for finite $\big(k, h, \varepsilon, \theta\big) > 0$, and θ sufficiently small, iterates of Algorithm B_1 satisfy assertions i), ii), iv) of Theorem 4; assertion iv) holds as well, provided $C\theta^2 \le \varepsilon$.*

The constraint $k \le \tilde{C}\varepsilon^4$ is a consequence of the contraction property by the use of Banach's fixed point theorem, and is a consequence of the bound in Lemma 3, iii). As is evidenced in [7, Remark 2.1], this bound is not pessimistic.

Proof. Step 1: Contraction property. Fix $j \ge 1$, and suppose that

$$\|P^{j-1}\|_h + \|N^{j-1}\|_h \le C\,. \tag{4.4.21}$$

We proceed similarly to Step 4 of the proof of Theorem 1; rather than (4.3.20), the crucial term is now

$$\begin{aligned}
&\Big|\big(\nabla e_\Psi^\ell, \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\ell-1})\nabla e_P^\ell\big) + \Big(\nabla\Psi^{j,\ell-1}\big\{\boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\ell-1}) - \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\ell-2})\big\}, \nabla e_P^\ell\Big)\Big| \\
&\quad \le 2\|\nabla e_\Psi^\ell\|_{L^2}\|\nabla e_P^\ell\|_{L^2} + C\varepsilon^{-1}\|\nabla\Psi^{j,\ell-1}\|_{L^6}\|e_P^{\ell-1}\|_{L^3}\|\nabla e_P^\ell\|_{L^2} \\
&\quad \le \frac{1}{4}\Big[\|\nabla e_P^\ell\|_{L^2}^2 + \|\nabla e_P^{\ell-1}\|_{L^2}^2\Big] + C\big[\|e_P^\ell\|_{L^2}^2 + \|e_N^\ell\|_{L^2}^2\big] \\
&\qquad\qquad + C\varepsilon^{-4}\big[\|P^{j-1}\|_h^4 + \|N^{j-1}\|_h^4\big]\|e_P^{\ell-1}\|_{L^2}^2\,,
\end{aligned}$$

since $\|e_\Psi^\ell\|_{L^2} \le C\|e_P^\ell - e_N^\ell\|_h$, and $\|\nabla\Psi^{j,\ell}\|_{L^6} \le \|P^{j-1}\|_h + \|N^{j-1}\|_h$, as a consequence of Lemma 5, ii). By putting things together, instead of (4.3.21) we arrive at

$$\begin{aligned}
&\Big[1 - Ck\Big]\Big[\|e_P^\ell\|_h^2 + \|e_N^\ell\|_h^2\Big] + \frac{k}{2}\Big[\|\nabla e_P^\ell\|_{L^2}^2 + \|\nabla e_N^\ell\|_{L^2}^2\Big] \\
&\quad \le Ck\varepsilon^{-4}\Big[\|e_P^{\ell-1}\|_{L^2}^2 + \|e_N^{\ell-1}\|_{L^2}^2\Big] + \frac{k}{4}\Big[\|\nabla e_P^{\ell-1}\|_{L^2}^2 + \|\nabla e_N^{\ell-1}\|_{L^2}^2\Big]\,.
\end{aligned}$$

Hence, the contraction property holds in case $k \leq \tilde{C}\varepsilon^4$, for some $\tilde{C} > 0$ sufficiently small.

Step 2: Derivation of a perturbed version of Scheme B. Fix $j \geq 1$. Suppose that for some $\bar{\ell} \geq 0$ the stopping criterion is met, such that $(P^{j,\bar{\ell}}, N^{j,\bar{\ell}}, \Psi^{j,\bar{\ell}}) = (P^j, N^j, \Psi^j)$. Then (4.4.17)–(4.4.19) may be restated as follows,

$$\big(d_t P^j, \Phi_1\big)_h + \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_\varepsilon(P^j)\nabla\Phi_1\Big) + \big(\nabla P^j, \nabla\Phi_1\big) = \Big(\nabla\Psi^j, \big\{\boldsymbol{\mathcal{S}}_\varepsilon(P^j) - \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\bar{\ell}-1})\big\}\nabla\Phi_1\Big), \tag{4.4.22}$$

$$\big(d_t N^j, \Phi_2\big)_h - \Big(\nabla\Psi^j, \boldsymbol{\mathcal{S}}_\varepsilon(N^j)\nabla\Phi_2\Big) + \big(\nabla N^j, \nabla\Phi_2\big) = -\Big(\nabla\Psi^j, \big\{\boldsymbol{\mathcal{S}}_\varepsilon(N^j) - \boldsymbol{\mathcal{S}}_\varepsilon(N^{j,\bar{\ell}-1})\big\}, \nabla\Phi_2\Big), \tag{4.4.23}$$

$$\big(\nabla\Psi^j, \nabla\Phi_3\big) = \big(P^j - N^j, \Phi_3\big)_h. \tag{4.4.24}$$

The term on the right-hand side of (4.4.22) is bounded as follows,

$$\Big|\Big(\nabla\Psi^j, \big\{\boldsymbol{\mathcal{S}}_\varepsilon(P^j) - \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\bar{\ell}-1})\big\}, \nabla\Phi_1\Big)\Big| \leq C\|\boldsymbol{\mathcal{S}}_\varepsilon(P^j) - \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\bar{\ell}-1})\|_{L^\infty}\|\nabla\Psi^j\|_{L^2}\|\nabla\Phi_1\|_{L^2}. \tag{4.4.25}$$

It is now easy to see that the a priori estimates from Theorem 4 remain valid for system (4.4.22)–(4.4.24): in order to validate i), we choose $\Phi_1 = -\Phi_2 = \Psi^j$ as before; the term on the right-hand side may then be absorbed on the left-hand side for sufficiently small θ, thanks to the bound $\|\nabla\Psi^j\|_{L^2} \leq \|P^j - N^j\|_h$. It is now straightforward to bound additional terms in iii), iv) by $C\theta^2 E(\Psi^0)$. In order to show a perturbed version of assertion ii), we use Lemma 3, i) to control terms five and six vom below by $\varepsilon k \sum_{j=1}^J \big[\|\nabla\mathcal{I}_h\big[F'_\varepsilon(P^j)\big]\|_{L^2}^2 + \|\nabla\mathcal{I}_h\big[F'_\varepsilon(P^j)\big]\|_{L^2}^2\big]$. Then, we bound the additional term in (4.4.22) as follows,

$$\begin{aligned}\Big|\Big(\nabla\Psi^j, \big\{\boldsymbol{\mathcal{S}}_\varepsilon(P^j) - \boldsymbol{\mathcal{S}}_\varepsilon(P^{j,\bar{\ell}-1})\big\}\nabla\mathcal{I}_h\big[F'_\varepsilon(P^j) - \Psi^j\big]\Big)\Big| \\ \leq \theta\|\nabla\Psi^j\|_{L^2}\|\nabla\mathcal{I}_h\big[F'_\varepsilon(P^j) - \Psi^j\big]\|_{L^2}.\end{aligned}$$

By Young's inequality, we may absorb this term in the third and fifth term of assertion ii) in Theorem 4, provided $C\theta^2 \leq \varepsilon$.

These uniform bounds are now sufficient to identify existing limits of solutions to Algorithm B_1 for $(k, h, \varepsilon, \theta) \to 0$. First, note that (4.4.21) is valid, and that the right-hand sides in (4.4.22), (4.4.23) vanish for $\theta \to 0$. Therefore, we may follow the arguments which preceed Theorem 5 to conclude convergence to weak solutions of (4.1.1)–(4.1.5). □

4.5 Extensions

The study of Schemes A and B in the previous sections was done for the classical Nernst-Planck-Poisson equations (4.1.1)–(4.1.3), in the case of vanishing Neumann boundary conditions. In this section, we discuss the extended model (4.1.8)–(4.1.10) with Dirichlet-Neumann boundary conditions (4.1.11); see [41, 20, 21] for further details regarding this model. Most of the previous results in Sections 4.3 and 4.4 may be obtained for corresponding discretizations; in this section, we generalize those from Sections 4.3 to problem (4.1.8)–(4.1.12). For this purpose, we adopt previous notations, and highlight differences in the argumentation.

Let $\tilde{V}_h := \big\{\Phi \in V_h : \Phi = 0 \text{ on } \Gamma_D\big\}$, $r(s) = s^\alpha$ for $\alpha \geq 1$, and $c \in L^\infty(\Omega)$ be given.

Scheme $\tilde{A}$. Let $\big(P^0, N^0\big) \in [V_h]^2$ be given. For every $j \geq 1$, find iterates $\big(P^j, N^j, \Psi^j\big) \in [V_h]^3$, such that $P^j = p_D$, $N^j = n_D$, $\Psi^j = \psi_D$ on Γ_D, and for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[\tilde{V}_h\big]^3$ holds

$$[d_t P^j, \Phi_1]_i + \big(P^j \nabla \Psi^j, \nabla \Phi_1\big) + \big(\nabla r(P^j), \nabla \Phi_1\big) = 0\,, \tag{4.5.1}$$

$$[d_t N^j, \Phi_2]_i - \big(N^j \nabla \Psi^j, \nabla \Phi_2\big) + \big(\nabla r(N^j), \nabla \Phi_2\big) = 0\,, \tag{4.5.2}$$

$$(\nabla \Psi^j, \nabla \Phi_3) = [P^j - N^j + c, \Phi_3]_i\,. \tag{4.5.3}$$

We study solvability of Scheme $\tilde{A}$, where our main focus is on the additional nonlinearity $r : \mathbb{R} \to \mathbb{R}$; for this purpose, we restrict to the case $c \equiv 0$, $\Gamma_D \equiv \emptyset$, and also put $[\cdot,\cdot]_i = (\cdot,\cdot)$. Our goal is to verify similar stability properties for iterates of Scheme $\tilde{A}$ to those for Scheme A; cf. Theorem 1.

Theorem 7. *Let (I1), (T1) be valid, $\alpha \geq 1$, $T \equiv t_J > 0$, $c \equiv 0$, $\Gamma_D = \emptyset$, and $[\cdot,\cdot]_2 = (\cdot,\cdot)$. Suppose that $0 < m \leq P^0, N^0 \leq 1$, and $k \leq Ch^2$, for some $C \equiv C(\alpha, m) > 0$ sufficiently small. For every $j \geq 1$, there exists a unique $\big(P^j, N^j, \Psi^j\big) \in \big[V_h\big]^3$ which solves Scheme $\tilde{A}$. Moreover,*

$$0 < m \leq P^j, N^j \leq 1 \qquad (1 \leq j \leq J)\,, \tag{4.5.4}$$

and there exists $C \equiv C(\alpha, m, \Omega) > 0$ such that for small $h > 0$,

i)
$$E(\Psi^J) + \frac{k^2}{2}\sum_{j=1}^{J} \|\nabla d_t \Psi^j\|_{L^2}^2 + k\sum_{j=1}^{j}\Big(P^j + N^j, |\nabla \Psi^j|^2\Big) + Ck\sum_{j=1}^{J}\|P^j - N^j\|_{L^{1+\alpha}}^{1+\alpha} \leq E(\Psi^0) + o(1)\,,$$

ii)
$$\frac{1}{2}\Big(\|P^J\|_{L^2}^2 + \|N^J\|_{L^2}^2\Big) + \frac{k^2}{2}\sum_{j=1}^{J}\Big(\|d_t P^j\|_{L^2}^2 + \|d_t N^j\|_{L^2}^2\Big) + \frac{\alpha}{2}k\sum_{j=1}^{j}\Big(\|[P^j]^{\frac{\alpha-1}{2}}\nabla P^j\|_{L^2}^2 + \|[N^j]^{\frac{\alpha-1}{2}}\nabla N^j\|_{L^2}^2\Big) \leq \frac{1}{2}\Big(\|P^0\|_{L^2}^2 + \|N^0\|_{L^2}^2\Big) + CT\max_{1\leq j\leq J} E(\Psi^j)\,,$$

iii)
$$k\sum_{j=1}^{J}\Big[\|d_t P^j\|_{[W^{1,2}]^*}^2 + \|d_t P^j\|_{[W^{1,2}]^*}^2\Big] \leq CT\Big[\|P^0\|_{L^2}^2 + \|N^0\|_{L^2}^2 + \max_{1\leq j\leq J} E(\Psi^j)\Big]\,.$$

As for the proof of Theorem 1, we use a fully practical simple fixed-point scheme, together with a suitable criterion to construct solutions of Scheme $\tilde{A}$.

Algorithm $\tilde{A}_1$. 1. For $j \geq 1$, set $(P^{j,0}, N^{j,0}) := (P^{j-1}, N^{j-1})$, and $\ell := 0$.

2. For $\ell \geq 1$, compute $\big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big) \in \big[V_h\big]^3$, where $\big(\Psi^{j,\ell}, 1\big) = 0$, such that for all $\big(\Phi_1, \Phi_2, \Phi_3\big) \in \big[V_h\big]^3$,

$$\frac{2}{k}\big(P^{j,\ell}, \Phi_1\big) + \Big(P^{j,\ell}\nabla \Psi^{j,\ell-1}, \nabla \Phi_1\Big) + \alpha\Big([P^{j,\ell-1}]^{\alpha-1}\nabla P^{j,\ell}, \nabla \Phi_1\Big) \tag{4.5.5}$$

$$= \frac{1}{k}\Big(P^{j-1} + P^{j,\ell-1}, \Phi_1\Big)\,, \tag{4.5.6}$$

$$\frac{2}{k}\big(N^{j,\ell}, \Phi_2\big) - \Big(N^{j,\ell}\nabla \Psi^{j,\ell-1}, \nabla \Phi_2\Big) + \alpha\Big([N^{j,\ell-1}]^{\alpha-1}\nabla N^{j,\ell}, \nabla \Phi_2\Big) \tag{4.5.7}$$

$$= \frac{1}{k}\big(N^{j-1} + N^{j,\ell-1}, \Phi_2\Big)\,, \tag{4.5.8}$$

$$\Big(\nabla \Psi^{j,\ell}, \nabla \Phi_3\Big) = \Big(P^{j,\ell} - N^{j,\ell}, \Phi_3\Big)\,. \tag{4.5.9}$$

3. For fixed $\theta > 0$, stop if

$$
\begin{aligned}
&\|\nabla\{\Psi^{j,\ell} - \Psi^{j,\ell-1}\}\|_{L^2} + \frac{1}{k}\Big[\|P^{j,\ell} - P^{j,\ell-1}\|_{L^2} + \|N^{j,\ell} - N^{j,\ell-1}\|_{L^2}\Big] \\
&+\alpha\Big[\big\|[P^{j,\ell}]^{\alpha-1} - [P^{j,\ell-1}]^{\alpha-1}\big\|_{L^\infty} + \big\|[N^{j,\ell}]^{\alpha-1} - [N^{j,\ell-1}]^{\alpha-1}\big\|_{L^\infty}\Big] \leq \theta\,, \qquad (4.5.10)
\end{aligned}
$$

set $\big(P^j, N^j, \Psi^j\big) := \big(P^{j,\ell}, N^{j,\ell}, \Psi^{j,\ell}\big)$, and go to 4.; otherwise, set $\ell \leftarrow \ell + 1$ and continue with 2.

4. Stop if $j + 1 = J$; set $j \leftarrow j + 1$ and go to 1. otherwise.

In the subsequent proof, we highlight necessary changes in the proof of Theorem 1.

Proof. A first relevant change happens in Step 2, where $k_{\beta\beta'}$ (and K) is now replaced by

$$
\tilde{k}_{\beta\beta'} := \alpha\Big([N^{j,\ell-1}]^{\alpha-1}\nabla\varphi_{\mathbf{x}_\beta}, \nabla\varphi_{\mathbf{x}'_\beta}\Big) \qquad (1 \leq \beta, \beta' \leq L)\,,
$$

(and $\tilde{K}$). As a consequence, in order to maintain strict positivity of diagonal entries of the modified system matrix $\tilde{\boldsymbol{\mathcal{A}}}$ (Step 2b), and strict diagonal dominance property (Step 2c), we need to establish

$$
0 < m \leq P^{1,\ell-1}, N^{1,\ell-1} \leq 1\,. \qquad (4.5.11)
$$

Step 3 has to be modified for this purpose: To verify the lower bound, we introduce $\hat{P}^{1,r} := P^{1,r} - m$, for $r = \ell - 1, \ell$, and $\hat{P}^0 := P^0 - 1$. Then, thanks to $\big(\nabla\Psi^{1,\ell}, \nabla\Psi_3\big) = \big(\hat{P}^{1,\ell} - \hat{N}^{1,\ell}, \Phi_3\big)$ for all $\Phi_3 \in V_h$, we obtain from (4.5.5)–(4.5.7),

$$
\begin{aligned}
&\frac{2}{k}\big(\hat{P}^{1,\ell}, \Phi_1\big) + \Big(\hat{P}^{1,\ell}\nabla\Psi^{1,\ell-1}, \nabla\Phi_1\Big) + \alpha\Big([\hat{P}^{1,\ell-1} + m]^{\alpha-1}\nabla\hat{P}^{1,\ell}, \nabla\Phi_1\Big) \qquad (4.5.12)\\
&\quad = \frac{1}{k}\Big(\hat{P}^0 + [1 - mk]\hat{P}^{1,\ell-1}, \Phi_1\Big) + m\big(\hat{N}^{1,\ell-1}, \Phi_1\big)\\
&\frac{2}{k}\big(\hat{N}^{1,\ell}, \Phi_2\big) - \Big(\hat{N}^{1,\ell}\nabla\Psi^{1,\ell-1}, \nabla\Phi_2\Big) + \alpha\Big([\hat{N}^{1,\ell-1} + m]^{\alpha-1}\nabla\hat{N}^{1,\ell}, \nabla\Phi_2\Big) \qquad (4.5.13)\\
&\quad = \frac{1}{k}\Big(\hat{N}^0 + [1 - mk]\hat{N}^{1,\ell-1}, \Phi_2\Big) + m\big(\hat{P}^{1,\ell-1}, \Phi_2\big)\,.
\end{aligned}
$$

Note that (4.5.12)–(4.5.13) is only a slightly modified version of (4.5.5)–(4.5.7); hence, we may run an inductive argument ($\ell \geq 1$) to verify that $0 \leq \hat{P}^{1,\ell}, \hat{N}^{1,\ell}$, due to M-matrix property for the system matrix of (4.5.12)–(4.5.13), and positivity of the right-hand sides.

Verification of the upper bound in (4.5.11) requires small changes of the argument in Step 3 of the proof of Theorem 1: Rather than (4.3.12), we now have

$$
\begin{aligned}
&\frac{2}{k}\big(\overline{P}^{1,\ell}, \Phi_1\big) + \Big(\big\{\overline{P}^{1,\ell} + 1\big\}\nabla\Psi^{1,\ell-1}, \nabla\Phi_1\Big) + \big([P^{1,\ell-1}]^{\alpha-1}\nabla\overline{P}^{1,\ell}, \nabla\Phi_1\big) \qquad (4.5.14)\\
&\quad = \frac{1}{k}\big(\overline{P}^{1,\ell-1} + \overline{P}^0, \Phi_1\big)\,,
\end{aligned}
$$

and (4.3.13) changes to

$$
\begin{aligned}
\frac{1}{k}\big\|[\Phi_1]^+\big\|_{L^2}^2 + \alpha m^{\alpha-1}\big\|\nabla[\Phi_1]^+\big\|_{L^2}^2 \quad \leq \quad & \frac{1}{k}\big([\Phi_1]^+, \Phi_1\big)_{L^2} + \alpha\Big([P^{1,\ell-1}]^{\alpha-1}\nabla[\Phi_1]^+, \nabla\Phi_1\Big)\\
& + \Big([\Phi_1]^-\nabla\Psi^{1,\ell-1}, \nabla[\Phi_1]^+\Big) \qquad \forall\, \Phi_1 \in V_h\,. \qquad (4.5.15)
\end{aligned}
$$

We may now follow the argumentation as before to validate the upper bound in (4.5.11).

In Step 4, we now also have to account for the additional nonlinearity: the second terms in (4.3.17), (4.3.18) change to

$$\alpha\Big([P^{1,\ell-1}]^{\alpha-1}\nabla P^{1,\ell} - [P^{1,\ell-2}]^{\alpha-1}\nabla P^{1,\ell-1}, \nabla\Phi_1\Big)$$
$$\text{resp.} \qquad \alpha\Big([N^{1,\ell-1}]^{\alpha-1}\nabla N^{1,\ell} - [N^{1,\ell-2}]^{\alpha-1}\nabla N^{1,\ell-1}, \nabla\Phi_2\Big)\,.$$

For simplicity, we only deal with the first term for $\Phi_1 = e_P^\ell$, which may be controlled as follows,

$$\begin{aligned}
&\alpha\Big([P^{1,\ell-2}]^{\alpha-1}\nabla e_P^\ell + \Big[[P^{1,\ell-1}]^{\alpha-1} - [P^{1,\ell-2}]^{\alpha-1}\Big]\nabla P^{1,\ell}, \nabla e_P^\ell\Big) \\
&\geq \alpha m^{\alpha-1}\|\nabla e_P^\ell\|_{L^2}^2 - 2\alpha(\alpha-1)\max_{1\leq\beta\leq 2}\|[P^{1,\ell-\beta}]^{\alpha-2}\|_{L^\infty}\|e_P^{\ell-1}\|_{L^2}\|\nabla P^{1,\ell}\|_{L^\infty}\|\nabla e_P^\ell\|_{L^2} \\
&\geq \frac{\alpha}{2}m^{\alpha-1}\|\nabla e_P^\ell\|_{L^2}^2 - C\|e_P^{\ell-1}\|_{L^2}^2\|\nabla P^{1,\ell}\|_{L^\infty}^2\,.
\end{aligned}$$

By inverse estimate, and Step 3 above, the contraction property then follows for $C = C(\alpha, m) > 0$ sufficiently small, and values $k \leq Ch^2$.

In Step 5, we verify assertions i)–iii). Assertion i) follows for

$$\big(\Phi_1, \Phi_2, \Phi_3\big) = \big(\Psi^j, -\Psi^j, P_1[r(P^j) - r(N^j)]\big)$$

in (4.5.1)–(4.5.3), thanks to the following algebraic relation for all $\zeta, \eta \in \mathbb{R}^d$, (for $C_1 > 0$)

$$\big\langle |\zeta|^{\alpha-1}\zeta - |\eta|^{\alpha-1}\eta, \zeta - \eta\big\rangle \geq C_1|\zeta - \eta|^{1+\alpha}\,,$$

and the upper bounds from Step 3 to validate

$$\begin{aligned}
&\Big|\Big(P^j - N^j, [P_1 \pm \mathrm{Id}][r(P^j) - r(N^j)]\Big)\Big| \\
&\geq C_1\|P^j - N^j\|_{L^{1+\alpha}}^{1+\alpha} - C\big\|[P_1 - \mathrm{Id}][r(P^j) - r(N^j)]\big\|_{L^1} \\
&\geq C_1\|P^j - N^j\|_{L^{1+\alpha}}^{1+\alpha} - C\big\|[P_1 - \mathrm{Id}][r(P^j) - r(N^j)]\big\|_{L^2}\,.
\end{aligned} \tag{4.5.16}$$

We use standard L^2-estimate for the Poisson problem, and $W^{1,2}$-stability of the Ritz projection to e.g. conclude that

$$\big\|[P_1 - \mathrm{Id}]r(P^j)\big\|_{L^2} \leq Ch\big\|[P_1 - \mathrm{Id}]r(P^j)\big\|_{W^{1,2}} \leq C(\alpha)h\|P^j\|_{W^{1,2}}\,.$$

Hence, it remains to verify bounds $k\sum_{j=1}^J\big[\|\nabla P^j\|_{L^2}^2 + \|\nabla N^j\|_{L^2}^2\big] \leq CT$ to control the last but one term on the right-hand side of (4.5.16) by $o(1)$, for $h \to 0$. This is an (independent) consequence of assertion ii), where we use $\big(\Phi_1, \Phi_2\big) = \big(P^j, N^j\big)$ in (4.5.1)–(4.5.2) and sum over all iteration steps.

Assertion iii) follows as in Step 5 of the proof of Theorem 1. □

A corresponding version of Theorem 2, with stopping criterion (4.5.10) is straight-forward to show for Algorithm $\tilde{A}_1$. Finally, the uniform bounds in Theorem 7, i)–iii) yield to property (4.3.32), and to construct weak solutions of (4.1.8)–(4.1.10), (4.1.11)–(4.1.12) for the case addressed in Theorem 7, it suffices to additionally show

$$\alpha\Big([\overline{\mathcal{P}}_{k,h}]^{\alpha-1}\nabla\overline{\mathcal{P}}_{k,h}, \nabla\mathcal{I}_h\phi_1\Big) \to \alpha\Big([\hat{p}]^{\alpha-1}\nabla\hat{p}, \nabla\phi_1\Big) \qquad \forall\,\phi_1 \in C^\infty\big(\overline{\Omega_T}\big)\,.$$

But this result follows from $\nabla\mathcal{P}_{k,h} \rightharpoonup \nabla\hat{p}$ in $L^2(\Omega_T)$, as well as continuity of the mapping $x \mapsto x^{\alpha-1}$, and $\mathcal{P}_{k,h} \to \hat{p}$ in $L^q(\Omega_T)$ $(1 \leq q < \infty)$, which interpolates the results $(4.3.32)_2$ and $(4.3.32)_3$.

We collect these results in the following

Theorem 8. *Suppose (I1), (T1), and* $T \equiv t_J > 0$. *Let* $0 < m \leq P^0, N^0 \leq 1$, *and* $\big(p_0, n_0\big) \in [L^\infty\big(\Omega, [m,1]\big)]^2$, *and* $P^0 \to p_0$, $N^0 \to n_0$ *in* $L^2(\Omega)$. *Let* $\big(\mathcal{P}_{k,h}, \mathcal{N}_{k,h}, \mathbf{\Psi}_{k,h}\big) : \Omega_T \to [m,1]^2 \times \mathbb{R}$ *be constructed from the solution* $\big\{\big(P^j, N^j, \Psi^j\big)\big\}_{j=1}^J \in \big[V_h\big]^3$ *of Scheme* $\tilde{A}$ *by continuous interpolation. For* $\big(k,h\big) \to 0$, *there exists a convergent sequence* $\big\{\big(\mathcal{P}_{k,h}, \mathcal{N}_{k,h}, \mathbf{\Psi}_{k,h}\big)\big\}_{k,h}$, *whose limit is a weak solution of* (4.1.8)–(4.1.12), *with* $c \equiv 0$ *and* $\Gamma_D = \emptyset$, *i.e., properties (1)–(3) of Definition 1 are valid.*

Most of the results in Section 4.4 apply for an entropy based discretization of (4.1.8)–(4.1.12) as well; we leave details to the interested reader.

4.6 Computational Studies

In this section, we computationally compare the energy based Scheme A (resp. Algorithm A_1) with the entropy based Scheme B (resp. Algorithm B_1): conservation of mass, decay of energies, entropies, as well as non-negativity and maximum principle for iterates at finite scales is studied in academic Example 1. The modified problem (4.1.8)–(4.1.10), with data from [41, 20] is studied in Example 2. In the sequel, let $\mathbf{x} = \big(x_1, x_2\big)^\top$.

The first example compares evolution of smooth and L^∞-initial data with Schemes A and B.

Example 1. *Let* $\Omega := (0,1)^2 \subset \mathbb{R}^2$, *and* $T = 1$. *Assume vanishing Neumann boundary conditions for* $\big(P^j, N^j, \Psi^j\big)$, *for* $j \geq 1$, *and initial conditions*

i) $\big(x_1, x_2\big) \mapsto P^0\big((x_1,x_2)\big) = \cos(x_2)\,, \qquad \big(x_1, x_2\big) \mapsto N^0\big((x_1,x_2)\big) = \sin(x_1)\,,$

ii)
$$P^0\big((x_1,x_2)\big) = \begin{cases} 1\,, & (0,1)^2 \setminus \big\{(0,0.75)\times(0,1) \cup (0.75,1)\times(0,\frac{11}{20})\big\}\,, \\ 10^{-6}\,, & \textit{else,} \end{cases}$$
$$N^0\big((x_1,x_2)\big) = \begin{cases} 1\,, & (0,1)^2 \setminus \big\{(0,0.75)\times(0,1) \cup (0.75,1)\times(\frac{9}{20},1)\big\}\,, \\ 10^{-6}\,, & \textit{else.} \end{cases}$$

The computations which use Algorithm A_1 are done on a uniform mesh, and subsequent snapshots for initial data ii) are depicted in Figure 4.6.1; corresponding results are obtained with Scheme B, where $\varepsilon = 10^{-5}$ is used for F_ε. We observe more iterations to be necessary in i) to meet the stopping criterion, with $\theta = 10^{-4}$. In general, up to six iterations are necessary for Algorithm A_1, while those needed for Algorithm B_1 may reach up to the double of this value. Evolution of energies $j \mapsto E(\Psi^j)$ and entropies $j \mapsto W^j$ for both initial data are plotted in Figure 4.6.2, with results for Schemes A and B being indistinguishable.

The plots in Figure 4.6.2 motivate decay behavior for solutions according to Theorem 1, i) for different spatial refinements. In all computations, we observe no significant difference in the energy plots for Schemes A and B.

As has been pointed out in Theorem 1, acute-type meshes are necessary to validate an M-matrix property for the system matrix $\boldsymbol{\mathcal{A}}$ in Algorithm A_1; Figure 4.6.3 shows that solutions of Scheme A may become negative (i.e., -0.016 at time 0.002) in the case of highly distorted meshes; negative minimum values (i.e., -0.0047 at time 0.006) for $\{P^j\}$ for non-negative initial data for the same mesh are also found for Scheme B.

The second example is motivated from corresponding time-asymptotic studies of charge densities in a *pn*-junction diode in [41, 21, 20], and uses Scheme $\tilde{A}$ to solve (4.1.8)–(4.1.12). We remark that the following example considers a pn-diode in the switched-on regime and therefore neglects generation and recombination effects.

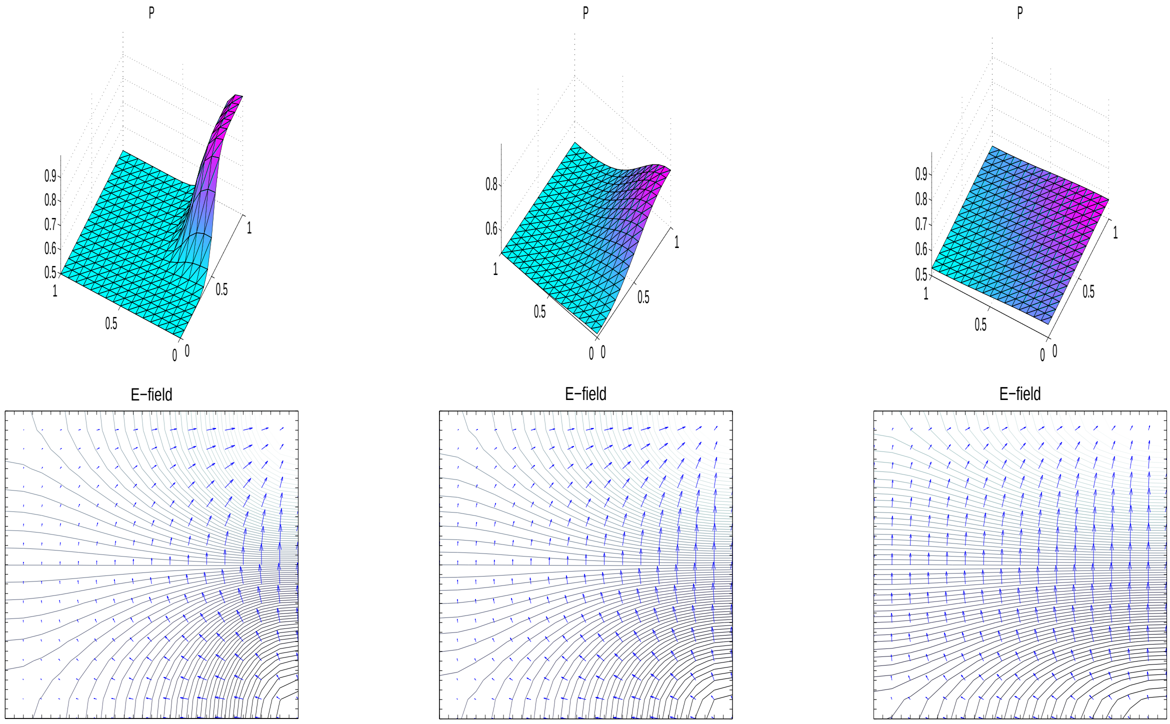


Figure 4.6.1: Example 1 (Scheme A): Snapshots of P^j (1st line), and Ψ^j (2nd line) at times $t = 0.002, 0.02, 0.1$ ($k = 0.002$, $h = 0.03125$).

Example 2. *Data for a pn-junction diode covering* $\Omega = (0,1)^2$ *are shown in Figure 4.6.4, and* $\alpha = \frac{5}{3}$. *We impose a doping profile* $C : \Omega \to \mathbb{R}$,

$$C(x_1, x_2) = \begin{cases} -1\,, & \textit{in the } p-\textit{region}, \\ +1\,, & \textit{in the } n-\textit{region}. \end{cases}$$

The Dirichlet boundary conditions are

$$\begin{aligned} n_D &= 0.1, \quad p_D = 0.9, \quad \psi_D = \tfrac{h(N_D)-h(P_D)}{2} \qquad \textit{on } y = 1,\ 0 \le x \le 0.25\,, \\ n_D &= 0.9, \quad p_D = 0.1, \quad \psi_D = \tfrac{h(N_D)-h(P_D)}{2} \qquad \textit{on } y = 0\,, \end{aligned}$$

where $h(s) = \int_1^s \frac{r'(\tau)}{\tau}\, d\tau$. *Elsewhere we put Neumann boundary conditions. We choose initial conditions*

$$p_0(x_1,x_2) = \begin{cases} 0\,, & \textit{in the } p-\textit{region}, \\ 1\,, & \textit{in the } n-\textit{region}. \end{cases} \quad \textit{and} \quad n_0(x_1,x_2) = \begin{cases} 1\,, & \textit{in the } p-\textit{region}, \\ 0\,, & \textit{in the } n-\textit{region}. \end{cases}$$

Scheme $\tilde{A}$ *is used to solve* (4.1.8)–(4.1.12).

Figure 4.6.5 shows snapshots of computed solutions at subsequent times; the plots in Figure 4.6.6 illustrate evolution of $j \mapsto E(\Psi^j)$ (energy) and $j \mapsto W^j$ (entropy) throughout the experiment, and maximum resp. minimum values for P^j.

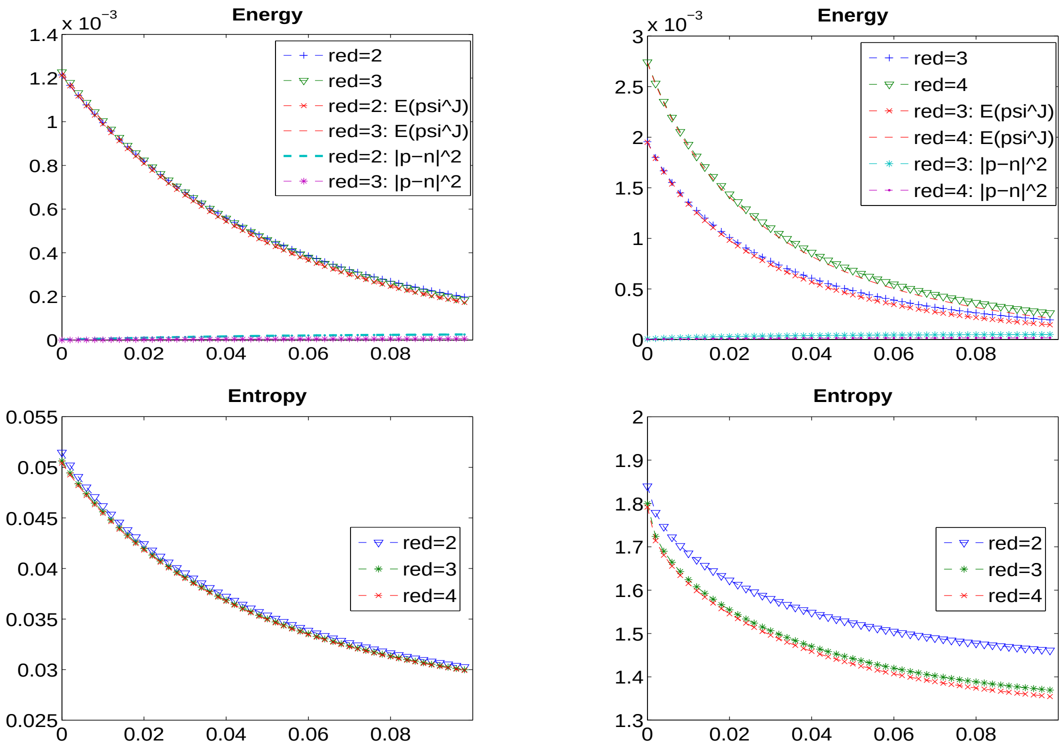


Figure 4.6.2: Example 1: Plot of evolving energies (1st line) and entropies (2nd line), using initial data i) (left), and ii) (right) ($k = 0.002$, $h = 0.0625$, $\varepsilon = 10^{-5}$).

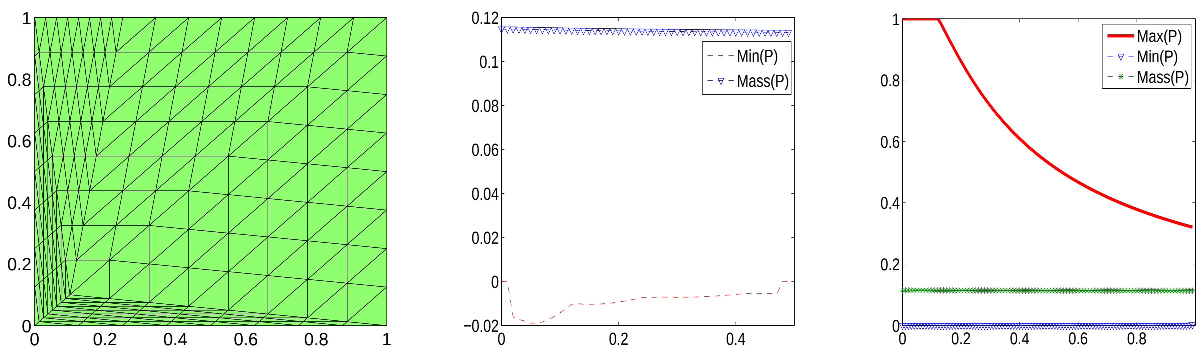


Figure 4.6.3: Example 1, ii): Plot of evolving minimum values of P^j on non-acute meshes, using Scheme A (middle), and Scheme B (right) ($k = 0.002$, $\varepsilon = 10^{-5}$).

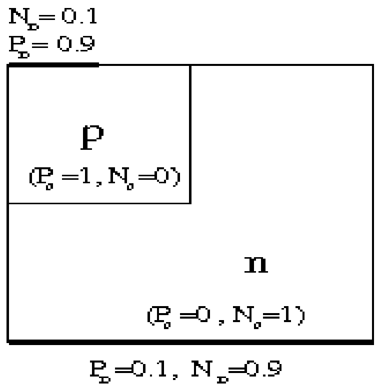


Figure 4.6.4: Example 2: Geometry of pn-junction diode.

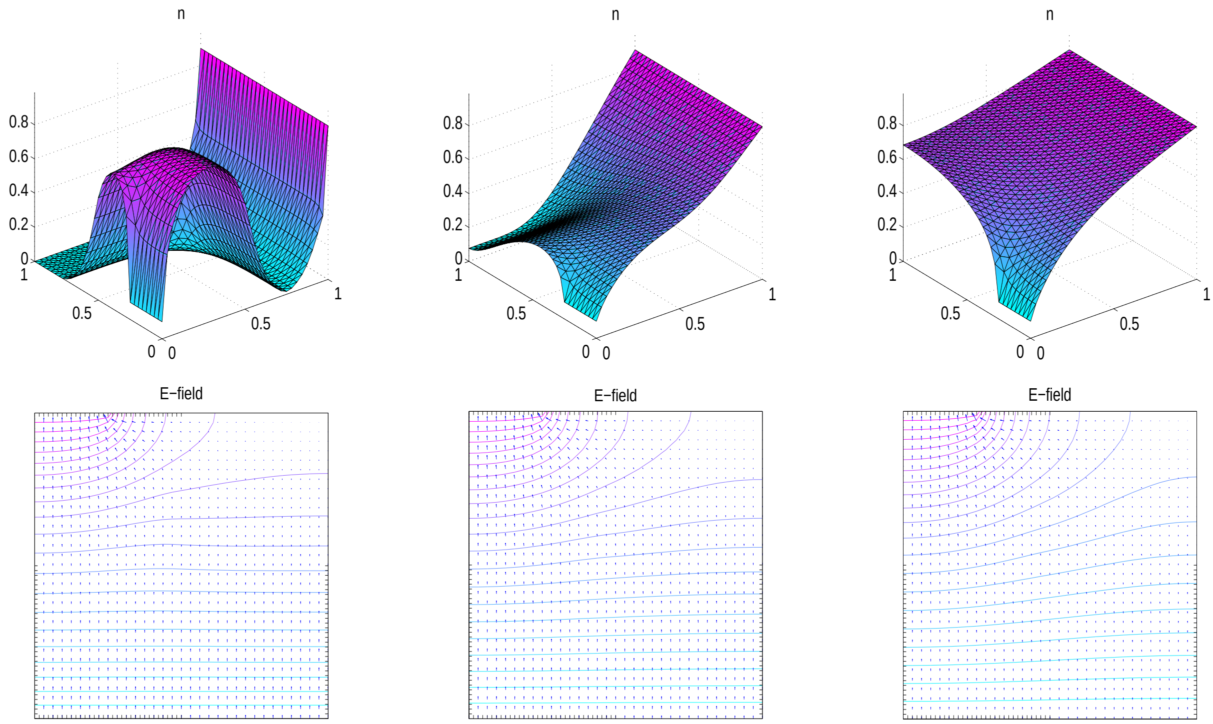


Figure 4.6.5: Example 2 (Scheme $\tilde{A}$): Snapshots of N^j (1st line), and Ψ^j (2nd line) at times $t = 0.002, 0.02, 4$. ($k = 0.002$, $h = 0.0625$).

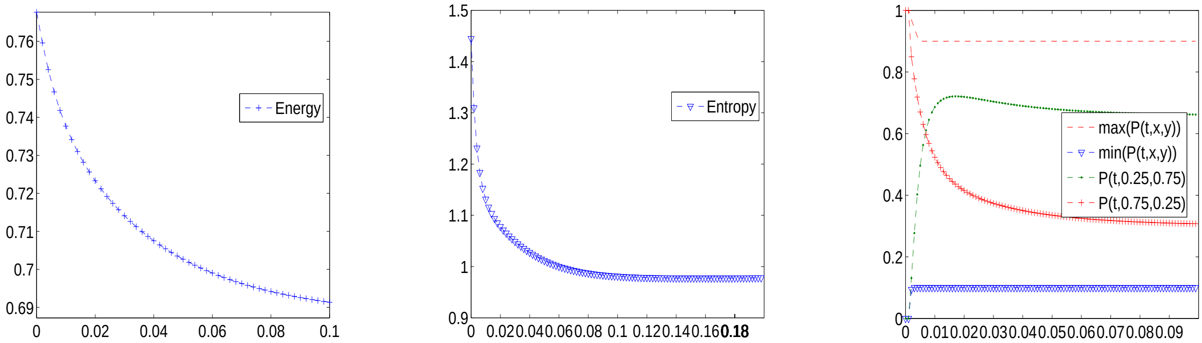


Figure 4.6.6: Example 2 (Scheme $\tilde{A}$): Plot of energy (left), entropy (middle), and minimum/maximum values of P^j (right) ($k = 0.002$, $h = 0.0625$).

Chapter 5

Convergent Finite Element Discretizations of the Navier-Stokes-Nernst-Planck-Poisson System

5.1 Introduction

We consider the following electrohydrodynamic model from [37, 60, 71]:

Let $\Omega \subset \mathbb{R}^N$ be a bounded Lipschitz domain and $T > 0$. Find a velocity field $\mathbf{u} : \Omega \times (0,T) \to \mathbb{R}^N$, concentrations of positive and negative charged species $n^\pm : \Omega \times (0,T) \to \mathbb{R}_{\geq 0}$, and a quasi-electrostatic potential $\psi : \Omega \times (0,T) \to \mathbb{R}$ such that

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} - \Delta \mathbf{u} + \nabla p = \mathbf{f}_C \qquad \text{in } \Omega_T := \Omega \times (0,T) \tag{5.1.1}$$

$$\operatorname{div} \mathbf{u} = 0 \qquad \text{in } \Omega_T \tag{5.1.2}$$

$$\mathbf{u} = 0 \qquad \text{on } \partial\Omega_T := \partial\Omega \times (0,T) \tag{5.1.3}$$

$$\partial_t n^+ + \operatorname{div}\big(J_{n^+}\big) = 0 \qquad \text{in } \Omega_T \tag{5.1.4}$$

$$\langle J_{n^+}, \mathbf{n} \rangle = 0 \qquad \text{on } \partial\Omega_T \tag{5.1.5}$$

$$\partial_t n^- + \operatorname{div}\big(J_{n^-}\big) = 0 \qquad \text{in } \Omega_T \tag{5.1.6}$$

$$\langle J_{n^-}, \mathbf{n} \rangle = 0 \qquad \text{on } \partial\Omega_T \tag{5.1.7}$$

$$-\Delta\psi = n^+ - n^- \qquad \text{in } \Omega_T \tag{5.1.8}$$

$$\langle \nabla\psi, \mathbf{n} \rangle = 0 \qquad \text{on } \partial\Omega_T \tag{5.1.9}$$

for

$$\begin{aligned} \mathbf{u}(\cdot,0) = \mathbf{u}_0, \qquad n^\pm(\cdot,0) = n_0^\pm\,, \\ J_{n^\pm} := \mp n^\pm \nabla\psi - \nabla n^\pm + \mathbf{u} n^\pm\,, \quad \text{and} \quad \mathbf{f}_C := -\big(n^+ - n^-\big)\,\nabla\psi\,. \end{aligned} \tag{5.1.10}$$

Well-posedness of this model has been shown in [71]: Weak solutions to the system (5.1.1)–(5.1.10) are constructed by Schauder's fixed point theorem; the concentrations $n^\pm$ are non-negative and bounded in $L^\infty(\Omega_T)$ which follows from Moser's iteration technique; in addition, weak solutions satisfy an energy and an entropy law obtained by the use of special test functions. The local existence of strong solutions is also verified in [71].

The goal of this work is to recover these characteristic properties of weak solutions in a fully discrete setting by using finite elements. A first step into this direction is [62], where boundedness, non-negativity, an energy, and an entropy law of solutions for the Nernst-Planck-Poisson sub-system (5.1.4)–(5.1.10) (for $\mathbf{u} \equiv \mathbf{0}$) are transferred from the continuous setting to a spatio-temporal finite element based discretization. Here, we consider the whole system (5.1.1)–(5.1.10). This induces an additional interaction with a fluid flow requiring sharper estimates to verify an M-matrix property for discretizations of equations (5.1.4) and (5.1.6).

Electrokinetic flows have many applications: An important class of microfluidic and nowadays especially nanofluidic systems aims to perform basic chemical analyses and other processing steps on a fluidic chip. Fluid motion in such chemical (bio)chip systems is often achieved by using electroosmotic flow which enjoys several advantages over pressure driven flows. Briefly, the electroosmotic flow produces a nearly uniform velocity profile which results in reduced sample species dispersion as compared to the velocity gradients associated with pressure-driven flows. This characteristic property enables such applications as fluid pumping, non-mechanical valves, mixing and molecular separation. Many of these systems also employ electrophoresis. This is another electrokinetic phenomena describing the Coulomb force driven motion of suspended molecular species in the solution. As on a chip electroosmotic and electrophoretic systems grow in complexity, the need of a detailed understanding and computational validation by experimental comparison for such flow models becomes more and more critical. Therefore reliable schemes seem to be of great importance for design optimization.

For an overview of the applied models describing the electrokinetic flows, it is often customary to distinguish between electroosmosis (no external driving force) and electrophoresis (arising by an external force). For a complete description of these two terms we refer to [37, 60]. However, we briefly introduce the principle ideas in the following:
We first mention the pure electroosmotic description. When an electrolyte is brought into contact with a solid surface, a spontaneous electrochemical reaction typically occurs between the two types of media resulting in a redistribution of charges. In the cases of interest, an electric double layer (EDL) is formed that consists of a charged solid surface and a region near the surface that supports a net excess of counter-ions. By the assumption that the concentration profile in the ionic region of the EDL can be described by the Boltzmann distribution, one obtains the Poisson-Boltzmann equation for the net charge density

$$-\Delta\Psi = \frac{-F}{\epsilon}\sum_{i=1}^{L} z_i c_{\infty,i} \exp\Big(-\frac{z_i e \Psi}{kT}\Big) =: -\frac{F}{\epsilon}\rho \tag{5.1.11}$$

which is usually considered only for one particle, i.e., $L = 1$. A second approximation is to consider only a symmetric electrolyte such that the right hand side in (5.1.11) reduces to a *sinh* function. In a third approximation, called the Debye-Hückel limit, one obtains the linear form of the Poisson-Boltzmann equation in case the term $\frac{ze\Psi}{kT}$ is small enough to replace the *sinh* by its argument. Finally, the velocity field $\mathbf{u}$ is described in an arbitrarily shaped micro- or nano-channel for an incompressible liquid via the linear Stokes equation for the Coulomb driving force $\mathbf{f}_C$ on the right hand side. This linear description allows now to consider separately the velocity components due to the electric field $\mathbf{u}_\psi$ and the pressure gradient $\mathbf{u}_p$, where $\mathbf{u} = \mathbf{u}_\psi + \mathbf{u}_p$ solves the linear Stokes equation

$$\begin{aligned} -\Delta\mathbf{u} &= \mathbf{f}_C - \nabla p \qquad \text{in } \Omega \\ \operatorname{div}\mathbf{u} &= 0 \qquad \text{in } \Omega \end{aligned} \tag{5.1.12}$$

Algorithm	Convergence	Scheme	Convergence	System
A_1	$\overset{(I),\,\theta\to 0}{\longrightarrow}$	A	$\overset{h,k\to 0}{\longrightarrow}$	weak solutions of (5.1.1)-(5.1.10)
		B	$\overset{h,k\to 0}{\longrightarrow}$	strong solutions of (5.1.1)-(5.1.10)

Figure 5.1.1: **Scheme A:** (I) = $\Big\{$M-matrix (strongly acute mesh, $h > 0$ small enough) ; existence via Banach's fixed point theorem $\big(k < \tilde{C}h^{\frac{N}{3}+\beta},\ \beta > 0\big)\Big\}$. **Scheme B** bases on Chorin's projection scheme.

for $\mathbf{f}_C = -\rho\nabla\psi$ analogously to the electrohydrodynamic model (5.1.1)–(5.1.10). In the computational part (Section 5.6) we investigate in Examples 1 and 2 the purely electroosmotic behavior especially in view of the energy and entropy property (Section 5.3) proposed in this article.

These electrophoretic phenomena are induced by applying an electric field, and result in the motion of colloidal particles or molecules suspended in ionic solutions. The application of the Stokes law $\mathbf{f}_v = 3\pi\mu d\mathbf{u}$ allows to balance the electrostatic force $q\nabla\Psi$ and the viscous drag $\mathbf{f}_v$ associated with its resulting motion. As a result we have

$$\mathbf{u} = \frac{q\nabla\Psi}{3\pi\mu d} \tag{5.1.13}$$

where q is the total charge on the molecule, $\nabla\Psi$ is the applied field, and d is the diameter of the Stokes sphere in a continuum flow. Hence, we consider the species in the liquid to be of sphere shape as in [71]. The above considerations are made for a stationary liquid. The idea that the electric double layer acts like a capacitor and suggests that the dynamics can be described in terms of equivalent circuits, where the double layer remains in quasi equilibrium with the neutral bulk is discussed and validated in the thin double layer limit by asymptotic analysis of the Nernst-Planck-Poisson equations [9]. Moreover, in [42], the Nernst-Planck-Poisson equations are recently modified to account for the effect of steric constraints on the dynamics. A more detailed description of the physical derivation and motivations concerning the electrohydrodynamic model (5.1.1)–(5.1.10) is given in [70].

In this paper we investigate the incompressible Navier-Stokes-Nernst-Planck-Poisson system (5.1.1)–(5.1.10) which is a more general description of electrokinetic flows compared to the above reduced models for electroosmosis and electrophoresis, see [37, 60]. First, we introduce a fully implicit Scheme A which allows for non-negativity and a discrete maximum principle for the concentrations, and further validates a discrete energy and entropy law for solutions. All results for Scheme A are obtained via an implementable Algorithm A_1 which is proven to converge to Scheme A for $\theta \to 0$, where $\theta > 0$ defines the threshold parameter of the stopping criterion in the fixed point iteration, see Figure 5.1.1. Hence, we verify existence and uniqueness of iterates for Algorithm A_1 via Banach's fixed point theorem, provided that $k \le Ch^{\frac{N}{3}+\beta}$ for any $\beta > 0$. Further, non-negativity and boundedness of iterates of the discrete Nernst-Planck equations in Algorithm A_1 are obtained via the M-matrix property, provided a compatibility constraint (see (5.2.6) below) for admissible finite element spaces is met, and used meshes are strongly acute. This latter compatibility requirement accounts for the coupling of the Nernst-Planck system with the incompressible Navier-Stokes system. Then iterates of Scheme A converge towards weak solutions of the system (5.1.1)–(5.1.10) for $h,\ k \to 0$. Moreover, we verify a discrete energy law, and in two dimensions a discrete entropy dissipation property at finite scales. The latter discrete (perturbed) entropy estimate is verified in two dimensions for the coupling $k \le Ch^2$ of the mesh parameters (h, k), and initial data satisfying $n_0^{\pm} \in H^1(\Omega)$. Hence, we have to require slightly more regularity on the initial concentrations $n_0^{\pm}$, and a dimensional restriction compared

to the continuous setting.
Let us briefly mention why the energy based approach convinces more than an entropy based approach introduced in [62], where an (unperturbed) entropy law holds without any mesh constraint for the Nernst-Planck-Poisson sub-system (5.1.4)–(5.1.10), for $\mathbf{u} \equiv 0$. An entropy based approach does not allow a constructive existence and uniqueness proof via a fully practical fixed point algorithm, enables only quasi-non-negativity of concentrations, does not easily allow for a discrete maximum principle and requires a perturbation of the momentum equation by the entropy-provider $\boldsymbol{\mathcal{S}}_\varepsilon(\cdot)$ to guarantee a discrete energy law.
In the second part of this article we propose a Scheme B based on Chorin's projection method [22, 61, 59] to construct discrete approximations, where iterates converge to the strong solution of the system (5.1.1)–(5.1.10) with optimal rates.The main advantage of Scheme B is its efficiency and the absence of theoretically required mesh constraints. But the solution of Scheme B cannot guarantee any more physically relevant properties, such as a discrete maximum principle for concentrations, a discrete energy, and an entropy law.
The results are given in Section 5.3; Section 5.2 introduces notation. The proofs are given in Section 5.4 for Scheme A, and in Section 5.5 for Scheme B. Comparative computational studies are reported in Section 5.6.

5.2 Preliminaries

5.2.1 Notation

We use the standard Lebesgue and Sobolev spaces [1]. To keep the notation simple, let $\|\cdot\| := \|\cdot\|_{L^2}$. The Poisson equation for vanishing Neumann conditions $g = 0$, that is

$$-\Delta u = f \qquad \text{in } \Omega\,, \qquad \frac{\partial u}{\partial \mathbf{n}} = g \qquad \text{on } \partial\Omega\,, \tag{5.2.1}$$

is of special interest to our analysis and concerns the following regularity estimate for $1 < p < \infty$

$$\|u\|_{W^{2,p}} \leq C\|f\|_{L^p}\,, \tag{5.2.2}$$

which is known to hold for the following assumption, [35]:

(A1) Let $\Omega \subset \mathbb{R}^N$ be an open and bounded domain with a $C^{1,1}$ boundary, or convex in the case of $N = 2$.

We frequently use the following spaces [50],

$$\begin{aligned}
\tilde{\boldsymbol{\mathcal{D}}}(\Omega) &= \{\mathbf{u} \in C_0^\infty(\Omega, \mathbb{R}^N) : \quad \operatorname{div} \mathbf{u} = 0 \quad \text{in } \Omega\}\,,\\
\mathbf{V}^{0,2}(\Omega) &= \text{the closure of } \tilde{\boldsymbol{\mathcal{D}}} \text{ in } L^2 = \overline{\tilde{\boldsymbol{\mathcal{D}}}}^{L^2}\,,\\
\mathbf{V}^{1,2}(\Omega) &= \text{the closure of } \tilde{\boldsymbol{\mathcal{D}}} \text{ in } H_0^1 = \overline{\tilde{\boldsymbol{\mathcal{D}}}}^{H_0^1}\,.
\end{aligned}$$

Subsequently, $\mathcal{T}_h$ denotes a quasi-uniform triangulation [16] of $\Omega \subset \mathbb{R}^N$ for $N = 2, 3$. Let $\mathcal{N}_h = \{\mathbf{x}_\ell\}_{\ell \in L}$ denote the set of all nodes of $\mathcal{T}_h$. We define *strongly acute meshes [36, 58]* as follows:

> The sum of the opposite angles to the common side of any two adjacent triangles is $\leq \pi - \theta$, with $\theta > 0$ independent of h.

This condition is sufficient to validate $k_{\beta\beta'} := \big(\nabla\varphi_\beta, \nabla\varphi_{\beta'}\big) \leq -C_\theta < 0$, for $\beta \neq \beta'$, for the stiffness matrix in three dimensions; here, φ_β is the nodal basis as introduced below. We make the assumption:

(A2) Let $\mathcal{T}_h$ be a strongly acute triangulation, or for $N = 2$ a Delaunay triangulation.

Let P_ℓ denote the set of all polynomials in two variables of degree $\leq \ell$. We introduce the following spaces

$$\begin{aligned} \mathbf{Y}_h &= \big\{\mathbf{U} \in C_0(\overline{\Omega}, \mathbb{R}^N) \,:\, \mathbf{U}|_K \in P_1(K, \mathbb{R}^N) \quad \forall K \in \mathcal{T}_h\big\} \\ Y_h &= \big\{\varphi \in C(\overline{\Omega}) \cap H^1(\Omega) \,:\, \varphi|_K \in P_1(K) \quad \forall K \in \mathcal{T}_h\big\} \qquad (5.2.3) \\ \mathbf{B}_h^\ell &= \big\{\mathbf{U} \in C_0(\overline{\Omega}, \mathbb{R}^N) \,:\, \mathbf{U}|_K \in P_\ell(K, \mathbb{R}^N) \cap H_0^1(K, \mathbb{R}^N) \quad \forall K \in \mathcal{T}_h\big\} \\ \mathbf{X}_h &= \mathbf{Y}_h \cap \mathbf{B}_h^3 \qquad (5.2.4) \\ M_h &= \big\{Q \in L_0^2(\Omega) \cap C(\overline{\Omega}) \,:\, Q|_K \in P_1(K)\big\}. \qquad (5.2.5) \end{aligned}$$

A well-known example [4] that satisfies the discrete inf-sup condition

$$\sup_{\mathbf{U} \in \mathbf{X}_h} \frac{(\operatorname{div} \mathbf{U}, Q)}{\|\nabla \mathbf{U}\|} \geq C\|Q\| \quad \forall Q \in M_h,$$

is the MINI-element defined by $\mathbf{X}_h$ in (5.2.4), and by M_h in (5.2.5). Let

$$\mathbf{V}_h = \big\{\mathbf{V} \in \mathbf{X}_h \,:\, (\operatorname{div} \mathbf{V}, Q) = 0 \quad \forall\, Q \in M_h\big\}.$$

The following compatibility condition of spaces

$$Y_h/\mathbb{R} \subset M_h\,, \qquad (5.2.6)$$

accounts for coupling effects in the electrohydrodynamical system (5.1.1)–(5.1.10). We use the nodal interpolation operator $\mathcal{I}_{Y_h} : C(\overline{\Omega}) \to Y_h$ such that

$$\mathcal{I}_{Y_h}\psi := \sum_{\mathbf{z} \in \mathcal{N}_h} \psi(\mathbf{z})\varphi_{\mathbf{z}}$$

where $\{\varphi_{\mathbf{z}} \,:\, \mathbf{z} \in \mathcal{N}_h\} \subset Y_h$ denotes the nodal basis of Y_h, and $\psi \in C(\overline{\Omega})$. For functions $\phi,\, \psi \in C(\overline{\Omega})$, we define mass-lumping as

$$\begin{aligned} (\phi,\, \psi)_h &:= \int_\Omega \mathcal{I}_{Y_h}\big(\phi\psi\big)\, d\mathbf{x} = \sum_{\mathbf{z} \in \mathcal{N}_h} \beta_{\mathbf{z}}\phi(\mathbf{z})\psi(\mathbf{z})\,, \\ \|\phi\|_h^2 &:= (\phi,\, \phi)_h, \end{aligned}$$

where $\beta_{\mathbf{z}} = \int_\Omega \varphi_{\mathbf{z}}\, d\mathbf{x}$ for $\mathbf{z} \in \mathcal{N}_h$. For all $\Phi,\, \Psi \in Y_h$ one immediately obtains

$$\begin{aligned} \|\Phi\| \leq \|\Phi\|_h &\leq (N+2)^{\frac{1}{2}}\|\Phi\|\,, \\ \big|(\Phi, \Psi)_h - (\Phi, \Psi)\big| &\leq Ch\|\Phi\|\|\nabla\Psi\|\,. \end{aligned} \qquad (5.2.7)$$

Moreover, in appropriate situations we use the convention with its induced norms

$$[\cdot,\cdot]_i := \begin{cases} (\cdot,\cdot) & \text{for } i = 1\,, \\ (\cdot,\cdot)_h & \text{for } i = 2\,, \end{cases} \qquad \|\Phi\|_i^2 := \begin{cases} (\Phi,\Phi) & \text{for } i = 1\,, \\ (\Phi,\Phi)_h & \text{for } i = 2\,. \end{cases}$$

We define the discrete Laplace operators $\mathcal{L}_h^{(i)} : H^1(\Omega) \to Y_h$ for $i = 1, 2$ by

$$\Big[-\mathcal{L}_h^{(i)}\phi, \Psi\Big]_i = -(\nabla\phi, \nabla\Psi) \qquad \forall\, \Psi \in Y_h\,. \qquad (5.2.8)$$

Note that there exists a constant $C > 0$, such that for all $\mathbf{\Phi} \in \mathbf{Y}_h$ and $i = 1, 2$ there holds

$$\|\mathcal{L}_h^{(i)}\mathbf{\Phi}\| \leq Ch^{-2}\|\mathbf{\Phi}\| \quad \text{and} \quad \|\mathcal{L}_h^{(i)}\mathbf{\Phi}\|_{L^\infty} \leq Ch^{-2}\|\mathbf{\Phi}\|_{L^\infty} \quad \forall \mathbf{\Phi} \in \mathbf{Y}_h. \tag{5.2.9}$$

The following discrete Sobolev inequalities generalize results in [38, Lemma 4.4] in the case $N = 3$, for $i = 1, 2$,

$$\begin{aligned} \|\nabla\mathbf{\Phi}\|_{L^3} &\leq C\|\nabla\mathbf{\Phi}\|^{\frac{6-N}{6}}\|\mathcal{L}_h^{(i)}\mathbf{\Phi}\|^{\frac{N}{6}} \quad \forall \mathbf{\Phi} \in \mathbf{Y}_h\,, \\ \|\nabla\Phi\|_{L^6} &\leq C\left(\|\mathcal{L}_h^{(i)}\Phi\| + \|\Phi\|_{H^1}\right) \quad \forall \Phi \in Y_h\,. \end{aligned} \tag{5.2.10}$$

In the sequel, we use the L^2-orthogonal projections $J_{\mathbf{V}_h} : L^2(\Omega, \mathbb{R}^N) \to \mathbf{V}_h$ and $J_{\mathbf{Y}_h} : L^2(\Omega, \mathbb{R}^N) \to \mathbf{Y}_h$, which satisfy for all $\mathbf{u} \in L^2(\Omega, \mathbb{R}^N)$

$$(\mathbf{u} - J_{\mathbf{V}_h}\mathbf{u}, \mathbf{V}) = 0 \quad \forall \mathbf{V} \in \mathbf{V}_h \tag{5.2.11}$$

$$(\mathbf{u} - J_{\mathbf{Y}_h}\mathbf{u}, \mathbf{Y}) = 0 \quad \forall \mathbf{Y} \in \mathbf{Y}_h\,. \tag{5.2.12}$$

The following estimates can be found in [38]:

$$\|\mathbf{u} - J_{\mathbf{V}_h}\mathbf{u}\| + h\|\nabla(\mathbf{u} - J_{\mathbf{V}_h}\mathbf{u})\| \leq Ch^2\|D^2\mathbf{u}\| \quad \forall \mathbf{u} \in \mathbf{V}^{1,2}(\Omega) \cap H^2(\Omega, \mathbb{R}^N), \tag{5.2.13}$$

$$\|\mathbf{u} - J_{\mathbf{V}_h}\mathbf{u}\| \leq Ch\|\nabla\mathbf{u}\| \quad \forall \mathbf{u} \in \mathbf{V}^{1,2}(\Omega)\,. \tag{5.2.14}$$

The same approximation results also hold for J_{Y_h} and $u \in H_0^1(\Omega) \cap H^2(\Omega)$.

5.2.2 Discrete time-derivatives and interpolations

Given a time-step size $k > 0$, and a sequence $\{U^j\}_{j=1}^J$ in some Banach space X, we set $d_t U^j := k^{-1}\{U^j - U^{j-1}\}$ for $j \geq 1$. Note that $(d_t U^j, U^j) = \frac{1}{2}d_t\|U^j\|^2 + \frac{k}{2}\|d_t U^j\|^2$, if X is a Hilbert space. Piecewise constant interpolations of $\{U^j\}_{j=1}^J$ are defined for $t \in [t_{j-1}, t_j)$, and $0 \leq j \leq J$ by

$$\underline{\mathcal{U}}(t) := U^{j-1} \quad \text{and} \quad \overline{\mathcal{U}}(t) := U^j\,,$$

and a piecewise affine interpolation on $[t_{j-1}, t_j)$ is defined by

$$\mathcal{U}(t) := \underline{\mathcal{U}} + \frac{\overline{\mathcal{U}} - \underline{\mathcal{U}}}{k}(t - t_{j-1})\,.$$

Further, we employ the spaces $\ell^p(0, t_J; X)$ for $1 \leq p \leq \infty$. These are the spaces of functions $\{\Phi^j\}_{j=0}^J$ with the bounded norms

$$\|\Phi^j\|_{\ell^p(0,t_J;X)} := \Big(k\sum_{j=0}^J \|\Phi^j\|_X^p\Big)^{\frac{1}{p}}\,, \qquad \|\Phi^j\|_{\ell^\infty(0,t_J;X)} := \max_{1\leq j\leq J}\|\Phi^j\|_X\,.$$

5.3 Main Results

We recall the notion of weak solutions for (5.1.1)–(5.1.10), cf. [71].

Definition 5.3.1. *(Weak solution)* Assume (A1), $N \leq 3$, and $0 < T < \infty$. We call $(\mathbf{u}, n^+, n^-, \psi)$ a weak solution of (5.1.1)-(5.1.10), if

i) it satisfies for $p = 2$, if $N = 2$, or for $p = \frac{4}{3}$, if $N = 3$, that

$$\begin{aligned} \mathbf{u} &\in L^2(0,T;\mathbf{V}^{1,2}(\Omega)) \cap L^\infty(0,T;\mathbf{V}^{0,2}(\Omega)) \cap W^{1,p}(0,T;\mathbf{V}^{-1,2}(\Omega)), \\ n^\pm &\in L^2(0,T;H^1(\Omega)) \cap L^\infty(\Omega_T) \cap W^{1,\frac{6}{5}}(0,T;(H^1(\Omega))^*), \\ \psi &\in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \end{aligned}$$

ii) it solves the equations (5.1.1)-(5.1.8) in the weak sense for the initial data

$$\mathbf{u}_0 \in \mathbf{V}^{0,2}(\Omega), \qquad n_0^\pm \in L^\infty(\Omega, \mathbb{R}_{\geq 0}), \tag{5.3.1}$$

where for $t \to 0$ holds

$$\mathbf{u}(\cdot,t) \rightharpoonup \mathbf{u}_0 \quad \text{in } L^2(\Omega,\mathbb{R}^N), \qquad n^\pm(\cdot,t) \rightharpoonup n_0^\pm \quad \text{in } L^2(\Omega), \tag{5.3.2}$$

iii) it satisfies the following boundary conditions in the trace sense for a.e. $t \in [0,T]$, i.e.,

$$\big\langle J_{n^\pm}, \mathbf{n}\big\rangle\big|_{\partial\Omega} = 0, \qquad \text{and} \quad \big\langle \nabla\psi, \mathbf{n}\big\rangle\big|_{\partial\Omega} = 0, \tag{5.3.3}$$

where $\mathbf{n} \in \mathbb{R}^N$ is the unit normal on the boundary of Ω,

iv) it fulfils for a.e. $t \in [0,T]$ the energy and entropy inequalities

$$E(t) + \int_0^t e(s) + d(s)\, ds \leq E(0) \tag{5.3.4}$$

$$W(t) + \int_0^t I^+(s) + I^-(s)\, ds \leq W(0), \tag{5.3.5}$$

where $W(t) := W_{NPP}(t) + W_{INS}(t)$, for

$$\begin{aligned} W_{NPP}(t) &:= \int_\Omega n^+\left(\log\left(n^+\right) - 1\right) + n^-\left(\log\left(n^-\right) - 1\right) + \frac{1}{2}\left|\nabla\psi\right|^2 + 2\, d\mathbf{x} \\ W_{INS}(t) &:= \int_\Omega \frac{1}{2}\left|\mathbf{u}\right|^2\, d\mathbf{x} + \int_0^t\int_\Omega \left|\nabla\mathbf{u}\right|^2\, d\mathbf{x}ds \\ I^\pm(t) &:= \int_\Omega n^\pm\left[\nabla\left(\log\left(n^\pm\right) - \psi\right)\right]^2\, d\mathbf{x} \\ E(t) &:= \frac{1}{2}\left[\|\mathbf{u}\|^2 + \|\nabla\psi\|^2\right] \\ e(t) &:= \|\nabla\mathbf{u}\|^2 + \|\Delta\psi\|^2 \\ d(t) &:= \int_\Omega \left(n^+ + n^-\right)\left|\nabla\psi\right|^2\, d\mathbf{x}\,. \end{aligned}$$

The term $E(t)$ in the above Definition 5.3.1 contains the physically motivated kinetic energy $E^1(\mathbf{u}) := \frac{1}{2}\|\mathbf{u}\|^2$, and the energy density of the electric field $E^2(\psi) := \frac{1}{2}\|\nabla\psi\|^2$; furthermore, the term $d(t)$ denotes the total electrical energy of the system.

To construct discrete approximations of the weak solutions given in Definition 5.3.1, we propose the following Scheme A. The main interest and hence the reason for the fully implicit character of the subsequently proposed Scheme A is to preserve all the characteristic properties of weak solutions given in the above Definition 5.3.1.

Scheme A:

(1). Set $\mathbf{U}^0 = J_{\mathbf{V}_h}\mathbf{u}_0$, and $\big((N^+)^0,(N^-)^0\big) := \big(J_{Y_h}n_0^+, J_{Y_h}n_0^-\big)$.

(2). For $j = 1,\ldots,J$, let $\mathbf{F}_C^j := -((N^+)^j - (N^-)^j)\nabla\Psi^j$. Find $(\,\mathbf{U}^j,\,(N^\pm)^j,\,\Psi^j) \in \mathbf{V}_h \times [Y_h]^3$ such that for all $(\,\mathbf{V},\,\Phi^\pm,\,\Phi\,) \in \mathbf{V}_h \times [Y_h]^3$, and for $i = 1,\,2$

$$
\begin{aligned}
&(\mathrm{d}_t\mathbf{U}^j,\mathbf{V}) + (\nabla\mathbf{U}^j,\nabla\mathbf{V}) + \epsilon(\nabla d_t\mathbf{U}^j,\nabla\mathbf{V}) + \big((\mathbf{U}^{j-1}\cdot\nabla)\mathbf{U}^j,\mathbf{V}\big)\\
&\qquad\qquad + \frac{1}{2}\big((\operatorname{div}\mathbf{U}^{j-1})\mathbf{U}^j,\mathbf{V}\big) = (\mathbf{F}_C^j,\mathbf{V})\,, \qquad (5.3.6)
\end{aligned}
$$

$$
\begin{aligned}
&[\mathrm{d}_t(N^\pm)^j,\Phi^\pm]_i + (\nabla(N^\pm)^j,\nabla\Phi^\pm) \pm \big((N^\pm)^j\nabla\Psi^j,\nabla\Phi^\pm\big)\\
&\qquad\qquad - (\mathbf{U}^j(N^\pm)^j,\nabla\Phi^\pm) = 0\,, \qquad (5.3.7)
\end{aligned}
$$

$$
(\nabla\Psi^j,\nabla\Phi) = [(N^+)^j - (N^-)^j,\Phi]_i\,, \qquad (5.3.8)
$$

where $\epsilon := h^\alpha$ with $0 < \alpha < \frac{6-N}{3}$.

In the scheme, the stabilization term $\epsilon\,\big(\nabla d_t\mathbf{U}^j,\nabla\mathbf{V}\big)$ is introduced, which serves its purpose to validate a corresponding M-matrix property for the sub-system (5.3.7)–(5.3.8) later, and hence accounts for the problematic nature of the coupled overall system. Since the Scheme A is fully implicit for a coupled nonlinear system, the use of an iterative solver is required; its implicit character allows to recover the properties of solutions from the continuous setting [71]. A corresponding discretization of the Nernst-Planck-Poisson system has been studied in [62]; however, the additional coupling with the Navier-Stokes equations causes major additional problems to effectively deal with (5.3.6)–(5.3.8) which e.g. motivates the term $\epsilon(\nabla d_t\mathbf{U}^j,\nabla\mathbf{V})$. See the discussion in Section 5.4.

Remark 5.3.2. Let us recall the entropy based scheme for the Nernst-Planck-Poisson equations (5.1.4)–(5.1.10) (with $\mathbf{u} \equiv \mathbf{0}$) introduced in [62]. We use the notion of an entropy-provider: For any $\varepsilon \in (0,1)$, and $\varepsilon \geq 1$ sufficiently large, we call $\boldsymbol{\mathcal{S}}_\varepsilon : Y_h \to \big[L^\infty(\Omega)\big]^{d\times d}$ an entropy-provider if for all $\Phi \in Y_h$

$$
\begin{aligned}
&\text{i)} && \boldsymbol{\mathcal{S}}_\varepsilon(\Phi) \text{ is symmetric and positive definite}\,,\\
&\text{ii)} && \boldsymbol{\mathcal{S}}_\varepsilon(\Phi)\nabla\mathcal{I}_h\big[F_\varepsilon'(\Phi)\big] = \nabla\Phi\,.
\end{aligned}
$$

This entropy based approach, which allows for an unperturbed entropy law in [62], leads to

Scheme A': Fix $0 < \varepsilon < 1$, and let $\big((N^+)^0,(N^-)^0\big) \in \big[Y_h\big]^2$, such that $\big((N^+)^0 - (N^-)^0, 1\big) = 0$. For every $j \geq 1$, find iterates $\big(\,(N^+)^j,(N^-)^j,\Psi^j\,\big) \in \big[Y_h\big]^3$, where $(\Psi^j,1) = 0$ such that for all $\big(\,\Phi_1,\Phi_2,\Phi_3\,\big) \in \big[Y_h\big]^3$ holds

$$
\big(d_t(N^+)^j,\Phi_1\big)_h + \Big(\nabla\Psi^j,\boldsymbol{\mathcal{S}}_\varepsilon\big((N^+)^j\big)\nabla\Phi_1\Big) + \big(\nabla(N^+)^j,\nabla\Phi_1\big) = 0\,, \qquad (5.3.9)
$$

$$
\big(d_t(N^-)^j,\Phi_2\big)_h - \Big(\nabla\Psi^j,\boldsymbol{\mathcal{S}}_\varepsilon\big((N^-)^j\big)\nabla\Phi_2\Big) + \big(\nabla(N^-)^j,\nabla\Phi_2\big) = 0\,, \qquad (5.3.10)
$$

$$
\big(\nabla\Psi^j,\nabla\Phi_3\big) = \big((N^+)^j - (N^-)^j,\Phi_3\big)_h\,. \qquad (5.3.11)
$$

In contrast, the extension of this Scheme A' to the electro-hydrodynamic model (5.1.1)–(5.1.10) requires to apply the entropy provider in the Coulomb force term $\mathbf{F}_C^j$ in the following way

$$
-(\boldsymbol{\mathcal{S}}_\varepsilon\big(N^+\big) - \boldsymbol{\mathcal{S}}_\varepsilon\big((N^-)^j\big))\nabla\Psi^j
$$

to verify a discrete energy law, and to compensate for the lack of a discrete maximum principle. This consequence and the weaker results mentioned in the introduction (Section 5.1) motivate to follow the energy based approach as realized with Scheme A.

With the kinetic energy $E^1(\mathbf{U}^j) := \frac{1}{2}\|\mathbf{U}^j\|^2$ and the electric energy density $E^2(\Psi^j) := \frac{1}{2}\|\nabla\Psi^j\|^2$ we define the energy of the electro-hydrodynamic system as

$$E(\mathbf{U}^j, \Psi^j) := \frac{1}{2}\Big[\|\mathbf{U}^j\|^2 + \|\nabla\Psi^j\|^2\Big]\,.$$

In below, the following compatibility condition (5.2.6) is needed to validate an $L^\infty(\Omega_T)$-bound for discrete concentrations. We state the first main result that is verified in Section 5.4.

Theorem 5.3.3. (Properties of Solutions for Scheme A) *Assume the initial conditions of Definition 5.3.1 ii), and (A1). Let (A2) and (5.2.6) be valid, and $h \le h_0(\Omega)$ be small enough, as well as $k \le \tilde{C}h^{\frac{N}{3}+\beta}$ for some $\beta > 0$, and $0 < T = t_J$. Let $0 \le (N^\pm)^0 \le 1$. Then for every $j \ge 1$, there exists a unique solution $(\,\mathbf{U}^j,\, \Pi^j,\, (N^\pm)^j,\, \Psi^j\,) \in \mathbf{V}_h \times M_h \times \big[Y_h\big]^3$, such that (5.3.6)–(5.3.8) hold. Furthermore,*

$$0 \le (N^\pm)^j \le 1 \qquad (1 \le j \le J),$$

and for $i = 1,\, 2$ it holds

i)
$$E(\mathbf{U}^J, \Psi^J) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^J\|^2 + k\sum_{j=1}^{J}\|\nabla\mathbf{U}^j\|^2 + k^2\sum_{j=1}^{J}\Big\{E(d_t\mathbf{U}^j, d_t\Psi^j) + \frac{\epsilon}{2}\|d_t\nabla\mathbf{U}^j\|^2\Big\}$$
$$+k\sum_{j=1}^{J}\Big[\|\nabla\mathbf{U}^j\|^2 + \|(N^+)^j - (N^-)^j\|_i^2\Big] + k\sum_{j=1}^{J}\Big(\big((N^+)^j + (N^-)^j\big), |\nabla\Psi^j|^2\Big)$$
$$= E(\mathbf{U}^0, \Psi^0) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^0\|^2\,,$$

ii)
$$\frac{1}{2}\Big\{\|\mathbf{U}^J\|^2 + \epsilon\|\nabla\mathbf{U}^J\|^2\Big\} + \frac{k^2}{2}\sum_{j=1}^{J}\Big\{\|d_t\mathbf{U}^j\|^2 + \epsilon\|\nabla d_t\mathbf{U}^j\|^2\Big\}$$
$$+k\sum_{j=1}^{J}\|\nabla\mathbf{U}^j\|^2 \le CE(\mathbf{U}^0, \Psi^0) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^0\|^2\,,$$

iii)
$$\frac{1}{2}\Big[\|(N^+)^J\|_i^2 + \|(N^-)^J\|_i^2\Big] + \frac{k^2}{2}\sum_{j=1}^{J}\Big[\|d_t(N^+)^j\|_i^2 + \|d_t(N^-)^j\|_i^2\Big] + \frac{k}{2}\sum_{j=1}^{J}\Big[\|\nabla(N^+)^j\|^2$$
$$+\|\nabla(N^-)^j\|^2\Big] \le CE(\mathbf{U}^0, \Psi^0) + \frac{1}{2}\Big[\|(N^+)^0\|_i^2 + \|(N^-)^0\|_i^2\Big]\,,$$

iv)
$$k\sum_{j=1}^{J}\Big[\|d_t(N^+)^j\|_{(H^1)^*}^2 + \|d_t(N^-)^j\|_{(H^1)^*}^2\Big] \le C\Big\{E(\mathbf{U}^0, \Psi^0) + \Big[\|(N^+)^0\|^2 + \|(N^-)^0\|^2\Big]\Big\}\,,$$

v)
$$k\sum_{j=1}^{J}\|d_t\mathbf{U}^j\|_{(\mathbf{V}^{1,2}\cap\mathbf{H}^2)^*}^q \le C\,,$$

where $q = 2$ for dimension $N = 2$, and $q = \frac{4}{3}$ for $N = 3$.

We introduce a practical Algorithm A_1 in Section 5.4 that is a simple fixed-point scheme, together with a suitable stopping criterion to verify the statements of Theorem 5.3.3.

Motivated by the entropy estimate established in [71] for (5.1.1)–(5.1.10), we recover the proof from there in a fully discrete setting. Therefore, we introduce the entropy functional

$$J \mapsto W^J := E\big(\mathbf{U}^J, \Psi^J\big) + \frac{\epsilon}{2}\|\nabla\mathbf{U}^J\|^2 + \int_\Omega\Big\{\mathcal{I}_{Y_h}\Big[F\Big((N^+)^J\Big) + F\Big((N^-)^J\Big)\Big] + 2\Big\}\,d\mathbf{x}\,, \tag{5.3.12}$$

where $F(x) := x(\log\, x\, - 1)$, and herewith we extend the version in [62].

Theorem 5.3.4. (Entropy Law for Scheme A) *Let* $n_0^\pm \in H^1(\Omega)$, *(A2), (5.2.6),* $N = 2$, *and* $k \leq Ch^2$ *be valid for some* $T := t_J > 0$. *Suppose that* $\delta \leq (N^\pm)^0 \leq 1$ *and some* $0 < \delta < \frac{1}{2}$, *and let* $\big\{\big(\mathbf{U}^j, (N^\pm)^j, \Psi^j\big)\big\}_{j=1}^J$ *solve the Scheme A for* $i = 2$, *i.e.,* $[\cdot,\cdot]_2 = (\cdot,\cdot)_h$. *Then, for all* $0 \leq j < j' \leq J$,

(5.3.13)

$$W^{j'} + \frac{k^2}{2}\sum_{l=j+1}^{j'}\Big[\|\nabla d_t\Psi^l\|^2 + \epsilon\|d_t\nabla\mathbf{U}^l\|^2\Big] + k\sum_{l=j+1}^{j'}\Big[\Big((N^+)^l, \big|\nabla\Psi^l + \mathcal{I}_h\big[F'((N^+)^l)\big]\big|^2\Big)$$
$$+ \|\nabla\mathbf{U}^l\|^2 + \Big((N^-)^l, \big|\nabla\big\{\Psi^l - \mathcal{I}_h\big[F'((N^-)^l)\big]\big\}\big|^2\Big)\Big]$$
$$\leq W^j + Ch\delta^{-4}\Big[E(\mathbf{U}^0, \Psi^0) + \|\nabla(N^+)^0\|_h^2 + \|\nabla(N^-)^0\|_h^2\Big]^2 .$$

The dissipation of $W^{j'}$ in (5.3.13) is then guaranteed for $h < C_W^{-1}\delta^4$.

The main convergence result concerning Scheme A is

Theorem 5.3.5. (Convergence of Scheme A) *Assume the initial conditions of Definition 5.3.1 ii). Suppose (A2), (5.2.6), and* $0 < t_J < \infty$. *Let* $0 \leq (N^+)^0, (N^-)^0 \leq 1$, $(n_0^+, n_0^-) \in \big[L^\infty(\Omega)\big]^2$, *as well as*

$$\mathbf{U}^0 \to \mathbf{u}_0 \text{ in } L^2(\Omega, \mathbb{R}^N), \text{ and } \quad (N^+)^0 \to n_0^+, \, (N^-)^0 \to n_0^- \text{ in } L^2(\Omega).$$

Let $(\boldsymbol{\mathcal{U}}, \mathbf{\Pi}, \mathcal{N}^\pm, \mathbf{\Psi})$ *be constructed from the solution* $\big\{\big(\mathbf{U}^j, \Pi^j, (N^\pm)^j, \Psi^j\big)\big\}_{j=1}^J \subset \mathbf{V}_h \times M_h \times \big[Y_h\big]^3$ *of Scheme A by piecewise affine interpolation as outlined in Section 5.2.2. Then, for* $h, k \to 0$ *such that* $k \leq Ch^{\frac{N}{3}+\beta}$ *for* $\beta > 0$, *there exists a convergent subsequence* $\big\{(\boldsymbol{\mathcal{U}}, \mathbf{\Pi}, \mathcal{N}^\pm, \mathbf{\Psi})\big\}_{k,h}$ *whose limit is a weak solution of (5.1.1)–(5.1.10).*

In Section 5.5, we analyze a time-splitting scheme based on Chorin's projection method [22]. In this scheme, the computation of iterates is fully decoupled in every time-step, which leads to significantly reduced computational resources. But this strategy sacrifices the discrete energy and entropy inequalities, which are relevant tools to characterize long-time asymptotics and convergence towards weak solutions. Therefore, the related numerical analysis requires the existence of (local) strong solutions which is verified for the system (5.1.1)–(5.1.10) in [71].

Definition 5.3.6. *(Strong solution)* Let $0 < T \leq \infty$. The weak solutions $(\mathbf{u}, n^+, n^-, \psi)$ are called strong solutions of (5.1.1)-(5.1.10), if

i)

$$\begin{aligned} \mathbf{u} &\in L^2(0,T;\mathbf{V}^{1,2}(\Omega) \cap \mathbf{V}^{2,2}(\Omega)) \cap W^{1,2}(0,T;\mathbf{V}^{0,2}(\Omega)) \\ n^\pm &\in L^2(0,T;H^2(\Omega)) \cap W^{1,2}(0,T;L^2(\Omega)) \\ \psi &\in C([0,T];H^2(\Omega)) \\ p &\in L^2(0,T;H^1(\Omega)/\mathbb{R}), \end{aligned}$$

where in dimension $N = 3$ the time $T = T(\mathbf{u}_0) > 0$ is finite,

ii) the initial conditions

(5.3.14) $$\mathbf{u}_0 \in \mathbf{V}^{1,2}(\Omega), \qquad n_0^\pm \in H^1(\Omega) \cap L^\infty(\Omega),$$

are attained for $t \to 0$,

(5.3.15) $$\mathbf{u}(\cdot,t) \to \mathbf{u}_0 \quad \text{in } L^2(\Omega,\mathbb{R}^N), \qquad n^\pm(\cdot,t) \to n_0^\pm \quad \text{in } L^2(\Omega),$$

iii) the boundary condition $\langle \nabla n^{\pm}, \mathbf{n}\rangle|_{\partial\Omega} = 0$ hold for all $t \in [0,T]$,

iv) for $N \leq 3$ and $t \in [0,T]$, the energy and entropy identities hold

$$E(t) + \int_0^t e(s) + d(s)\, ds = E(0), \tag{5.3.16}$$

$$W(t) + \int_0^t I^+(s) + I^-(s)\, ds = W(0)\,. \tag{5.3.17}$$

For convenience, we say that a strong solution $(\,\mathbf{u}, p, n^{\pm}, \psi\,)$ is in $\mathbf{S}$, if it satisfies the regularity properties i) of Definition 5.3.6. To approximate the strong solutions of Definition 5.3.6, we propose the following time-splitting

Scheme B: Let $j \geq 1$ and $\{\mathbf{u}^{j-1}, (n^{\pm})^{j-1}\}$, determine $\{\mathbf{u}^j, (n^{\pm})^j, \psi^j\} \in \mathbf{S}$ as follows:

1. Start with $\mathbf{u}^0 = \mathbf{u}_0$, and $(n^{\pm})^0 = n_0^{\pm}$.
2. Let $j \geq 1$. Compute $\psi^{j-1} \in H^1(\Omega)$ from
$$\begin{aligned} -\Delta\psi^{j-1} &= (n^+)^{j-1} - (n^-)^{j-1} \quad \text{in } \Omega \\ \langle \nabla\psi^{j-1}, \mathbf{n}\rangle &= 0 \quad \text{on } \partial\Omega\,. \end{aligned}$$
3. Compute $(n^{\pm})^j \in H^1(\Omega)$ via
$$\begin{aligned} \frac{1}{k}\big\{(n^{\pm})^j - (n^{\pm})^{j-1}\big\} - \Delta(n^{\pm})^j \pm \operatorname{div}((n^{\pm})^j\nabla\psi^{j-1}) + (\mathbf{u}^{j-1}\cdot\nabla)(n^{\pm})^j &= 0 \quad \text{in } \Omega \\ \langle \nabla(n^{\pm})^j \pm (n^{\pm})^j\nabla\psi^{j-1}, \mathbf{n}\rangle &= 0 \quad \text{on } \partial\Omega\,. \end{aligned}$$
4. Find $\tilde{\mathbf{u}}^j \in H_0^1(\Omega, \mathbb{R}^N)$ by solving
$$\begin{aligned} \frac{1}{k}\big\{\tilde{\mathbf{u}}^j - \mathbf{u}^{j-1}\big\} - \Delta\tilde{\mathbf{u}}^j + (\mathbf{u}^{j-1}\cdot\nabla)\tilde{\mathbf{u}}^j &= -\Big((n^+)^j - (n^-)^j\Big)\nabla\psi^{j-1} \\ \tilde{\mathbf{u}}^j &= 0 \quad \text{on } \partial\Omega\,. \end{aligned}$$
5. Determine the tuple $\{\mathbf{u}^j, p^j\} \in \mathbf{V}^{0,2} \times H^1/\mathbb{R}$ that solves the system
$$\frac{1}{k}\big\{\mathbf{u}^j - \tilde{\mathbf{u}}^j\big\} + \nabla p^j = 0\,, \qquad \operatorname{div}\mathbf{u}^j = 0 \quad \text{on } \Omega, \tag{5.3.18}$$
$$\langle \mathbf{u}^j, \mathbf{n}\rangle = 0 \quad \text{on } \partial\Omega\,. \tag{5.3.19}$$

Step 5 is Chorin's projection step. Using the div-operator in (5.3.18) amounts to solving a Laplace-Neumann problem for the pressure iterate,

$$-\Delta p^j = -\frac{1}{k}\operatorname{div}\tilde{\mathbf{u}}^j \quad \text{in } \Omega, \qquad \partial_{\mathbf{n}}\, p^j| = 0 \quad \text{on } \partial\Omega\,, \tag{5.3.20}$$

followed by an algebraic update for the present solenoidal velocity field,

$$\mathbf{u}^j = \tilde{\mathbf{u}}^j - k\nabla p^j \quad \text{in } \Omega\,. \tag{5.3.21}$$

The goal of the second part (Section 5.5) of this paper is to analyze Scheme B by investigating its stability and approximation properties. Therefore we propose a series of auxiliary problems to separately account for inherent time-discretization, decoupling effects, and those attributed to the quasi-compressibility constraint (5.3.20). For this purpose, the following notation is useful.

We say that

1. the quadruple $\Big(\mathbf{u},\, p,\, n^{\pm},\, \psi\Big) := \big\{\xi_i\big\}_{i=1}^4 \in \mathbf{S}$ satisfies property $(P1)$, if the following is satisfied for $i \in \{1,3\}$,

$$k\sum_{j=1}^{J}\Big\{\|d_t\xi_i^j\|_{H^1}^2 + \|d_t\xi_4^j\|_{H^2}^2\Big\} + \max_{1\le j\le J}\Big\{\|\mathrm{d}_t\xi_i^j\|^2 + \|\xi_i^j\|_{H^2}^2 + \|\xi_2^j\|_{H^1}^2 + \|\xi_4^j\|_{H^2}^2\Big\} \le C,$$

2. the quadruple $\{\xi_i^j\}_{i=1}^4 \in \mathbf{S}$ satisfies property $(P2)_l$, for $l \in \{0,1\}$, if the following approximation properties are satisfied:

$$\max_{0\le j\le J}\Bigg\{\|\mathbf{u}(t_j) - \xi_1^j\| + \tau_l^j\|p(t_j) - \xi_2^j\|_{H^{-1}} + \|\psi(t_j) - \xi_4^j\| + \|\psi(t_j) - \xi_4^j\|_{H^1} + \|n^{\pm}(t_j) - \xi_3^j\|$$
$$+ \sqrt{k}\Big(\|\mathbf{u}(t_j) - \xi_1^j\|_{H^1} + \sqrt{\tau_l^j}\|p(t_j) - \xi_2^j\| + \|n^{\pm}(t_j) - \xi_3^j\|_{H^1}\Big)\Bigg\} \le Ck\,,$$

where

$$\tau_l^j := \begin{cases} 1\,, & \text{if } l = 0\,,\\ \min\big\{1, t_j\big\}\,, & \text{if } l = 1\,.\end{cases}$$

The property $(P2)_0$ is used in the analysis of Scheme B. The generic constant C is independent of k, and depends only on the given data. In the following theorem, we state the main result concerning optimal convergence behaviour of the solution obtained via Scheme B.

Theorem 5.3.7. (Convergence of Scheme B) *Suppose (A1), the initial and boundary conditions from Definition 5.3.6 and additionally* $\mathbf{u}_0,\, n_0^{\pm} \in H^2(\Omega)$. *Then the solution*

$$\big\{\mathbf{u}^j, (n^+)^j, (n^-)^j, \psi^j\big\}_{j=1}^J \subset \mathbf{S}$$

of Scheme B satisfies the properties $(P1)$ *and* $(P2)_1$ *for sufficiently small time-steps* $k \le k_0(t_J)$.

If we additionally include the error effects of a corresponding space discretization which uses the setup of (5.2.3)–(5.2.5), we immediately get the

Theorem 5.3.8. (Convergence of Scheme B) *Let* $\big\{\mathbf{U}^j,\, P^j\,(N^{\pm})^j,\, (\Psi)^j\big\}_{j=1}^J \subset \mathbf{V}_h \times M_h \times Y_h$ *be the solution of a fully discrete version of Scheme B (see (5.5.57) of Section 5.5.4), and* $(\mathbf{u},\, p,\, n^{\pm},\, \psi) \in \mathbf{S}$ *be the strong solution of (5.1.1)–(5.1.10) under the additional requirement* $\mathbf{u}_0,\, n_0^{\pm} \in H^2(\Omega)$. *Then*

$$\max_{1\le j\le J}\big\{\|\mathbf{u}(t_j) - \mathbf{U}^j\| + \|\psi(t_j) - \Psi^j\| + \|\psi(t_j) - \Psi^j\|_{H^1} + \|n^{\pm}(t_j) - (N^{\pm})^j\|\big\} \le C\left(k + h^2\right)$$
$$\max_{1\le j\le J}\left\{\|\mathbf{u}(t_j) - \mathbf{U}^j\|_{H^1} + \sqrt{\tau_l^j}\|p(t_j) - P^j\| + \|n^{\pm}(t_j) - (N^{\pm})^j\|_{H^1}\right\} \le C\left(\sqrt{k} + h\right)\,.$$

5.4 Proof of the Results for Scheme A

5.4.1 Existence and Uniqueness of Solutions for Scheme A, Theorem 5.3.3

The M-matrix property of the system matrix for the subsystem (5.3.7)–(5.3.8), and (5.2.6) are key tools to guarantee solvability of Scheme A, non-negativity and boundedness of the iterates $\big\{((N^+)^j,\, (N^-)^j)\big\}_{j\ge 0}$. For the subsequent proof of Theorem 5.3.3, we introduce a practical Algorithm A_1 which asserts the existence and the uniqueness of iterates.

Algorithm $\mathbf{A}_1$. 1. Let $\Big(\mathbf{U}^0, (N^\pm)^0\Big) \in \mathbf{V}_h \times [Y_h]^2$, such that $\Big((N^+)^0 - (N^-)^0, 1\Big) = 0$. For $j \geq 1$, set $\Big((N^+)^{j,0}, (N^-)^{j,0}\Big) := \Big((N^+)^{j-1}, (N^-)^{j-1}\Big)$, and $\ell := 0$.
2. For $\ell \geq 1$, compute $\Big(\mathbf{U}^{j,\ell}, (N^\pm)^{j,\ell}, \Psi^{j,\ell-1}\Big) \in \mathbf{V}_h \times [Y_h]^3$ that solve for all $\Big(\mathbf{V}, \Phi^\pm, \Phi\Big) \in \mathbf{V}_h \times [Y_h]^3$, $i = 1, 2$, and $\mathbf{F}_C^{j,\ell-1} := -\big((N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}\big)\nabla\Psi^{j,\ell-1}$,

$$\Big(\nabla\Psi^{j,\ell-1}, \nabla\Phi\Big) = \Big[(N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}, \Phi\Big]_i\,, \tag{5.4.1}$$

$$\begin{aligned}&\frac{1}{k}\Big(\mathbf{U}^{j,\ell}, \mathbf{V}\Big) + \frac{h^\alpha}{k}\Big(\nabla\mathbf{U}^{j,\ell}, \nabla\mathbf{V}\Big) + \Big(\nabla\mathbf{U}^{j,\ell}, \nabla\mathbf{V}\Big) + \Big((\mathbf{U}^{j-1}\cdot\nabla)\mathbf{U}^{j,\ell}, \mathbf{V}\Big)\\ &\quad+\frac{1}{2}\Big((\mathrm{div}\mathbf{U}^{j-1})\mathbf{U}^{j,\ell}, \mathbf{V}\Big) = \Big(\mathbf{F}_C^{j,\ell-1}, \mathbf{V}\Big) + \frac{1}{k}\Big(\mathbf{U}^{j-1}, \mathbf{V}\Big) + \frac{h^\alpha}{k}\Big(\nabla\mathbf{U}^{j-1}, \nabla\mathbf{V}\Big)\,,\end{aligned} \tag{5.4.2}$$

$$\begin{aligned}&\frac{1}{k}\Big[(N^\pm)^{j,\ell}, \Phi^\pm\Big]_i \pm \Big((N^\pm)^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi^\pm\Big) + \Big(\nabla(N^\pm)^{j,\ell}, \nabla\Phi^\pm\Big)\\ &\qquad -\Big(\mathbf{U}^{j,\ell-1}(N^\pm)^{j,\ell}, \nabla\Phi^\pm\Big) = \frac{1}{k}\Big[(N^\pm)^{j-1}, \Phi^\pm\Big]_i\,.\end{aligned} \tag{5.4.3}$$

3. Stop, if for fixed $\theta > 0$ we have

$$\begin{aligned}&\|\mathbf{U}^{j,\ell} - \mathbf{U}^{j,\ell-1}\| + \|\nabla\{\Psi^{j,\ell} - \Psi^{j,\ell-1}\}\|\\ &+ \Big(\|(N^+)^{j,\ell} - (N^+)^{j,\ell-1}\|_{L^\infty} + \|(N^-)^{j,\ell} - (N^-)^{j,\ell-1}\|_{L^\infty}\Big) \leq \theta\end{aligned} \tag{5.4.4}$$

and go to 4.; set $\ell \leftarrow \ell + 1$ and continue with 2. otherwise.
4. Stop, if $j + 1 = J$; set $j \leftarrow j + 1$ and go to 1. otherwise.

We first achieve $0 \leq (N^\pm)^{1,\ell} \leq 1$ for $\ell \geq 1$; after the verification of a contraction property for iterates, we can identify

$$\big(\mathbf{U}^1,\, (N^\pm)^1,\, \Psi^1\big) := \lim_{\ell\to\infty}\big(\mathbf{U}^{1,\ell},\, (N^\pm)^{1,\ell},\, \Psi^{1,\ell}\big) \in \mathbf{V}_h \times [V_h]^3 \tag{5.4.5}$$

as the unique solution of Scheme A for $j = 1$. Finally, the results can be extended to $1 \leq j \leq J$ by repeating the same procedure for every time-step j.

Proof. (of Theorem 3.3) *Step 1:* (Stability for $\Psi^{j,\ell-1}$) Let $0 \leq (N^+)^{j,\ell-1}, (N^-)^{j,\ell-1} \leq 1$. The solution $\Psi^{j,\ell-1} \in Y_h$ of (5.4.1) may be interpreted as the Ritz projection of $\psi^{j,\ell-1} \in H^1(\Omega)/\mathbb{R}$, i.e., $\Psi^{1,\ell-1} = P_1\psi^{1,\ell-1}$, such that $\big(\Psi^{1,\ell-1}, 1\big) = 0$, and

$$\Big(\nabla\psi^{j,\ell-1}, \nabla\phi\Big) = \Big[(N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}, \phi\Big]_i \qquad \forall\phi \in H^1(\Omega) \cap C(\overline{\Omega})\,,$$

where by assumption $\big((N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}, 1\big) = 0$. By the $W^{1,p}(\Omega)$-stability of P_1, cf. [16, Theorem 8.5.3], there holds $\big\|\Psi^{j,\ell-1}\big\|_{W^{1,\gamma'}} \leq C\,\big\|\psi^{j,\ell-1}\big\|_{W^{1,\gamma'}}$. By Sobolev embedding, the right hand side is bounded by $C\,\big\|(N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}\big\|_{L^{\gamma'}}$, for $1 \leq \gamma' < \infty$, for $N = 2$, and $1 \leq \gamma' \leq 6$ in the case of $N = 3$.

Step 2: (A priori estimates for Algorithm A_1) After testing the equation (5.4.2) with $k\mathbf{U}^{j,\ell}$ we obtain

$$\Big\|\mathbf{U}^{j,\ell}\Big\|^2 + h^\alpha\,\Big\|\nabla\mathbf{U}^{j,\ell}\Big\|^2 + k\,\Big\|\nabla\mathbf{U}^{j,\ell}\Big\|^2 \leq \mathrm{(I)} + \mathrm{(II)} + \mathrm{(III)}\,, \tag{5.4.6}$$

where

$$
\begin{aligned}
\text{(I)} &:= \left|\Big(\mathbf{U}^{j-1}, \mathbf{U}^{j,\ell}\Big)\right| \le \frac{1}{2}\left\|\mathbf{U}^{j-1}\right\|^2 + \frac{1}{2}\left\|\mathbf{U}^{j,\ell}\right\|^2 , \\
\text{(II)} &:= h^\alpha \left|\Big(\nabla\mathbf{U}^{j-1}, \nabla\mathbf{U}^{j,\ell}\Big)\right| \le \frac{h^\alpha}{2}\left\|\nabla\mathbf{U}^{j-1}\right\|^2 + \frac{h^\alpha}{2}\left\|\nabla\mathbf{U}^{j,\ell}\right\|^2 , \\
\text{(III)} &:= k\left|\Big(\Big\{(N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}\Big\}\nabla\Psi^{j,\ell-1}, \mathbf{U}^{j,\ell}\Big)\right| \\
&\le kC\left\{\left\|(N^+)^{j,\ell-1}\right\| + \left\|(N^-)^{j,\ell-1}\right\|\right\}\left\|\nabla\Psi^{j,\ell-1}\right\|_{L^6}\left\|\nabla\mathbf{U}^{j,\ell}\right\| \\
&\le kC\left\|\nabla\Psi^{j,\ell-1}\right\|_{L^6}^2\left\{\left\|(N^+)^{j,\ell-1}\right\|^2 + \left\|(N^-)^{j,\ell-1}\right\|^2\right\} + \frac{k}{2}\left\|\nabla\mathbf{U}^{j,\ell}\right\|^2 .
\end{aligned}
$$

Therefore, we arrive at

$$
\begin{aligned}
\frac{1}{2}\|\mathbf{U}^{j,\ell}\|^2 + \frac{h^\alpha}{2}\|\nabla\mathbf{U}^{j,\ell}\|^2 + \frac{k}{2}\|\nabla\mathbf{U}^{j,\ell}\|^2 \le C\Big\{&\|\mathbf{U}^{j-1}\|^2 + h^\alpha\|\nabla\mathbf{U}^{j-1}\|^2 \\
&+ k\left\|\nabla\Psi^{j,\ell-1}\right\|_{L^6}^2\Big[\|(N^+)^{j,\ell-1}\|^2 + \|(N^-)^{j,\ell-1}\|^2\Big]\Big\} .
\end{aligned}
\tag{5.4.7}
$$

Hence, the right hand side depends on $\ell \ge 1$. Therefore, in the following steps, we use an inductive argument, by showing that the right hand side of (5.4.7) is in fact uniformly bounded in $\ell \ge 1$ by the uniform boundedness of $(N^\pm)^{j,\ell}$ from Step 4.

Step 3: (M-matrix property) To establish the M-matrix property for a sub-system of Algorithm A_1, let $\mathcal{A}$ be the system matrix corresponding to the equations (5.4.3), with the convective term depending on $\mathbf{U}^{j,\ell-1}$, i.e.,

$$
\Big(\mathbf{U}^{j,\ell-1}\varphi_\beta, \nabla\varphi_{\beta'}\Big) =: \Big\{\mathcal{D}(\mathbf{U}^{j,\ell-1})\Big\}_{\beta\beta'} =: d_{\beta\beta'} ,
$$

where $\{\varphi_\beta\}_{\beta=1}^L$ is the canonical basis of Y_h. And correspondingly, we define for $i = 1, 2$

$$
\begin{aligned}
&\Big(\varphi_\beta\nabla\Psi^{j,\ell-1}, \nabla\varphi_{\beta'}\Big) =: \Big\{\mathcal{C}(\Psi^{j,\ell-1})\Big\}_{\beta\beta'} =: c_{\beta\beta'} \\
&\Big(\nabla\varphi_\beta, \nabla\varphi_{\beta'}\Big) =: \{\mathcal{K}\}_{\beta\beta'} =: k_{\beta\beta'} \\
&\Big[\varphi_\beta, \varphi_{\beta'}\Big]_i =: \Big\{\mathcal{M}^{(i)}\Big\}_{\beta\beta'} =: m^{(i)}_{\beta\beta'} .
\end{aligned}
\tag{5.4.8}
$$

Here, $\mathcal{M}^{(1)}$ is the mass and $\mathcal{M}^{(2)}$ the lumped mass matrix. Hence, the system matrix $\{\mathcal{A}\}_{\beta\beta'} := a_{\beta\beta'}$ for (5.4.3) becomes

$$
\mathcal{A} := \begin{pmatrix} \mathcal{A}^+ & \mathbf{0} \\ \mathbf{0} & \mathcal{A}^- \end{pmatrix} ,
\tag{5.4.9}
$$

for $\mathcal{A}^\pm := \frac{1}{k}\mathcal{M}^{(i)} \pm \mathcal{C}(\Psi^{j,\ell-1}) + \mathcal{K} - \mathcal{D}(\mathbf{U}^{j,\ell-1})$ such that $\mathcal{A}[\mathbf{x}^{j,\ell}, \mathbf{y}^{j,\ell}]^\top = \mathbf{f}^{j,\ell}$, where

$$
(N^+)^{j,\ell} := \sum_{\beta=1}^L x_\beta^{j,\ell}\varphi_\beta , \qquad (N^-)^{j,\ell} := \sum_{\beta=1}^L y_\beta^{j,\ell}\varphi_\beta ,
\tag{5.4.10}
$$

with the right hand sides $f_\beta^{j,\ell} := \frac{1}{k}\Big((N^+)^{j-1}, \varphi_\beta\Big)$, and $f_{L+\beta}^{j,\ell} := \frac{1}{k}\Big((N^-)^{j-1}, \varphi_\beta\Big)$, for $1 \le \beta \le L$.

Since the stiffness matrix $\mathcal{K}$ is already an M-matrix, we guarantee its dominating influence as part of $\mathcal{A}^\pm$ by a dimensional argument.

(a) Non-positivity of off-diagonal entries, i.e., $a_{\beta\beta'} \le 0$ for all $\beta \ne \beta'$: Since $\mathcal{T}_h$ is strongly acute, there exists C_{θ_0}, such that $k_{\beta\beta'} \le -C_{\theta_0} h^{N-2} < 0$ uniformly for $h > 0$, for any pair of adjacent nodes. The remaining entries are bounded as follows,

(5.4.11)
$$\big|\big(\mathbf{U}^{j,\ell-1}\varphi_\beta, \nabla\varphi_{\beta'}\big)\big| \le \|\mathbf{U}^{j,\ell-1}\|_{L^\infty}\|\varphi_\beta\nabla\varphi_{\beta'}\|_{L^1} \le Ch^{N-1-\frac{N}{6}}\|\mathbf{U}^{j,\ell-1}\|_{L^6} \le Ch^{\frac{5N}{6}-\frac{\alpha}{2}-1},$$

because of (5.4.7). Hence, we require $N-2 < \frac{5N}{6} - 1 - \frac{\alpha}{2}$ by a dimensional argument between $k_{\beta\beta'}$ and $d_{\beta\beta'}$, which amounts to $0 < \alpha < \frac{6-N}{3}$. Similarly, we proceed with $\mathcal{C}(\Psi^{j,\ell-1})$ for γ' as in Step 1 with $\gamma^{-1} + \gamma'^{-1} = 1$ in the following way

$$\big|\big(\varphi_\beta\nabla\Psi^{j,\ell-1}, \nabla\varphi_{\beta'}\big)\big| \le \|\nabla\Psi^{j,\ell-1}\|_{L^{\gamma'}}\|\varphi_\beta\nabla\varphi_{\beta'}\|_{L^\gamma} \le Ch^{\frac{N}{\gamma}-1}. \tag{5.4.12}$$

Repeating the dimensional argument from above between $k_{\beta\beta'}$ and $c_{\beta\beta'}$ provides $N-2 < \frac{N}{\gamma} - 1$. Hence, $N < \frac{\gamma}{\gamma-1} = \gamma' \sim \frac{2N}{N-2}$, where " $\sim$ " = " $<$ " if $N = 2$ and " $\sim$ " = " $\le$ " if $N = 3$. Therefore (a) holds for $h \le h_0(\Omega)$ small enough.

(b) Strict positivity of the diagonal entries of $\mathcal{A}$: We have to verify that

$$\frac{1}{k} m^{(i)}_{\beta\beta} + k_{\beta\beta} \pm c_{\beta\beta}(\Psi^{1,\ell-1}) - d_{\beta\beta}(\mathbf{U}^{1,\ell-1}) > 0\,.$$

We know that $\frac{1}{k} m^{(i)}_{\beta\beta} \ge c_{\theta_0} h^N$, and $k_{\beta\beta} \ge c_{\theta_0} h^{N-2}$, for some $c_{\theta_0} > 0$. Moreover, from (5.4.11) and (5.4.12) we obtain

$$|c_{\beta\beta}| + |d_{\beta\beta}| \le Ch^{\frac{5N}{6}-1-\frac{\alpha}{2}} + Ch^{\frac{N}{\gamma}-1} =: \eta(h)\,. \tag{5.4.13}$$

Hence $c_{\theta_0} h^{N-2} - \eta(h) > 0$ is guaranteed by the same dimensional argument as in (a) for small enough $h \le h_0(\Omega)$.

(c) $\mathcal{A}$ strictly diagonal dominant, i.e., $\sum_{\beta'\ne\beta} |a_{\beta\beta'}| < a_{\beta\beta}$: We use the fact that the number of neighboring nodes $\mathbf{x}_{\beta'} \in \mathcal{N}_h$ for each $\mathbf{x}_\beta$ is bounded independently of $h > 0$. Hence, there exists a constant $\overline{C} := \overline{C}\big(\{\#\beta' : k_{\beta\beta'} \ne 0\}\big) > 0$, such that for $k,\, h > 0$ sufficiently small

$$\begin{aligned} a_{\beta\beta} &\ge \frac{1}{k} c_{K_\beta} h^N + c_{K_\beta} h^{N-2} - \eta(h) > \overline{C} \max_{\beta\ne\beta'} |a_{\beta\beta'}| \\ &= \overline{C}\Big|-C_{\theta_0} h^{N-2} - \eta(h)\Big| \ge \sum_{\beta\ne\beta'} |a_{\beta\beta'}|\,, \end{aligned} \tag{5.4.14}$$

where we used (b) for the first inequality and (a) and for the second inequality, and in both cases (5.4.13). Hence assertion (c) is verified for small enough $h \le h_0(\Omega)$ and $k \le k_0(\Omega)$.

The verification of (a)–(c) guarantees the M-matrix property of $\mathcal{A}$ for small enough $h \le h_0(\Omega)$ and $k \le k_0(\Omega)$. This property additionally implies the non-negativity of $((N^+)^{1,\ell},\, (N^-)^{1,\ell})$.

Step 4: (Boundedness of $0 \le (N^\pm)^{1,\ell} \le 1$) Under the assumption $(N^\pm)^0 \le 1$ and $(N^\pm)^{1,\ell-1} \le 1$, we have $(\overline{N}^\pm)^{1,\ell-1} \le 0$ for $(\overline{N}^\pm)^{1,\ell-1} := (N^\pm)^{1,\ell-1} - 1$ and also $(\overline{N}^\pm)^0 \le 0$. Then for every $\Phi \in Y_h$, we have

$$\begin{aligned} &\frac{1}{k}\Big[(\overline{N}^\pm)^{1,\ell}, \Phi\Big]_i + \Big(\nabla(\overline{N}^\pm)^{1,\ell}, \nabla\Phi\Big) \pm \Big(\{(\overline{N}^\pm)^{1,\ell} + 1\}\nabla\Psi^{1,\ell-1}, \nabla\Phi\Big) \\ &\qquad + \Big(\mathbf{U}^{1,\ell-1}\{(\overline{N}^\pm)^{1,\ell} + 1\}, \nabla\Phi\Big) = \frac{1}{k}\Big[(\overline{N}^\pm)^0, \Phi\Big]_i\,. \end{aligned} \tag{5.4.15}$$

Via the M-matrix property of $\mathcal{A}$ for the equation (5.4.3) we have

$$\begin{aligned}
&\frac{1}{k}\Big[\Phi-[\Phi]_+,[\Phi]_+\Big]_i+\Big([\Phi]_-\nabla\Psi^{1,\ell-1},\nabla[\Phi]_+\Big)+\Big(\nabla\{\Phi-[\Phi]_+\},\nabla[\Phi]_+\Big)\\
&\qquad\qquad+\Big(\mathbf{U}^{j,\ell-1}[\Phi]_-,\nabla[\Phi]_+\Big)\\
&\geq\frac{1}{k}\big[[\Phi]_-,[\Phi]_+\big]_i+\Big([\Phi]_-\nabla\Psi^{1,\ell-1},\nabla[\Phi]_+\Big)+\big(\nabla[\Phi]_-,\nabla[\Phi]_+\big)+\Big(\mathbf{U}^{j,\ell-1}[\Phi]_-,\nabla[\Phi]_+\Big)\\
&\geq\sum_{\beta,\beta'}a_{\beta\beta'}[\Phi]_+(\mathbf{x}_\beta)[\Phi]_-(\mathbf{x}_{\beta'})\geq 0\,,
\end{aligned}$$

where $[\cdot]_-:=\mathcal{I}_{Y_h}\min\{\cdot,0\}$, $[\cdot]_+:=\mathcal{I}_{Y_h}\max\{\cdot,0\}$, and $\Phi\in Y_h$. Since $\Phi=[\Phi]_++[\Phi]_-$ for all $\Phi\in Y_h$, the definition (5.4.9) of $a_{\beta\beta'}$ then directly implies

$$\begin{aligned}
\frac{1}{k}\|[\Phi]_+\|_i^2+\|\nabla[\Phi]_+\|^2\leq&\frac{1}{k}\Big[[\Phi]_+,\Phi\Big]_i+\Big(\nabla[\Phi]_+,\nabla\Phi\Big)\\
&\pm\Big([\Phi]_-\nabla\Psi^{1,\ell-1},\nabla[\Phi]_+\Big)+\Big(\mathbf{U}^{1,\ell-1}[\Phi]_-,\nabla[\Phi]_+\Big)\,.
\end{aligned}\tag{5.4.16}$$

Testing the equation (5.4.15) with $\Phi=\big[(\overline{N}^{\pm})^{1,\ell}\big]_+$ implies with (5.4.16) the inequality

$$\begin{aligned}
\frac{1}{k}\Big\|[(\overline{N}^{\pm})^{1,\ell}]_+\Big\|_i^2+\Big\|\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\Big\|^2\leq&\Big|\Big(\big\{[(\overline{N}^{\pm})^{1,\ell}]_++1\big\}\nabla\Psi^{1,\ell-1},\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\Big)\Big|\\
&+\Big|\Big(\mathbf{U}^{1,\ell-1}\big\{[(\overline{N}^{\pm})^{1,\ell}]_++1\big\},\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\Big)\Big|\,,
\end{aligned}\tag{5.4.17}$$

where we already skipped $\frac{1}{k}\Big[(\overline{N}^{\pm})^0,\Big[(\overline{N}^{\pm})^{1,\ell}\Big]_+\Big]_i\leq 0$ on the right hand side. We use the interpolation of L^3 between L^2 and H^1, and $\Big(\mathrm{div}\big(\mathbf{U}^{1,\ell-1}\big),[(\overline{N}^{\pm})^{1,\ell}]_+\Big)=0$ which holds by (5.2.6) to estimate the last term in (5.4.17) as

$$\begin{aligned}
&\Big|\Big(\mathbf{U}^{1,\ell-1}\big\{[(\overline{N}^{\pm})^{1,\ell}]_++1\big\},\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\Big)\Big|\leq\|\mathbf{U}^{1,\ell-1}\|_{L^6}\|[(\overline{N}^{\pm})^{1,\ell}]_+\|_{L^3}\|\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\|\\
&\leq C\|\nabla\mathbf{U}^{1,\ell-1}\|\|[(\overline{N}^{\pm})^{1,\ell}]_+\|^{\theta}\|\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\|^{2-\theta}\\
&\leq\Big[Ch^{-\frac{\alpha}{2}}\Big(h^{\frac{\alpha}{2}}\|\nabla\mathbf{U}^{1,\ell-1}\|\Big)\Big]^{\frac{2}{\theta}}\Big\|\big[(\overline{N}^{\pm})^{1,\ell}\big]_+\Big\|^2+\frac{1}{4}\Big\|\nabla\big[(\overline{N}^{\pm})^{1,\ell}\big]_+\Big\|^2,
\end{aligned}\tag{5.4.18}$$

for $\theta=\frac{6-N}{6}$ and the multiplication of $\|\nabla\mathbf{U}^{1,\ell-1}\|$ with $h^{-\frac{\alpha}{2}}h^{\frac{\alpha}{2}}$. The first term on the right hand side of (5.4.17) we control with the help of

$$\begin{aligned}
\Big(\nabla\Psi^{1,\ell-1},\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\Big)&=\Big((\overline{N}^{+})^{1,\ell-1}-(\overline{N}^{-})^{1,\ell-1},[(\overline{N}^{\pm})^{1,\ell}]_+\Big)\\
&\leq\frac{1}{2}\Big\|(\overline{N}^{+})^{1,\ell-1}-(\overline{N}^{-})^{1,\ell-1}\Big\|_i^2+\frac{1}{2}\Big\|(\overline{N}^{\pm})^{1,\ell-1}\Big\|_i^2
\end{aligned}$$

and the interpolation of L^3 between L^2 and H^1 to obtain the bound

$$\Big|\Big([(\overline{N}^{\pm})^{1,\ell}]_+\nabla\Psi^{1,\ell-1},\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\Big)\Big|\leq C\|[(\overline{N}^{\pm})^{1,\ell}]_+\|_i^2\|\nabla\Psi^{1,\ell-1}\|_{L^6}^{\frac{2}{\theta}}+\frac{1}{2}\|\nabla[(\overline{N}^{\pm})^{1,\ell}]_+\|_{L^2}^2\,.\tag{5.4.19}$$

Putting now the bounds of (5.4.18) and (5.4.19) on the left hand side of (5.4.17) results in

$$\begin{aligned}
&\frac{1}{k}\Big\{\frac{1}{2}-Ck\Big(\|\nabla\Psi^{1,\ell-1}\|_{L^6}^{\frac{2}{\theta}}+\Big\|(\overline{N}^{+})^{1,\ell-1}-(\overline{N}^{-})^{1,\ell-1}\Big\|^2\Big)\\
&\qquad-Ckh^{\alpha\frac{N-6}{6}}\Big(h^{\alpha}\Big\|\nabla\mathbf{U}^{j,\ell-1}\Big\|^2\Big)^{\frac{1}{\theta}}\Big\}\|([\overline{N}^{\pm})^{1,\ell}]_+\|_i^2+\frac{1}{2}\|\nabla([\overline{N}^{\pm})^{1,\ell}]_+\|^2\leq 0\,.
\end{aligned}\tag{5.4.20}$$

Hence, only $k \leq Ch^\delta$ for $\delta > 0$ is required to validate the assertion.

Step 5: (Contraction property) We define $\mathbf{e}_\mathbf{u}^\ell := \mathbf{U}^{j,\ell} - \mathbf{U}^{j,\ell-1}$, and for $N^\pm$ correspondingly $e_{n^\pm}^\ell$. First, we consider the terms

$$\big(\mathrm{NP}^\pm\big)^{j,\ell} := \Big(\mathbf{U}^{j,\ell-1}(N^\pm)^{j,\ell}, \nabla\Phi^\pm\Big)\,. \tag{5.4.21}$$

We control the error term $e_{n^+}^\ell$ arising from $\big(\mathrm{NP}^+\big)^{j,\ell}$ via Hölder's inequality for $p_1 = \infty$, $p_2 = 2$, $p_3 = 2$, and inverse estimates from L^∞ to L^6 for $\Phi^+ = e_{n^+}^\ell$ as follows,

$$\begin{aligned}\Big|\big(\mathrm{NP}^+\big)^{j,\ell} - \big(\mathrm{NP}^+\big)^{j,\ell-1}\Big| &\leq \Big|\Big(\mathbf{e}_\mathbf{u}^{\ell-1}(N^+)^{j,\ell}, \nabla e_{n^+}^\ell\Big)\Big| + \Big|\Big(\mathbf{U}^{j,\ell-2} e_{n^+}^\ell, \nabla e_{n^+}^\ell\Big)\Big| \\ &\leq C\|\mathbf{e}_\mathbf{u}^{\ell-1}\|^2 + \frac{1}{10}\|\nabla e_{n^+}^\ell\|^2 + Ch^{-\frac{N}{3}}\big\|\mathbf{U}^{j,\ell-2}\big\|_{L^6}^2 \|e_{n^+}^\ell\|^2 \\ &\leq C\|\mathbf{e}_\mathbf{u}^{\ell-1}\|^2 + \frac{1}{10}\|\nabla e_{n^+}^\ell\|^2 + Ch^{-\frac{N}{3}-\alpha}\|e_{n^+}^\ell\|^2\,,\end{aligned} \tag{5.4.22}$$

where $0 < \alpha < \frac{6-N}{3}$. In the same way we treat (NP^-). Next, we estimate errors arising from

$$\Big(\mathrm{NL}^\pm\Big)^{j,\ell} := \Big((N^\pm)^{j,\ell}\nabla\Psi^{j,\ell-1}, \nabla\Phi^\pm\Big)$$

by

$$\begin{aligned}\Big|\Big(\mathrm{NL}^+\Big)^{j,\ell} - \Big(\mathrm{NL}^+\Big)^{j,\ell-1}\Big| &\leq \Big|\Big(e_{n^\pm}^\ell\nabla\Psi^{j,\ell-1}, \nabla e_{n^\pm}^\ell\Big)\Big| + \Big|\Big((N^\pm)^{j,\ell-1}\nabla e_\psi^{\ell-1}, \nabla e_{n^\pm}^\ell\Big)\Big| \\ &\leq C\Big[\|e_{n^+}^{\ell-1}\|^2 + \|e_{n^-}^{\ell-1}\|^2\Big] + C\Big[\|\nabla\Psi^{j,\ell-1}\|_{L^6}^4 + \frac{1}{2}\Big]\|e_{n^+}^\ell\|_i^2 + \frac{1}{10}\|\nabla e_{n^+}^\ell\|^2\end{aligned} \tag{5.4.23}$$

and in the same way for (NL^-). Hence, we obtain for the Nernst-Planck-Poisson system

$$\begin{aligned}[1 - Ck - Ckh^{-\frac{N}{3}-\alpha}]\Big\{\|e_{n^+}^\ell\|^2 + \|e_{n^-}^\ell\|^2\Big\} + \frac{4k}{5}\Big\{\|\nabla e_{n^+}^\ell\|^2 + \|\nabla e_{n^-}^\ell\|^2\Big\} \\ \leq Ck\Big\{\|e_{n^+}^{\ell-1}\|^2 + \|e_{n^-}^{\ell-1}\|^2\Big\} + kC\|\mathbf{e}_\mathbf{u}^{\ell-1}\|^2\,.\end{aligned}$$

It leaves to control the error $\mathbf{e}_\mathbf{u}^\ell$ concerning to the momentum equation (5.4.2) for $\mathbf{V} = \mathbf{e}_\mathbf{u}^\ell$ as

$$\begin{aligned}\frac{1}{k}\Big(\mathbf{e}_\mathbf{u}^\ell, \mathbf{V}\Big) + \frac{h^\alpha}{k}\Big(\nabla\mathbf{e}_\mathbf{u}^\ell, \nabla\mathbf{V}\Big) + \Big(\nabla\mathbf{e}_\mathbf{u}^\ell, \nabla\mathbf{V}\Big) &\leq \Big|\Big(\{e_{n^+}^{\ell-1} - e_{n^-}^{\ell-1}\}\nabla\Psi^{j,\ell-1}, \mathbf{V}\Big)\Big| \\ &+ \Big|\Big(\{(N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}\}\nabla e_\psi^{\ell-1}, \mathbf{V}\Big)\Big|\,,\end{aligned} \tag{5.4.24}$$

where we already skipped the terms disappearing by the skew symmetry of the convective term. We use Step 4 and (5.4.1) to control the last term on the right hand side in (5.4.24) as follows

$$\begin{aligned}\Big|\Big(\{(N^+)^{j,\ell-1} - (N^-)^{j,\ell-1}\}\nabla e_\psi^{\ell-1}, \mathbf{e}_\mathbf{u}^\ell\Big)\Big| &\leq C\|\mathbf{e}_\mathbf{u}^\ell\|^2 + \|\nabla e_\psi^{\ell-1}\|^2 \\ &\leq C\|\mathbf{e}_\mathbf{u}^\ell\|^2 + C\Big[\|e_{n^+}^{\ell-1}\|^2 + \|e_{n^-}^{\ell-1}\|^2\Big]\,.\end{aligned} \tag{5.4.25}$$

The following control of the remaining term in (5.4.24) for $\theta = \frac{6-N}{6}$

$$\begin{aligned}\Big|\Big(\{e_{n^+}^{\ell-1} - e_{n^-}^{\ell-1}\}\nabla\Psi^{j,\ell-1}, \mathbf{e}_\mathbf{u}^\ell\Big)\Big| &\leq \frac{1}{10}\Big(\theta\left[\left\|e_{n^+}^{\ell-1}\right\|^2 + \left\|e_{n^-}^{\ell-1}\right\|^2\right] \\ &\quad + (1-\theta)\left[\left\|\nabla e_{n^+}^{\ell-1}\right\|^2 + \left\|\nabla e_{n^-}^{\ell-1}\right\|^2\right]\Big) + C\left\|\nabla\Psi^{j,\ell-1}\right\|_{L^6}^2\|\mathbf{e}_\mathbf{u}^\ell\|^2 \\ &\leq \frac{1}{10}\left[\left\|e_{n^+}^{\ell-1}\right\|^2 + \left\|e_{n^-}^{\ell-1}\right\|^2\right] + \frac{N}{60}\left[\left\|\nabla e_{n^+}^{\ell-1}\right\|^2 + \left\|\nabla e_{n^-}^{\ell-1}\right\|^2\right] \\ &\quad + C\left\|\nabla\Psi^{j,\ell-1}\right\|_{L^6}^2\left\|\mathbf{e}_\mathbf{u}^\ell\right\|^2\end{aligned}$$

finally implies the inequality

(5.4.26)

$$\begin{aligned}\big[1-Ck-Ckh^{-\frac{N}{3}-\alpha}\big]\Big\{\|\mathbf{e}_{\mathbf{u}}^{\ell}\|^2+\|e_{n^+}^{\ell}\|_i^2+\|e_{n^-}^{\ell}\|_i^2\Big\}+\frac{4k}{5}\Big\{\|\nabla\mathbf{e}_{\mathbf{u}}^{\ell}\|^2+\|\nabla e_{n^+}^{\ell}\|^2+\|\nabla e_{n^-}^{\ell}\|^2\Big\}\\ \le kC\Big\{\|\mathbf{e}_{\mathbf{u}}^{\ell-1}\|^2+\|e_{n^+}^{\ell-1}\|_i^2+\|e_{n^-}^{\ell-1}\|_i^2\Big\}+\frac{3k}{5}\Big\{\|\nabla\mathbf{e}_{\mathbf{u}}^{\ell-1}\|^2+\|\nabla e_{n^+}^{\ell-1}\|^2+\|\nabla e_{n^-}^{\ell-1}\|^2\Big\}.\end{aligned}$$

Hence, we have the contraction for $k\le k_0(\Omega)$ small enough satisfying the the mesh constraint $k\le\tilde{C}h^{\frac{N}{3}+\alpha}$ which is equivalent to $k\le\tilde{C}h^{\frac{N}{3}+\beta}$ for $\beta>0$, since α satisfies $0<\alpha<\frac{6-N}{3}$ due to Step 3.

Step 6: (Convergence of Algorithm A_1) Fix $j\ge 1$. In the following, we denote the step that reaches the fixed point for the first time in Algorithm A_1 with $\overline{\ell}$.

Lemma 5.4.1. *i) Assume the initial conditions of Definition 3.2.6 ii). Suppose (A1), (A2), (5.2.6), and fix $T=t_J>0$, and let $k\le k_0(\Omega)$ and $h\le h_0(\Omega)$ be sufficiently small with $k\le Ch^{\frac{N}{3}+\beta}$ for any $\beta>0$. Then for every $0\le j\le J$, there exists a unique solution $\big(\mathbf{U}^{j,\overline{\ell}},(N^{\pm})^{j,\overline{\ell}},\Psi^{j,\overline{\ell}},\Pi^{j,\overline{\ell}}\big)\in\mathbf{V}_h\times\big[Y_h\big]^3\times M_h$ of Algorithm A_1, such that $0\le(N^{\pm})^{j,\ell}\le 1$. Moreover, $\big\{\mathbf{U}^{j,\overline{\ell}},(N^{\pm})^{j,\overline{\ell}},\Psi^{j,\overline{\ell}},\Pi^{j,\overline{\ell}}\big\}_{1\le j\le J}$ satisfies the assertions i)–v) of Theorem 5.3.3 for $[\cdot,\cdot]_1=(\cdot,\cdot)$, where each of the right hand sides is increased by $C\theta^2t_J$. In addition,*

$$\big(\mathbf{U}^{j,\ell},(N^{\pm})^{j,\ell},\Psi^{j,\ell},\Pi^{j,\ell}\big)\to\big(\mathbf{U}^{j},(N^{\pm})^{j},\Psi^{j},\Pi^{j}\big)$$

as $\theta\to 0$ for every $j\ge 1$, and the limit solves Scheme A.
ii) If $n_0^{\pm}\in W^{1,2}(\Omega)$, then assertion i) holds also for $[\cdot,\cdot]_2=(\cdot,\cdot)_h$.

Proof. (of Lemma 5.4.1) *i)* We first restate the nonlinear terms in Algorithm A_1, i.e., (5.4.1)–(5.4.3). First we consider (5.4.3). The term depending on $\Psi^{j,\ell-1}$ we may be restated as

$$\begin{aligned}\Big((N^{\pm})^{j,\overline{\ell}}\nabla\Psi^{j,\overline{\ell}-1},\nabla\Phi^{\pm}\Big)&=\Big((N^{\pm})^{j,\overline{\ell}}\nabla\Psi^{j,\overline{\ell}},\nabla\Phi^{\pm}\Big)\\&\quad-\Big((N^{\pm})^{j,\overline{\ell}}\big\{\nabla\Psi^{j,\overline{\ell}}-\nabla\Psi^{j,\overline{\ell}-1}\big\},\nabla\Phi^{\pm}\Big),\end{aligned}$$

where the last term can be controlled by

$$\le\|(N^{\pm})^{j,\overline{\ell}}\|_{L^\infty}\|\nabla\Psi^{j,\overline{\ell}}-\nabla\Psi^{j,\overline{\ell}-1}\|\|\nabla\Phi^{\pm}\|\le\|\nabla\Phi^{\pm}\|\theta\,. \tag{5.4.27}$$

The second relevant term in (5.4.3) is rewritten in the following way,

$$-\Big(\mathbf{U}^{j,\overline{\ell}-1}(N^{\pm})^{j,\overline{\ell}},\nabla\Phi^{\pm}\Big)=-\Big(\mathbf{U}^{j,\overline{\ell}}(N^{\pm})^{j,\overline{\ell}},\nabla\Phi^{\pm}\Big)+\Big(\big\{\mathbf{U}^{j,\overline{\ell}}-\mathbf{U}^{j,\overline{\ell}-1}\big\}(N^{\pm})^{j,\overline{\ell}},\nabla\Phi^{\pm}\Big),$$

where the last term, which contains the error $\mathbf{U}^j-\mathbf{U}^{j,\overline{\ell}-1}$, is estimated as

$$\le\|\mathbf{U}^j-\mathbf{U}^{j,\overline{\ell}-1}\|\|(N^{\pm})^{j,\overline{\ell}}\|_{L^\infty}\|\nabla\Phi^{\pm}\|\le\|\nabla\Phi^{\pm}\|\theta\,. \tag{5.4.28}$$

Consider the eqaution (5.4.2). The only relevant term is the Coulomb force $\mathbf{F}_C^{j,\overline{\ell}-1}$ rewritten as

$$\begin{aligned}-\Big(\big((N^+)^{j,\overline{\ell}-1}-(N^-)^{j,\overline{\ell}-1}\big)\nabla\Psi^{j,\overline{\ell}-1},\mathbf{V}\Big)&=-\Big(\big((N^+)^{j,\overline{\ell}}-(N^-)^{j,\overline{\ell}}\big)\nabla\Psi^{j,\overline{\ell}},\mathbf{V}\Big)\\&\quad+\Big(\Big\{\big\{(N^+)^{j,\overline{\ell}}-(N^+)^{j,\overline{\ell}-1}\big\}-\big\{(N^-)^{j,\overline{\ell}}-(N^-)^{j,\overline{\ell}-1}\big\}\nabla\Psi^{j,\overline{\ell}},\mathbf{V}\Big)\\&\quad+\Big(\big\{(N^+)^{j,\overline{\ell}-1}-(N^-)^{j,\overline{\ell}-1}\big\}\nabla\big\{\Psi^{j,\overline{\ell}}-\Psi^{j,\overline{\ell}-1}\big\},\mathbf{V}\Big),\end{aligned} \tag{5.4.29}$$

which may be controlled by

$$
\begin{aligned}
(5.4.30)\qquad &\leq \Big[\|(N^+)^{j,\bar\ell} - (N^-)^{j,\bar\ell-1}\|_{L^\infty} + \|(N^-)^{j,\bar\ell} - (N^-)^{j,\bar\ell-1}\|_{L^\infty}\Big]\|\nabla\Psi^{j,\bar\ell}\|\|\mathbf{V}\| \\
&+ \|(N^+)^{j,\bar\ell-1} - (N^-)^{j,\bar\ell-1}\|_{L^\infty}\|\nabla(\Psi^{j,\bar\ell} - \Psi^{j,\bar\ell-1})\|\|\mathbf{V}\| \leq C\|\mathbf{V}\|\theta\,.
\end{aligned}
$$

As a consequence, $\Big(\mathbf{U}^{j,\bar\ell},\, N^{\pm})^{j,\bar\ell}\Big)$ solves Scheme A, with perturbed right hand sides controllable through (5.4.4). After passing to the limit $\theta \to 0$, iterates of Algorithm A_1 solve Scheme A.
ii) A direct consequence of i) and (5.2.7). □

Step 7: (Properties *i)–v)*) For assertion *i)* we test equation (5.3.6) with $\mathbf{V} = \mathbf{U}^j$ and sum it with the Nernst-Planck-Poisson equation (5.3.7)–(5.3.8) tested with $\Big(\Phi^+, \Phi^-, \Phi\Big) = \Big(\Psi^j, -\Psi^j, (N^+)^j - (N^-)^j\Big)$. The second assertion uses Step 4 for $\mathbf{V} := \mathbf{U}^j$. The assertion *iii)* is verified by testing with $\Phi^\pm := (N^\pm)^j$. To control the discrete time derivatives *iv)* for $i = 2$, we use the $H^1(\Omega)$-stability of the L^2-projection $J_{Y_h} : L^2(\Omega) \to Y_h$ and its orthogonality property $\Big(\varphi - J_{Y_h}\varphi, \Phi\Big) = 0$ for all $\Phi \in Y_h$ and Step 4 to conclude

(5.4.31)

$$
\begin{aligned}
\|d_t(N^+)^j\|_{(H^1)^*} &\leq \sup_{\varphi\in H^1}\frac{\big(d_t(N^+)^j, J_{Y_h}\varphi\big)_h}{\|\varphi\|_{H^1}} + \sup_{\varphi\in H^1}\frac{\big|\big(d_t(N^+)^j, J_{Y_h}\varphi\big) - \big(d_t(N^+), J_{Y_h}\varphi\big)_h\big|}{\|\varphi\|_{H^1}} \\
&\leq C\Big[\|\nabla\Psi^j\| + \|\nabla(N^+)^j\| + \|\mathbf{U}^j\| + Ch\|d_t(N^+)^j\|\Big]
\end{aligned}
$$

and the subsequent estimate

$$
(5.4.32)\qquad \|d_t(N^+)^j\|_h^2 \leq \Big[\|\nabla\Psi^j\| + \|\nabla(N^+)^j\| + \|\mathbf{U}^j\|\Big]\|\nabla d_t(N^+)^j\|\,.
$$

Finally, it leaves to verify *v)*. Choose $\mathbf{V} = J_{\mathbf{V}_h}\mathbf{v}$ for any $\mathbf{v} \in \mathbf{V}^{1,2}\cap H^2(\Omega,\mathbb{R}^N)$ in (5.3.6), use the approximation respectively the stability properties of $J_{\mathbf{V}_h}$, Sobolev's inequality and interpolation of L^3 between L^2 and H^1. In details, that means

$$
(5.4.33)\qquad \|d_t\mathbf{U}^j\|_{(\mathbf{V}^{1,2}\cap\mathbf{H^2})^*} \leq C\sup_{\mathbf{v}\in\mathbf{V}^{1,2}\cap\mathbf{H^2}}\frac{(d_t\mathbf{U}^j,\mathbf{v})}{\|\Delta\mathbf{v}\|} = C\sup_{\mathbf{v}\in\mathbf{V}^{1,2}\cap\mathbf{H^2}}\frac{(d_t\mathbf{U}^j, J_{\mathbf{V}_h}\mathbf{v})}{\|\Delta\mathbf{v}\|} = (\mathrm{I})\,.
$$

The numerator in (I) we control with the help of equation (5.3.6)

(5.4.34)

$$
\begin{aligned}
|(d_t\mathbf{U}^j, J_{\mathbf{V}_h}\mathbf{v})| \leq C\Big\{&\|\mathbf{U}^{j-1}\|_{L^3}\|\nabla\mathbf{U}^j\| + \|\nabla\mathbf{U}^{j-1}\|\|\mathbf{U}^j\|_{L^3} + \|\nabla\mathbf{U}^j\| + C\|\nabla\Psi^j\|\Big\}\|\Delta\mathbf{v}\| \\
&+ \Big|\Big(h^\alpha d_t\nabla\mathbf{U}^j, \nabla J_{\mathbf{V}_h}\mathbf{v}\Big)\Big|
\end{aligned}
$$

and the last term is controlled by the stability (5.2.13) of the projection $J_{\mathbf{V}_h}$ as

$$
\begin{aligned}
\Big|\Big(h^\alpha d_t\nabla\mathbf{U}^j, \nabla J_{\mathbf{V}_h}\mathbf{v}\Big)\Big| &\leq \big|\big(h^\alpha\nabla d_t\mathbf{U}^j, \nabla\left\{J_{\mathbf{V}_h}\mathbf{v} - \mathbf{v}\right\}\big)\big| + \big|\big(h^\alpha\nabla d_t\mathbf{U}^j, \nabla\mathbf{v}\big)\big| \\
&\leq Ch^{-1}\left\|h^\alpha d_t\mathbf{U}^j\right\|\left\|\nabla\left\{J_{\mathbf{V}_h}\mathbf{v} - \mathbf{v}\right\}\right\| + \left\|h^\alpha d_t\mathbf{U}^j\right\|\left\|\mathcal{L}_h^{(1)}\mathbf{v}\right\| \\
&\leq C\left\|\Delta\mathbf{v}\right\|\left\|h^\alpha d_t\mathbf{U}^j\right\|\,.
\end{aligned}
$$

The latter estimate uses the inequality $\left\|\mathcal{L}_h^{(1)}\mathbf{v}\right\| \leq \|\Delta\mathbf{v}\|$, which we verify in the following. We use the definition (5.2.8) and the identity $\left(-J_{\mathbf{V}_h}\mathcal{L}_h^{(1)}\mathbf{v}, \boldsymbol{\varphi}\right) = \left(-\mathcal{L}_h^{(1)}\mathbf{v}, \boldsymbol{\varphi}\right)$ for all $\boldsymbol{\varphi} \in \mathbf{V}_h$. Hence, upon using $\varphi := -J_{\mathbf{V}_h}\mathcal{L}_h^{(1)}\mathbf{v}$ in (5.2.8) leads to

$$\begin{aligned}\left\|-J_{\mathbf{V}_h}\mathcal{L}_h^{(1)}\mathbf{v}\right\|^2 \leq \left\|\mathcal{L}_h^{(1)}\mathbf{v}\right\|^2 &= \left(\nabla\mathbf{v}, -\nabla\mathcal{L}_h^{(1)}\mathbf{v}\right) \\ &= \left(-\Delta\mathbf{v}, -\mathcal{L}_h^{(1)}\mathbf{v}\right) \leq \|\Delta\mathbf{v}\|\left\|\mathcal{L}_h^{(1)}\mathbf{v}\right\|.\end{aligned} \tag{5.4.35}$$

It leaves to bound $k\sum_{j=1}^{J}\|h^\alpha d_t\mathbf{U}^j\|^2$. Let $\mathbf{V}^j \in \mathbf{V}_h$ be the solution of

$$\left(\nabla\mathbf{V}^j, \nabla\mathbf{\Phi}\right) = \left(d_t\mathbf{U}^j, \mathbf{\Phi}\right) \qquad \text{for all } \mathbf{\Phi} \in \mathbf{V}_h \tag{5.4.36}$$

Hence, we test (5.3.6) with $h^\alpha\mathbf{V}^j$ and use (5.4.36) to obtain for the linear terms

$$\begin{aligned}\left(d_t\mathbf{U}^j, h^\alpha\mathbf{V}^j\right) &= h^\alpha\left(\nabla\mathbf{V}^j, \nabla\mathbf{V}^j\right) = h^\alpha\left\|\nabla\mathbf{V}^j\right\|^2 \\ \left(\nabla\mathbf{U}^j, \nabla h^\alpha\mathbf{V}^j\right) &= h^\alpha\left(d_t\mathbf{U}^j, \mathbf{U}^j\right) = \frac{h^\alpha}{2}d_t\left\|\mathbf{U}^j\right\|^2 + h^\alpha\frac{k}{2}\left\|d_t\mathbf{U}^j\right\|^2 \\ \left(h^\alpha\nabla d_t\mathbf{U}^j, \nabla h^\alpha\mathbf{V}^j\right) &= h^{2\alpha}\left(d_t\mathbf{U}^j, d_t\mathbf{U}^j\right) = \left\|h^\alpha d_t\mathbf{U}^j\right\|^2,\end{aligned}$$

and the nonlinear terms become

$$\begin{aligned}\left(\left(\mathbf{U}^{j-1}\cdot\nabla\right)\mathbf{U}^j, h^\alpha\mathbf{V}^j\right) &\leq C\|\nabla\mathbf{U}^j\|\|\mathbf{U}^{j-1}\|_{L^3}\|h^\alpha d_t\mathbf{U}^j\| \\ &\leq C\|\mathbf{U}^{j-1}\|^2\|\nabla\mathbf{U}^j\|^2 + \frac{1}{4}\|h^\alpha d_t\mathbf{U}^j\|^2 \\ &\leq CE(\mathbf{U}^0, \Psi^0)\|\nabla\mathbf{U}^j\|^2 + \frac{1}{4}\|h^\alpha d_t\mathbf{U}^j\|^2 \\ \frac{1}{2}\left(\operatorname{div}\left(\mathbf{U}^{j-1}\right)\mathbf{U}^j, h^\alpha\mathbf{V}^j\right) &\leq C\|\nabla\mathbf{U}^{j-1}\|^2\|\mathbf{U}^j\|^2 + \frac{1}{4}\|h^\alpha d_t\mathbf{U}^j\|^2 \\ &\leq CE(\mathbf{U}^0, \Psi^0)\|\nabla\mathbf{U}^{j-1}\|^2 + \frac{1}{4}\|h^\alpha d_t\mathbf{U}^j\|^2 \\ \left(\left\{(N^+)^j - (N^-)^j\right\}\nabla\Psi^j, h^\alpha\mathbf{V}^j\right) &\leq C\left\|(N^+)^j - (N^-)^j\right\|_i^2 + \frac{1}{4}\|h^\alpha d_t\mathbf{U}^j\|^2,\end{aligned}$$

where the inequality

$$\left\|h^\alpha\nabla\mathbf{V}^j\right\|^2 \leq C\left\|h^\alpha d_t\mathbf{U}^j\right\|\left\|h^\alpha\mathbf{V}^j\right\| \leq C\left\|h^\alpha d_t\mathbf{U}^j\right\|\left\|h^\alpha\nabla\mathbf{V}^j\right\|,$$

enters due to Poincaré's inequality and (5.4.36). We finally end up with

$$\begin{aligned}\frac{h^\alpha}{2}\|\mathbf{U}^J\|^2 + h^\alpha\frac{k^2}{2}\sum_{j=1}^{J}\|d_t\mathbf{U}^j\|^2 + \frac{k}{4}\sum_{j=1}^{J}\|h^\alpha d_t\mathbf{U}^j\|^2 + h^\alpha\frac{k}{2}\sum_{j=1}^{J}\|\nabla\mathbf{V}^j\|^2 \\ \leq C\left\{E(\mathbf{U}^0, \Psi^0) + 1\right\}E(\mathbf{U}^0, \Psi^0).\end{aligned}$$

This implies the assertion v). □

The proof of the Theorem 5.3.3 is constructive in the sense that it is achieved by the introduction of the practically valuable Algorithm A_1 that terminates by the contraction property respectively the convergence property of Step 7. In the following Section 5.4.2, we establish the entropy property of Scheme A.

5.4.2 Proof of the Entropy Estimate, Theorem 5.3.4

We need the following preliminary estimates which only hold in dimension $N = 2$.

Lemma 5.4.2. *Suppose $n_0^{\pm} \in H^1(\Omega)$, (A1), $N = 2$ and $k \leq \tilde{C}h^2$ for $\tilde{C} > 0$ sufficiently small. Let $0 \leq (N^{\pm})^0 \leq 1$, and choose $[\cdot,\cdot]_2 = (\cdot,\cdot)_h$ in Scheme A. Then the solution $\{(\mathbf{U}^j, (N^{\pm})^j, \Psi^j)\}_{j=1}^J$ of Scheme A satisfies for every $T = t_J > 0$*

$$
\begin{aligned}
i) \qquad & \max_{1\leq j\leq J}\Big(\frac{1}{2} - Ckh^{-2}\Big)\Big[\|\nabla(N^+)^j\|^2 + \|\nabla(N^-)^j\|^2\Big] + \frac{k^2}{2}\sum_{j=1}^J\Big[\|\nabla d_t(N^+)^j\|^2 \\
& +\|\nabla d_t(N^-)^j\|^2\Big] + \frac{k}{2}\sum_{j=1}^J\Big[\|\mathcal{L}_h^{(2)}(N^+)^j\|_h^2 + \|\mathcal{L}_h^{(2)}(N^-)^j\|_h^2\Big] \leq C\Big[E(\mathbf{U}^0,\Psi^0) \\
& +\|\nabla(N^+)^0\|^2 + \|\nabla(N^-)^0\|^2\Big], \\
ii) \qquad & k\sum_{j=1}^J\Big[\|d_t(N^+)^j\|^2 + \|d_t(N^-)^j\|^2\Big] \leq C\Big[E(\mathbf{U}^0,\Psi^0) + \|\nabla(N^+)^0\|^2 + \|\nabla(N^-)^0\|^2\Big],
\end{aligned}
$$

where i) is only uniformly controlled in t_J for $N = 2$.

Proof. i) Choose $\Phi^{\pm} = -\mathcal{L}_h^{(2)}(N^{\pm})^j$ in (5.3.7). We compute with Hölder's inequality for the exponents $p_1 = 2$, $p_2 = p_3 = 4$ and $N = 2$

$$
\begin{aligned}
&\big|\big(\mathbf{U}^j(N^{\pm})^j, -\nabla\mathcal{L}_h^{(2)}(N^{\pm})^j\big)\big| \leq \Big|\Big(\big(\mathrm{div}\mathbf{U}^j\big)(N^{\pm})^j, \mathcal{L}_h^{(2)}(N^{\pm})^j\Big)\Big| + \Big|\Big(\mathbf{U}^j\nabla(N^{\pm})^j, \mathcal{L}_h^{(2)}(N^{\pm})^j\Big)\Big| \\
&\quad \leq C\left\|\nabla\mathbf{U}^j\right\|^2 + \frac{1}{4}\left\|\mathcal{L}_h^{(2)}(N^{\pm})^j\right\|_h^2 + C\left\|\mathbf{U}^j\right\|\left\|\nabla\mathbf{U}^j\right\|\left\|\nabla(N^{\pm})^j\right\|\left\|\mathcal{L}_h^{(2)}(N^{\pm})^j\right\| + \frac{1}{8}\left\|\mathcal{L}_h^{(2)}(N^{\pm})^j\right\|_h^2 \\
&\quad \leq C\left\|\nabla\mathbf{U}^j\right\|^2 + CE(\mathbf{U}^0,\Psi^0)\left\|\nabla\mathbf{U}^j\right\|^2\left\|\nabla(N^{\pm})^j\right\|^2 + \frac{1}{2}\left\|\mathcal{L}_h^{(2)}(N^{\pm})^j\right\|_h^2,
\end{aligned}
$$

where the interpolation inequality

$$
\|\boldsymbol{\varphi}\|_{L^4} \leq C\,\|\boldsymbol{\varphi}\|^{\frac{1}{2}}\,\|\nabla\boldsymbol{\varphi}\|^{\frac{1}{2}} \qquad \text{for all } \boldsymbol{\varphi} \in H^1(\Omega,\mathbb{R}^2)
$$

enters. The latter estimate applies analogously to $(N^-)^j$. As in [62, Lemma 3.1], we obtain the bound

$$
\Big((N^{\pm})^j\nabla\Psi^j, \nabla\mathcal{L}_h^{(2)}(N^{\pm})^j\Big) \leq C\left[\left\|(N^+)^j - (N^-)^j\right\|_h^2 + \left\|\nabla(N^+)\right\|^4\right] + \frac{1}{4}\left\|\mathcal{L}_h^{(2)}(N^+)^j\right\|_h^2.
$$

Adding up everything results in

$$
\begin{aligned}
&\Big(\frac{1}{2} - Ckh^{-2}\Big)\Big[\|\nabla(N^+)^J\|^2 + \|\nabla(N^-)^J\|^2\Big] + \frac{k^2}{2}\sum_{j=1}^{J}\Big[\|\nabla d_t(N^+)^j\|^2 \\
&+\|\nabla d_t(N^-)^j\|^2\Big] + \frac{k}{2}\sum_{j=1}^{J}\Big[\|\mathcal{L}_h^{(2)}(N^+)^j\|_h^2 + \|\mathcal{L}_h^{(2)}(N^-)^j\|_h^2\Big] \\
&\leq Ck\sum_{j=1}^{J-1}\Big\{\|\mathbf{U}^j\|^2 + \|\nabla\mathbf{U}^j\|^2 + CE(\mathbf{U}^0,\Psi^0)\|\nabla\mathbf{U}^j\|^2\left[\left\|\nabla(N^+)^j\right\|^2 + \left\|\nabla(N^-)^j\right\|^2\right] \\
&\quad +\|(N^+)^j - (N^-)^j\|_h^2 + \|\nabla(N^+)^j\|^4 + \|\nabla(N^-)^j\|^4\Big\} \\
&\quad +\frac{1}{2}\left\{\|\nabla(N^+)^0\|^2 + \|\nabla(N^-)^0\|^2\right\} \\
&\leq C\exp\Big[Ck\sum_{j=1}^{J-1}\left\{\|\nabla(N^+)^j\|^2 + \|\nabla(N^-)^j\|^2\right\}\Big]\Big\{E(\mathbf{U}^0,\Psi^0) \\
&\qquad +\|\nabla(N^+)^0\|^2 + \|\nabla(N^-)^0\|^2\Big\},
\end{aligned}
$$

where the last inequality follows from Theorem 5.3.3 together with the discrete Gronwall inequality. Moreover, the right hand side is uniformly bounded in time due to Poincaré's inequality $\|\mathbf{U}^j\| \leq C\|\nabla\mathbf{U}^j\|$.
ii) Choose $\Phi^+ = d_t(N^+)^j$ in (5.3.7) and then treat the terms on the right hand side as in *i)*. □

Now, we can give the proof for the entropy inequality. For this purpose, we borrow arguments from [62]. Since $(N^+)^j, (N^-)^j \geq \delta$, for $j \geq 0$, we may choose $\Phi^+ = \mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j$ in (5.3.7),

$$
\begin{aligned}
&\Big[d_t(N^+)^j, F'((N^+)^j)\Big]_2 + \big[d_t(N^+)^j, \Psi^j\big]_2 + \big(\mathbf{U}^j(N^\pm)^j, \nabla\Phi^\pm\big) \\
&= -\Big((N^+)^j\nabla\Psi^j, \nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j\big\}\Big) - \Big(\nabla(N^+)^j, \nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j\big\}\Big)\,.
\end{aligned} \tag{5.4.37}
$$

We use the identity $(N^+)^j\nabla F'((N^+)^j) = \nabla(N^+)^j$ to estimate the right hand side of (5.4.37)

$$
\begin{aligned}
&= -\Big((N^+)^j\nabla\big\{F'((N^+)^j) + \Psi^j\big\}, \nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j\big\}\Big) \\
&\leq -\Big((N^+)^j, \big|\nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j\big\}\big|^2\Big) + \\
&\quad +\|\nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j\big\}\|_{L^2}\Big[\|\nabla\big\{F'((N^+)^j) - \mathcal{I}_h\big[F'((N^+)^j)\big]\big\}\|_{L^2}\Big]\,.
\end{aligned}
$$

We employ $W^{1,2}$-stability of the interpolation operator to bound the first factor of the last term by $2\big[E(\Psi^0) + \delta^{-2}\|\nabla(N^+)^j\|_{L^2}^2\big]$. For the second factor, we use standard interpolation estimates for each element $K \in \mathcal{T}_h$, and $D^2(N^+)^j\big|_K = 0$ for all $K \in \mathcal{T}_h$,

$$
\begin{aligned}
\Big(\sum_{K\in\mathcal{T}_h}\|\nabla\big\{F'((N^+)^j) - \mathcal{I}_h\big[F'((N^+)^j)\big]\big\}\|_{L^2(K)}^2\Big)^{1/2} &\leq Ch\Big(\sum_{K\in\mathcal{T}_h}\|D^2F'((N^+)^j)\|_{L^2(K)}^2\Big)^{1/2} \\
&\leq Ch\delta^{-2}\|\nabla(N^+)^j\|_{L^4}^2\,.
\end{aligned} \tag{5.4.38}
$$

The remaining term in (5.4.37) is controlled as follows,

$$
\begin{aligned}
&\Big(\mathbf{U}^j (N^+)^j, \nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] + \Psi^j\big\}\Big) + \Big(\mathbf{U}^j (N^-)^j, \nabla\big\{\mathcal{I}_h\big[F'((N^-)^j)\big] - \Psi^j\big\}\Big) \\
&\quad - \Big(\big((N^+)^j - (N^-)^j\big)\nabla\Psi^j, \mathbf{U}^j\Big) \\
&= \Big(\mathbf{U}^j (N^+)^j, \nabla\mathcal{I}_h\big[F'((N^+)^j)\big]\Big) - \Big(\mathbf{U}^j (N^-)^j, \nabla\mathcal{I}_h\big[F'((N^-)^j)\big]\Big) \\
&= \Big(\mathbf{U}^j (N^+)^j, \nabla\big\{\mathcal{I}_h\big[F'((N^+)^j)\big] - F'((N^+)^j)\big\}\Big) \\
&\quad - \Big(\mathbf{U}^j (N^-)^j, \nabla\big\{\mathcal{I}_h\big[F'((N^-)^j)\big] - F'((N^-)^j)\big\}\Big) \\
&\quad + \Big(\mathbf{U}^j (N^+)^j, \nabla F'((N^+)^j)\Big) - \Big(\mathbf{U}^j (N^-)^j, \nabla F'((N^-)^j)\Big) \\
&\le \|(N^+)^j\|_{L^\infty}\|\mathbf{U}^j\|Ch\delta^{-2}\|\nabla(N^+)^j\|^2_{L^4} + \|(N^-)^j\|_{L^\infty}\|\mathbf{U}^j\|Ch\delta^{-2}\|\nabla(N^-)^j\|^2_{L^4}\,,
\end{aligned}
\tag{5.4.39}
$$

where again (5.4.38) enters in the last inequality and we use $(N^\pm)^j\nabla F'((N^\pm)^j) = \nabla(N^\pm)^j$ together with

$$
\Big(\mathbf{U}^j,\nabla\big((N^+)^j + (N^-)^j\big)\Big) = -\Big(\operatorname{div}\mathbf{U}^j, \big((N^+)^j + (N^-)^j\big)\Big) = 0\,,
\tag{5.4.40}
$$

by the compatibility property (5.2.6) of M_h and Y_h. The control on the norms $\|\nabla(N^\pm)^j\|^2_{L^4}$ is given by Lemma 5.4.2 and the Sobolev embedding

$$
\big\|\nabla(N^\pm)^j\big\|_{L^6} \le C\left(\Big\|\mathcal{L}_h^{(2)}(N^\pm)^j\Big\| + \big\|(N^\pm)^j\big\|_{H^1}\right)\,,
$$

see (5.2.10). Now putting (5.4.37) and (5.4.39) together, summing up over iteration steps yields the entropy law (5.3.13).

5.4.3 Proof of the Convergence of Scheme A, Theorem 5.3.5

Step 1: (Extraction of convergent subsequences) The a priori estimates achieved in the last tow sections allow to apply well-established standard results to conclude convergence of a subsequence to a weak solution in the sense of Definition 5.3.1. For notational brevity, we omit the subindices $\cdot_{hk}$ in the subsequent considerations. For $k, h \to 0$, we have

$$
\begin{aligned}
&\overline{\mathcal{N}}^\pm, \underline{\mathcal{N}}^\pm, \mathcal{N}^\pm \rightharpoonup \hat{n}^\pm && \text{in } L^2\Big(0,T;H^1(\Omega)\Big) \cap W^{1,2}\Big(0,T;\big(H^1(\Omega)\big)^*\Big)\,, \\
&\overline{\mathcal{N}}^\pm, \underline{\mathcal{N}}^\pm, \mathcal{N}^\pm \overset{*}{\rightharpoonup} \hat{n}^\pm && \text{in } L^\infty\big(\Omega_T\big)\,, \\
&\overline{\mathcal{N}}^\pm, \underline{\mathcal{N}}^\pm, \mathcal{N}^\pm \to \hat{n}^\pm && \text{in } L^2(\Omega_T)\,, \\
&\nabla\overline{\mathbf{\Psi}}, \nabla\underline{\mathbf{\Psi}}, \nabla\mathbf{\Psi} \overset{*}{\rightharpoonup} \nabla\hat{\psi} && \text{in } L^\infty\Big(0,T;L^2(\Omega)\Big)\,, \\
&\overline{\boldsymbol{\mathcal{U}}}, \underline{\boldsymbol{\mathcal{U}}}, \boldsymbol{\mathcal{U}} \overset{*}{\rightharpoonup} \hat{\mathbf{u}} && \text{in } L^\infty(0,T;L^2(\Omega,\mathbb{R}^N))\,, \\
&\overline{\boldsymbol{\mathcal{U}}}, \underline{\boldsymbol{\mathcal{U}}}, \boldsymbol{\mathcal{U}} \rightharpoonup \hat{\mathbf{u}} && \text{in } L^2(0,T;H^1(\Omega,\mathbb{R}^N))\,, \\
&\overline{\boldsymbol{\mathcal{U}}}, \underline{\boldsymbol{\mathcal{U}}}, \boldsymbol{\mathcal{U}} \rightharpoonup \hat{\mathbf{u}} && \text{in } W^{1,\frac{4}{3}}(0,T;[\mathbf{V}^{1,2} \cap H^2(\Omega,\mathbb{R}^N)]^*)\,, \\
&\overline{\boldsymbol{\mathcal{U}}}, \underline{\boldsymbol{\mathcal{U}}}, \boldsymbol{\mathcal{U}} \to \hat{\mathbf{u}} && \text{in } L^2(0,T;L^2(\Omega,\mathbb{R}^N))\,,
\end{aligned}
\tag{5.4.41}
$$

where the property $(5.4.41)_4$ is a consequence of Aubin-Lions' compactness result validated by the property v) of Theorem 5.3.3. Further, since for $t \in [t_{j-1}, t_j]$

$$
\boldsymbol{\mathcal{U}} - \overline{\boldsymbol{\mathcal{U}}} = \boldsymbol{\mathcal{U}} - \mathbf{U}^j = \frac{t - t_j}{k}\Big(\mathbf{U}^j - \mathbf{U}^{j-1}\Big)\,,
$$

we have the relation

$$
\begin{aligned}
\|\boldsymbol{\mathcal{U}} - \overline{\boldsymbol{\mathcal{U}}}\|^2_{L^2(0,T;L^2)} &= \sum_{j=1}^{J} \left\{ \|\mathbf{U}^j - \mathbf{U}^{j-1}\|^2 \int_{t_{j-1}}^{t_j} \Big(\frac{t-t_j}{k}\Big)^2 \mathrm{d}t \right\} \\
&= \frac{k}{3} \sum_{j=1}^{J} \|\mathbf{U}^j - \mathbf{U}^{j-1}\|^2 = \frac{k^3}{3} \sum_{j=1}^{J} \|d_t \mathbf{U}^j\|^2 \,,
\end{aligned} \tag{5.4.42}
$$

which tends to zero for $k \to 0$. Hence with Theorem 5.3.3 ii) the sequences $\boldsymbol{\mathcal{U}}$ and $\overline{\boldsymbol{\mathcal{U}}}$ respectively $\underline{\boldsymbol{\mathcal{U}}}$ converge to the same limit as $h,\, k \to 0$.

Step 2: (Passing to the limit) We may restate (5.3.6) for any $\mathbf{v} \in \tilde{\boldsymbol{\mathcal{D}}}$, with $\mathbf{V} := J_{\mathbf{V}_h}\mathbf{v} \in \mathbf{V}_h$, which satisfies $\mathbf{V} \to \mathbf{v}$ in $\mathbf{W}^{1,p}(\Omega)\,(h \to 0)$, for all $1 \leq p \leq \frac{2N}{N-2}$ and $\omega(t)$ a continuously differentiable function on $[0,T]$ with $\omega(T) = 0$ in the following way: For every $t > 0$, find $\boldsymbol{\mathcal{U}}(t,\cdot) \in \mathbf{V}_h$ such that

$$
\begin{aligned}
\Big((\boldsymbol{\mathcal{U}})_t, \omega(t)\mathbf{V}\Big) + \Big(\nabla\overline{\boldsymbol{\mathcal{U}}}, \omega(t)\nabla\mathbf{V}\Big) + h^\alpha \Big(\nabla(\boldsymbol{\mathcal{U}})_t, \omega(t)\nabla\mathbf{V}\Big) \\
+ \Big((\underline{\boldsymbol{\mathcal{U}}}\cdot\nabla)\overline{\boldsymbol{\mathcal{U}}}, \omega(t)\mathbf{V}\Big) = \Big(\overline{\mathbf{F}}_C, \omega(t)\mathbf{V}\Big)\,,
\end{aligned} \tag{5.4.43}
$$

where $\overline{\mathbf{F}}_C := -\Big(\overline{\mathcal{N}}^+ - \overline{\mathcal{N}}^-\Big)\nabla\overline{\boldsymbol{\Psi}}$. Integrate (5.4.43) in t, and integrate the first and third term by parts to get

$$
\begin{aligned}
\int_0^T \Big\{ -\Big(\boldsymbol{\mathcal{U}}, \omega'(t)\mathbf{V}\Big) + \Big(\nabla\overline{\boldsymbol{\mathcal{U}}}, \omega(t)\nabla\mathbf{V}\Big) - h^\alpha\Big(\nabla\boldsymbol{\mathcal{U}}, \omega'(t)\nabla\mathbf{V}\Big) \\
+ \Big((\underline{\boldsymbol{\mathcal{U}}}\cdot\nabla)\overline{\boldsymbol{\mathcal{U}}}, \omega(t)\mathbf{V}\Big)\Big\}\, dt = \Big(\boldsymbol{\mathcal{U}}(0), \omega(0)\mathbf{V}\Big) + \int_0^T \Big(\overline{\mathbf{F}}_C, \omega(t)\mathbf{V}\Big)\, dt\,.
\end{aligned} \tag{5.4.44}
$$

We now pass to the limit in (5.4.44) with the sequence $h, k \to 0$ using essentially (5.4.41) and (5.4.42). In the limit we find

$$
\begin{aligned}
\int_0^T \Big\{ -\Big(\mathbf{u}, \omega'(t)\mathbf{v}\Big) + \Big(\nabla\mathbf{u}, \omega(t)\nabla\mathbf{v}\Big) \\
+ \Big((\mathbf{u}\cdot\nabla)\mathbf{u}, \omega(t)\mathbf{v}\Big)\Big\}\, dt = \Big(\mathbf{u}_0, \omega(0)\mathbf{v}\Big) + \int_0^T \Big(\mathbf{F}_C, \omega(t)\mathbf{v}\Big)\, dt\,.
\end{aligned} \tag{5.4.45}
$$

Now writing, in particular, (5.4.45) with $\omega \in C_0^\infty([0,T))$ we see that $\mathbf{u}$ satisfies (5.1.1) in the sense of distributions and by density also in the weak sense. Finally, it remains to prove that $\mathbf{u}(0) = \mathbf{u}_0$. For this we multiply (5.1.1) by $\omega\mathbf{v}$ and integrate. After integrating the first term by parts, we get

$$
\begin{aligned}
\int_0^T \Big\{ -\Big(\mathbf{u}, \omega'(t)\mathbf{v}\Big) + \Big(\nabla\mathbf{u}, \omega(t)\nabla\mathbf{v}\Big) \\
+ \Big((\mathbf{u}\cdot\nabla)\mathbf{u}, \omega(t)\mathbf{v}\Big)\Big\}\, dt = \Big(\mathbf{u}(0), \omega(0)\mathbf{v}\Big) + \int_0^T \Big(\mathbf{F}_C, \omega(t)\mathbf{v}\Big)\, dt\,.
\end{aligned}
$$

By comparison with (5.4.45),

$$
(\mathbf{u}(0) - \mathbf{u}_0, \mathbf{v})\,\omega(0) = 0\,.
$$

We can choose ω with $\omega(0) = 1$; thus

$$
(\mathbf{u}(0) - \mathbf{u}_0, \mathbf{v}) = 0 \qquad \text{for all } \mathbf{v} \in \mathbf{V}^{1,2}\,.
$$

The convergence of the Nernst-Planck-Poisson part may be verified as in [62] where the additional convective term for $k,\, h \to 0$

$$\int_0^T \left(\overline{\mathcal{UN}}^{\pm}, \nabla J_{Y_h}\phi^{\pm}\right)\, dt \to \int_0^T \left(\mathbf{u}n^{\pm}, \nabla\phi^{\pm}\right)\, dt \qquad \text{for all } \phi^{\pm} \in H^1(\Omega)\,,$$

by $(5.4.41)_3$ and $(5.4.41)_8$. Finally, in the sense of an overall-convergence in the Algorithm A_1 we may let $\theta, h, k \to 0$. As a consequence, the solutions of Algorithm A_1 converge to weak solutions of the system (5.1.1)–(5.1.10).

5.5 Analysis of Scheme B and Proofs

5.5.1 Semi-Discretization in Time, Theorem 5.3.7

Since each step of Scheme B introduces different discretization, splitting and perturbation errors, we introduce suitable auxiliary problems to analyze the ongoing error behavior of the proposed scheme, and we verify the properties $(P1)$ and $(P2)_l$, $l \in \{0,1\}$ (see Section 5.3) for each of it.

Auxiliary Problem A: We analyze the error originating from the fully implicit time discretization.
Let the initial data $\left(\mathbf{u}_A^0,\, (n^{\pm})_A^0\right)$ be given by (5.3.14), determine $\left\{\mathbf{u}_A^j,\, p_A^j,\, (n^{\pm})_A^j,\, \psi_A^j\right\}_{j=1}^J \subset \mathbf{S}$ that solves

$$\begin{aligned}
&(5.5.1) && d_t\mathbf{u}_A^j - \Delta\mathbf{u}_A^j + (\mathbf{u}_A^j\cdot\nabla)\mathbf{u}_A^j + \nabla p_A^j = -\big((n^+)_A^j - (n^-)_A^j\big)\nabla\psi_A^j\,,\\
&(5.5.2) && \operatorname{div}\mathbf{u}_A^j = 0\,,\\
&(5.5.3) && d_t(n^{\pm})_A^j \mp \operatorname{div}\big((n^{\pm})_A^j\nabla\psi_A^j\big) - \Delta(n^{\pm})_A^j + \mathbf{u}_A^j\cdot\nabla(n^{\pm})_A^j = 0\,,\\
&(5.5.4) && -\Delta\psi_A^j = (n^+)_A^j - (n^-)_A^j\,.
\end{aligned}$$

We gather the results concerning this auxiliary Problem A in Lemma 5.5.3.

Auxiliary Problem B: This auxiliary problem analyses the error caused by the semi-implicit coupling of the Coulomb force term in the Navier-Stokes equation (5.5.5) and the concentration equations (5.5.7), as well as a semi-implicit treatment of convective term.
Let the initial data $\left(\mathbf{u}_B^0,\, (n^{\pm})_B^0\right)$ be given by (5.3.14), determine $\left\{\mathbf{u}_B^j,\, p_B^j,\, (n^{\pm})_B^j,\, \psi_B^j\right\}_{j=1}^J \subset \mathbf{S}$ that solves

$$\begin{aligned}
&(5.5.5) && d_t\mathbf{u}_B^j - \Delta\mathbf{u}_B^{j-1} + (\mathbf{u}_B^j\cdot\nabla)\mathbf{u}_B^j + \nabla p_B^j = -\big((n^+)_B^j - (n^-)_B^j\big)\nabla\psi_B^{j-1}\,,\\
&(5.5.6) && \operatorname{div}\mathbf{u}_B^j = 0\,,\\
&(5.5.7) && d_t(n^{\pm})_B^j \mp \operatorname{div}\big((n^{\pm})_B^j\nabla\psi_B^{j-1}\big) - \Delta(n^{\pm})_B^j + \mathbf{u}_B^{j-1}\cdot\nabla(n^{\pm})_B^j = 0\,,\\
&(5.5.8) && -\Delta\psi_B^{j-1} = (n^+)_B^{j-1} - (n^-)_B^{j-1}\,.
\end{aligned}$$

The results on convergence and stability behavior are collected in Lemma 5.5.4.

Auxiliary Problem C: This problem investigates the influence of Chorin's projection scheme.

Let the initial data $\left(\mathbf{u}_C^0,\, (n^{\pm})_C^0\right)$ be given by (5.3.14), and let $\left\{(n^{\pm})_B^{j-1},\, \psi_B^{j-1}\right\}_{j=1}^J$ be given by Problem B, compute the iterates $\left(\mathbf{u}_C^j,\, p_C^j\right) \in \mathbf{V}^{1,2}\times H^1/\mathbb{R}$ that solve

$$\begin{aligned}
&(5.5.9) && d_t\mathbf{u}_C^j - \Delta\mathbf{u}_C^j + (P_{\mathbf{V}^{0,2}}\mathbf{u}_C^{j-1}\cdot\nabla)\mathbf{u}_C^j + \nabla p_C^j = -\big((n^+)_C^j - (n^-)_C^j\big)\nabla\psi_C^{j-1}\,,\\
&(5.5.10) && \operatorname{div}\mathbf{u}_C^j - k\Delta p_C^j = 0\,, \quad \partial_{\mathbf{n}}p_C^j|_{\partial\Omega} = 0\,,
\end{aligned}$$

where $P_{\mathbf{V}^{0,2}}$ denotes the L^2-projection onto the space $\mathbf{V}^{0,2}$.

Results concerning the analysis of Problem C are presented in Lemma 5.5.6.

Auxiliary Problem D: Chorin's projection method causes some recoupling effects which originate from a semi-explicit treatment of concentrations and velocity field.
Let the initial data $\big(\mathbf{u}_D^0,\, (n^\pm)_D^0\big)$ be given by (5.3.14), determine $\big\{\mathbf{u}_D^j,\, p_D^j,\, (n^\pm)_D^j,\, \psi_D^j\big\} \subset \mathbf{S}$ that solve

$$d_t\mathbf{u}_D^j - \Delta\mathbf{u}_D^j + (P_{V^{0,2}}\mathbf{u}_D^{j-1}\cdot\nabla)\mathbf{u}_D^j + \nabla p_D^{j-1} = -\big((n^+)_D^j - (n^-)_D^j\big)\nabla\psi_D^{j-1}\,, \tag{5.5.11}$$

$$\operatorname{div}\mathbf{u}_D^j - k\Delta p_D^j = 0\,, \quad \partial_{\mathbf{n}} p_D^j|_{\partial\Omega} = 0\,, \tag{5.5.12}$$

$$d_t(n^\pm)_D^j \pm \operatorname{div}\big((n^\pm)_D^j\nabla\psi_D^{j-1}\big) - \Delta(n^\pm)_D^j + (P_{V^{0,2}}\mathbf{u}_D^{j-1}\cdot)\nabla(n^\pm)_D^j = 0\,, \tag{5.5.13}$$

$$-\Delta\psi_D^{j-1} = (n^+)_D^{j-1} - (n^-)_D^{j-1}\,. \tag{5.5.14}$$

Lemma 5.5.7 provides both, stability and convergence results concerning Problem D.

Chorin's projection method has been analyzed in [61, 59]. The right hand side of equation (5.1.1) satisfies $\mathbf{f}_C := \big(n^+ - n^-\big)\nabla\psi \in C([0,T];L^2(\Omega,\mathbb{R}^N))$, since $n_t^\pm \in L^2(0,T;H^{-1}(\Omega))$ and $n^\pm \in L^2(0,T;H^1(\Omega))$ directly imply $n^\pm \in C([0,T];L^2(\Omega))$ and by (A1), $\psi \in C([0,T];H^2(\Omega))$. This setup of regularities allows to apply results from [61] regarding Chorin's projection scheme for the incompressible Navier-Stokes equations.

Lemma 5.5.1. *Assume (A1), the initial and boundary conditions of Definition 5.3.6,* $\mathbf{u}_0 \in H^2(\Omega,\mathbb{R}^N)$*,* $n_0^\pm \in H^2(\Omega)$*, and* $\mathbf{f}_C \in C([0,T];L^2(\Omega))$*. Let* $\{\tilde{\mathbf{u}}^j,\, p^j\}_{j=1}^J$ *be the (semi-)discrete solution of Chorin's method, i.e., Step 4 and Step 5 of Scheme B accordingly adjusted, whereas* $\{\mathbf{u}(t_j),\, p(t_j)\}_{j=1}^J$ *is the strong solution of the Navier-Stokes equations (5.1.1), for times* $0 < t_j < t_J$*. Then, for sufficiently small time-steps* $k \le k_0(t_J)$ *and* $\tau^j := \min\{1, t_j\}$*, there exists a constant* C *which only depends on the data of the problem, such that the following hold*

1. *convergence estimates*

$$\max_{1\le j\le J}\big\{\|\mathbf{u}(t_j) - \tilde{\mathbf{u}}^j\| + \tau^j\|p(t_j) - p^j\|_{H^{-1}}\big\} \le Ck, \tag{5.5.15}$$

$$\max_{1\le j\le J}\big\{\|\mathbf{u}(t_j) - \tilde{\mathbf{u}}^j\|_{H^1} + \sqrt{\tau^j}\|p(t_j) - p^j\|\big\} \le C\sqrt{k}. \tag{5.5.16}$$

2. *stability result*

$$\max_{1\le j\le J}\Big\{\|d_t\tilde{\mathbf{u}}^j\| + \|\tilde{\mathbf{u}}^j\|_{H^2} + \|p^j\|_{H^1}\Big\} + k\sum_{j=1}^J \|d_t\tilde{\mathbf{u}}^j\|_{H^1}^2 \le C. \tag{5.5.17}$$

5.5.2 A priori estimates of the continuous problem (5.1.1)–(5.1.10)

The results on strong solutions in [71] immediately imply

Lemma 5.5.2. *Let* $\big\{\mathbf{u},\, p,\, n^\pm,\, \psi_0\big\} \in \mathbf{S}$ *be the strong solution of (5.1.1)–(5.1.10) for initial and boundary data required in Definition 5.3.6, and* $\mathbf{u}_0 \in H^2(\Omega,\mathbb{R}^N)$*,* $n_0^\pm \in H^2(\Omega)$*. Then we have the following a priori bounds,*

$$\sup_{(0,t_J]}\Big\{\|\mathbf{u}_t\|^2 + \|n_t^\pm\|^2 + \|\mathbf{u}\|_{H^2}^2 + \|n^\pm\|_{H^2}^2\Big\} + \int_0^{t_J}\Big\{\|\nabla\mathbf{u}_t\|^2 + \|\nabla n_t^\pm\|^2\Big\}\,ds \le C\,. \tag{5.5.18}$$

The analysis in the next Section 5.5.3 requires higher order time-derivatives of $\mathbf{u}$ and $n^{\pm}$. This involves time-weights τ to control rough initial perturbations, see [38]. We directly refer to the cited literature for the needed standard arguments which yield to

$$\int_0^{t_J} \tau\Big\{\|\mathbf{u}_{tt}\|^2_{\mathbf{V}^{-1,2}} + \|n^{\pm}_{tt}\|^2_{(H^1)^*}\Big\} ds \le C\,. \tag{5.5.19}$$

The following sections provide main arguments which validate property $(P1)$ for every auxiliary Problem A through D and $(P2)_0$ for the Problems A and B, and $(P2)_1$ for C and D.

5.5.3 Properties of the Auxiliary Problems A through D

For better readability we skip convective terms in the error analysis in the above auxiliary problems.

It is known that the convective terms do not cause any severe problems; for the sake of better readability of the proofs we will skip the convective terms containing the fluid velocity as $\mathbf{u}$, $\mathbf{u}_A$, $\mathbf{u}_B$, $\mathbf{u}_C$, or $\mathbf{u}_D$ in the subsequent analysis of the auxiliary Problems A through D.

Lemma 5.5.3. (Problem A) *The solution to Problem A satisfies the properties* $(P1)$ *and* $(P2)_0$ *for sufficiently small time-steps* $k \le k_0(t_J)$.

Proof. The property (P1) is immediately verified by means of arguments that are used for the a priori estimates, see Lemma 5.5.2. Moreover, the apriori bounds for the auxiliary problem are obtained as in Theorem 5.3.3 due to its fully implicit structure. We introduce the abbreviations

$$\begin{aligned} \mathbf{e}^j &:= \mathbf{u}(t_j) - \mathbf{u}_A^j\,, & \pi^j &:= p(t_j) - p_A^j\,,\\ (\eta^{\pm})^j &= n^{\pm}(t_j) - (n^{\pm})_A^j\,, & \zeta^j &:= \psi(t_j) - \psi_A^j\,. \end{aligned}$$

The corresponding error equations are

$$\begin{aligned} d_t\mathbf{e}^j - \Delta\mathbf{e}^j + \nabla\pi^j &= R^j(\mathbf{u})\\ -\big((\eta^+)^j - (\eta^-)^j\big)\nabla\psi(t_j) &- \big((n^+)_A^j - (n^-)_A^j\big)\nabla\zeta^j, \end{aligned} \tag{5.5.20}$$

$$\operatorname{div}\mathbf{e}^j = 0, \tag{5.5.21}$$

$$d_t(\eta^{\pm})^j - \Delta(\eta^{\pm})^j \mp \operatorname{div}\big((\eta^{\pm})^j\nabla\psi(t_j)\big) \mp \operatorname{div}\big((n^{\pm})_A^j\nabla\zeta^j\big) = R^j(n^{\pm})\,, \tag{5.5.22}$$

$$-\Delta\zeta^j = (\eta^+)^j - (\eta^-)^j, \tag{5.5.23}$$

where for $\varphi = n^{\pm}$ or $\mathbf{u}$, we set

$$R^j(\varphi) := -\frac{1}{k}\int_{t_{j-1}}^{t_j} (s-t_j)\varphi_{tt}(s)\,\mathrm{d}s. \tag{5.5.24}$$

If we test (5.5.20) with $\mathbf{e}^j$, (5.5.22) with $(\eta^{\pm})^j$, and (5.5.23) with ζ^j, we obtain

(5.5.25)

$$\begin{aligned} &d_t\Big\{\|\mathbf{e}^j\|^2 + \|(\eta^+)^j\|^2 + \|(\eta^-)^j\|^2\Big\} + k\Big\{\|d_t\mathbf{e}^j\|^2 + \|d_t(\eta^+)^j\|^2 + \|d_t(\eta^-)^j\|^2\Big\}\\ &\quad + \frac{2}{5}\Big\{\|\nabla\mathbf{e}^j\|^2 + \|\nabla(\eta^+)^j\|^2 + \|\nabla(\eta^-)^j\|^2\Big\}\\ &\le C\Big\{\Big[\|R^j(\mathbf{u})\|^2_{\mathbf{V}^{-1,2}} + \|R^j(\eta^+)\|^2_{(H^1)^*} + \|R^j(\eta^-)\|^2_{(H^1)^*}\Big]\\ &\quad + \Big[\|\psi(t_j)\|^2_{H^2} + \|\psi(t_j)\|^{\frac{2}{\theta}}_{H^2} + \|(n^+)_A^j\|^2_{H^1} + \|(n^-)_A^j\|^2_{H^1} + 1\Big]\big(\|(\eta^+)^j\|^2 + \|(\eta^-)^j\|^2\big)\Big\}. \end{aligned}$$

by the Sobolev embedding $\|\mathbf{u}(t_j)\|_{L^\infty} \leq C\|\mathbf{u}(t_j)\|_{H^2}$, the Hölder inequality for the exponents $p_1 = 2$, $p_2 = 3$, $p_3 = 6$ and the Sobolev inequalities. We only give the estimate of the special term that requires the Gagliardo-Nirenberg inequality for $\theta = \frac{6-N}{6}$. We have

$$\begin{aligned}\Big|\Big((\eta^\pm)^j\nabla\psi(t_j), \nabla(\eta^\pm)^j\Big)\Big| &\leq C\|\psi(t_j)\|_{H^2}\|(\eta^\pm)^j\|^\theta\|\nabla(\eta^\pm)^j\|^{2-\theta} \\ &\leq C\|\psi(t_j)\|_{H^2}^{\frac{12}{6-N}}\|(\eta^\pm)^j\|^2 + \frac{1}{10}\|\nabla(\eta^\pm)^j\|^2\,,\end{aligned} \tag{5.5.26}$$

where we applied Young's inequality for the conjugate exponents $p = \frac{12}{6-N}$ and $p' = \frac{12}{6+N}$ in the last line of (5.5.26). The regularity of strong solutions results in

$$k\sum_{j=0}^{J}\|R^j(\varphi)\|_X^2 \leq Ck^{-1}\sum_{j=0}^{J}\int_{t_{j-1}}^{t_j}(s-t_j)^2\,\mathrm{d}s\int_{t_{j-1}}^{t_j}\|\varphi_{tt}(s)\|_X^2\,\mathrm{d}s \leq Ck^2\,, \tag{5.5.27}$$

where

$$X := \begin{cases}\mathbf{V}^{-1,2} & \text{for } \varphi = \mathbf{u}\,,\\ \left(H^1\right)^* & \text{for } \varphi = n^\pm\,.\end{cases}$$

Thus the discrete version of Gronwall's inequality finalizes the error property $(P2)_0$. □

The latter proof shows optimal rates of convergence for the auxiliary Problem A that satisfies a discrete energy law which implies property $(P2)$ for its iterates. The following Problem B involves a splitting strategy preventing a discrete energy law; in order to cope with this deficiency effectively, we apply an inductive argument and rely on regularity properties for iterates of Problem A.

Lemma 5.5.4. (Problem B) *The solution to Problem B satisfies the properties* $(P1)$ *and* $(P2)_0$*, provided again that the time-step size* $k \leq k_0(t_J)$ *is chosen sufficiently small.*

Proof. As in Lemma 5.5.3, we introduce

$$\begin{aligned}\mathbf{e}^j &:= \mathbf{u}_A^j - \mathbf{u}_B^j\,, &\qquad \pi^j &:= p_A^j - p_B^j\,,\\ (\eta^\pm)^j &:= (n^\pm)_A^j - (n^\pm)_B^j\,, & \zeta^j &:= \psi_A^j - \psi_B^j\,,\end{aligned}$$

with the corresponding error equations

$$\begin{aligned}d_t\mathbf{e}^j - \Delta\mathbf{e}^j + \nabla\pi^j = k\Big(\big((n^+)_A^j - (n^-)_A^j\big)\nabla d_t\psi_A^j\Big) &+ \Big(\big((\eta^+)^j - (\eta^-)^j\big)\nabla\psi_A^{j-1}\Big)\\ &+\Big(\big((n^+)_B^j - (n^-)_B^j\big)\nabla\zeta^{j-1}\Big)\end{aligned} \tag{5.5.28}$$

$$\operatorname{div}\mathbf{e}^j = 0, \tag{5.5.29}$$

$$\begin{aligned}d_t(\eta^\pm)^j - \Delta(\eta^\pm)^j \mp k\operatorname{div}\big((n^\pm)_A^j d_t\nabla\psi_A^j\big) &\mp \operatorname{div}\big((\eta^\pm)^j\nabla\psi_A^{j-1}\big)\\ &\mp\operatorname{div}\big((n^\pm)_B^j\nabla\zeta^{j-1}\big) = 0,\end{aligned} \tag{5.5.30}$$

$$-\Delta\zeta^{j-1} = (\eta^+)^{j-1} - (\eta^-)^{j-1}, \tag{5.5.31}$$

Step 1: (*Property* $(P1)$) The verification of $(P1)$ is done by Step 2.

Step 2: (*Property* $(P2)_0$) We test equation equation (5.5.30) with $(\eta^\pm)^j$, i.e.,

$$\frac{1}{2}d_t\|(\eta^\pm)^j\|^2 + \frac{k}{2}\|d_t(\eta^\pm)^j\|^2 + \|\nabla(\eta^\pm)^j\|^2 \leq \text{(I)} + \text{(II)} + \text{(III)} \tag{5.5.32}$$

where we estimate the terms on the right hand side in the following using the (L^2, L^3, L^6)-decomposition

$$
\begin{aligned}
\text{(I)} &:= k\left|\left((n^\pm)^j_A d_t\nabla\psi^j_A, \nabla(\eta^\pm)^j\right)\right| \le k^2C\|d_t\psi^j_A\|^2_{H^2}\|(n^\pm)^j_A\|^2_{H^1} + \frac{1}{4}\|\nabla(\eta^\pm)^j\|^2\\
\text{(II)} &:= \left|\left((\eta^\pm)^j\nabla\psi^{j-1}_A, \nabla(\eta^\pm)^j\right)\right| \le C\|\psi^{j-1}_A\|^{\frac{12}{6-N}}_{H^2}\|(\eta^\pm)^j\|^2 + \frac{1}{8}\|\nabla(\eta^\pm)^j\|^2\\
\text{(III)} &:= \left|\left((n^\pm)^j_A\nabla\zeta^{j-1}, \nabla(\eta^\pm)^j\right)\right| + \left|\left((\eta^\pm)^j\nabla\zeta^{j-1}, \nabla(\eta^\pm)^j\right)\right| \le C\left\|(n^\pm)^j_A\right\|^2_{H^2}\left\|\nabla\zeta^{j-1}\right\|^2\\
&\qquad + \frac{1}{4}\left\|\nabla(\eta^\pm)^j\right\|^2 + \text{(P1)}\,,
\end{aligned}
$$

where on

$$
\text{(P1)} := C\left[\|(\eta^+)^{j-1}\|^{\frac{12}{6-N}} + \|(\eta^-)^{j-1}\|^{\frac{12}{6-N}}\right]\left\|(\eta^\pm)^j\right\|^2
$$

we have to employ an inductive argument. It leaves to test (5.5.28) with $\mathbf{e}^j$, i.e.,

$$
\frac{1}{2}d_t\left\|\mathbf{e}^j\right\|^2 + \frac{k}{2}\left\|d_t\mathbf{e}^j\right\| + \left\|\nabla\mathbf{e}^j\right\|^2 \le \text{(I)} + \text{(II)} + \text{(III)} \tag{5.5.33}
$$

where the terms on the right hand side are estimated thanks to (5.5.31) by

$$
\begin{aligned}
\text{(I)} &:= k\left|\left(\left\{(n^+)^j_A - (n^-)^j_A\right\}\nabla d_t\psi^j_A, \mathbf{e}^j\right)\right|\\
&\le k^2C\left\|d_t\psi^j_A\right\|^2_{H^2}\left[\left\|(n^+)^j_A\right\|^2 + \left\|(n^-)^j_A\right\|^2\right] + \frac{1}{8}\left\|\nabla\mathbf{e}^j\right\|^2\\
\text{(II)} &:= \left|\left(\left\{(\eta^+)^j - (\eta^-)^j\right\}\nabla\psi^{j-1}_A, \mathbf{e}^j\right)\right| \le C\left\|\psi^{j-1}_A\right\|^2_{H^2}\left[\left\|(\eta^+)^j\right\|^2 + \left\|(\eta^-)^j\right\|^2\right] + \frac{1}{8}\left\|\nabla\mathbf{e}^j\right\|^2\\
\text{(III)} &:= \left|\left(\left\{(n^+)^j_A - (\eta^+)^j - (n^-)^j_A + (\eta^-)^j\right\}\nabla\zeta^{j-1}, \mathbf{e}^j\right)\right|\\
&\le C\left[\left\|(n^+)^j_A\right\|^2_{H^2} + \left\|(n^-)^j_A\right\|^2_{H^2}\right]\left\|\mathbf{e}^j\right\|^2 + \frac{1}{8}\left[\left\|(\eta^+)^{j-1}\right\|^2 + \left\|(\eta^-)^{j-1}\right\|^2\right] + \text{(P2)}\,.
\end{aligned}
$$

On the term

$$
\begin{aligned}
\text{(P2)} := \left|\left(\left\{-(\eta^+)^j + (\eta^-)^j\right\}\nabla\zeta^{j-1}, \mathbf{e}^j\right)\right| &\le C\left[\left\|(\eta^+)^{j-1}\right\|^2 + \left\|(\eta^-)^{j-1}\right\|^2\right]\left\|\mathbf{e}^j\right\|^2\\
+ \frac{1}{8}\left[\left\|(\eta^+)^j\right\|^2 + \left\|\nabla(\eta^+)^j\right\|^2 + \left\|(\eta^-)^j\right\|^2 + \left\|\nabla(\eta^-)^j\right\|^2\right]
\end{aligned}
$$

in (III) together with $(P1)$ we employ the following inductive argument:

Claim: For $T = t_J$, there exist constants $C_i(\Omega, t_J)$, $i = 1, 2$, such that for $0 \le \ell \le J$ and $k \le k_0(C_1, C_2, \Omega_T)$, we have

$$
\begin{aligned}
&\frac{1}{2}\left[\left\|\mathbf{e}^\ell\right\|^2 + \left\|(\eta^+)^\ell\right\|^2 + \left\|(\eta^-)^\ell\right\|^2\right] + \beta k^2\sum_{j=1}^{\ell}\left[\left\|d_t\mathbf{e}^j\right\|^2 + \left\|d_t(\eta^+)^j\right\|^2 + \left\|d_t(\eta^-)^j\right\|^2\right]\\
&\quad + \alpha k\sum_{j=1}^{\ell}\left[\left\|\nabla\mathbf{e}^j\right\|^2 + \left\|\nabla(\eta^+)^j\right\|^2 + \left\|\nabla(\eta^-)^j\right\|^2\right] \le C_1k^2\exp\left(C_2t_\ell\right).
\end{aligned} \tag{5.5.34}
$$

The constant $C_1 = C_1(\Omega_T) > 0$ bounds the solutions of Problem A; $C_2 = C_2(C_1, \Omega_T) > 0$ will be chosen sufficiently large for the following inductive argument. First, we verify (5.5.34) for

$\ell = 1$: Summation of (5.5.32) and (5.5.33) by setting $j = 1$ and using $\eta^0 = 0$, $\mathbf{e}^0 = \mathbf{0}$ easily validates (5.5.34).
We come to the induction step $\ell - 1 \to \ell$: Adding (5.5.32) and (5.5.33) and a subsequent summation over $1 \le j \le \ell$ verifies (5.5.34) again by using Gronwall's inequality for $k \le k_0(C_1, C_2, t_J)$ sufficiently small, since by $(P2)_0$ for iterates of Problem A,

$$\begin{aligned}
&\frac{1}{2}\left[\left\|\mathbf{e}^\ell\right\|^2 + \left\|(\eta^+)^\ell\right\|^2 + \left\|(\eta^-)^\ell\right\|^2\right] + \beta k^2 \sum_{j=1}^{\ell}\left[\|d_t\mathbf{e}^j\|^2 + \|d_t(\eta^+)^j\|^2 + \|d_t(\eta^-)^j\|^2\right]\\
&+ \alpha k \sum_{j=1}^{\ell}\left[\|\nabla \mathbf{e}^j\|^2 + \|\nabla(\eta^+)^j\|^2 + \|\nabla(\eta^-)^j\|^2\right]\\
&\le k^3 C_1 \sum_{j=1}^{\ell}\left\|d_t\psi_A^j\right\|_{H^2}^2\left[\left\|(n^+)_A^j\right\|_{H^1}^2 + \left\|(n^-)_A^j\right\|_{H^1}^2\right]\\
&+ kC_1 \sum_{j=1}^{\ell}\left[1 + \left\|(n^\pm)_A^j\right\|^2\right]\left[\|(\eta^+)^{j-1}\|^2 + \|(\eta^-)^{j-1}\|^2\right]\\
&+ kC_1 \sum_{j=1}^{\ell}\left[+\left\|\psi_A^{j-1}\right\|_{H^2}^{\frac{12}{6-N}} + \left\|\psi_A^{j-1}\right\|_{H^2}^2 + \left\|(n^+)_A^j\right\|_{H^2}^2\right.\\
&\qquad\left. + \left\|(n^-)_A^j\right\|_{H^2}^2\right]\left[\|\mathbf{e}^j\|^2 + \|(\eta^+)^j\|^2 + \|(\eta^-)^j\|^2\right]\\
&+ kC_1 \sum_{j=1}^{\ell}\left[\|(\eta^+)^{j-1}\|^2 + \|(\eta^-)^{j-1}\|^2\right]\|\mathbf{e}^j\|^2 + \frac{1}{2}\left[\|\mathbf{e}^0\|^2 + \|(\eta^+)^0\|^2 + \|(\eta^-)^0\|^2\right]\\
&+ kC_1 \sum_{j=1}^{\ell}\left[\|(\eta^+)^j\|^{\frac{6-N}{6}} + \|(\eta^-)^j\|^{\frac{6-N}{6}}\right]\left[\|(\eta^+)^j\|^2 + \|(\eta^-)^j\|^2\right]\\
&\le k^2C_1^2 + C_1^2 t_\ell k^2 \exp(C_2 t_\ell) + kC_1^2 \sum_{j=1}^{\ell}\left[\|\mathbf{e}^j\|^2 + \|(\eta^+)^j\|^2 + \|(\eta^-)^j\|^2\right]\\
&+ kC_1^2 k^2 \exp(C_2 t_\ell)\sum_{j=1}^{\ell}\|\mathbf{e}^j\|^2 + 2k\left[C_1^2 t_\ell k^2 \exp(C_2 t_\ell)\right]^{\frac{12}{6-N}}\sum_{j=1}^{\ell}\left[\|(\eta^+)^j\|^2 + \|(\eta^-)^j\|^2\right]\\
&\quad + \frac{1}{2}\left[\|\mathbf{e}^0\|^2 + \|(\eta^+)^0\|^2 + \|(\eta^-)^0\|^2\right],
\end{aligned}$$

which results with Gronwall's inequality and $\mathbf{e}^0 = \mathbf{0}$, $(\eta^\pm)^0 = 0$ to

$$\left(\frac{1}{2} - C_2 k\right)\left[\left\|\mathbf{e}^\ell\right\|^2 + \left\|(\eta^+)^\ell\right\|^2 + \left\|(\eta^-)^\ell\right\|^2\right] \le C_1 k^2 \exp\left(5\left[k^2 C_1^2 t_\ell \exp(C_2 t_\ell)\right]^5\right). \tag{5.5.35}$$

Hence, for $k \le k_0(C_1, C_2, \Omega_T)$ small enough, we have for all $0 \le \ell \le J$

$$5\left[C_1 k^2 \exp(C_2 t_J)\right]^5 \le C_2 .$$

Therefore, the right hand side in (5.5.35) becomes $C_1 k^2 \exp(C_2 t_\ell)$ and the induction is verified.
□

Remark 5.5.5. This inductive argument corresponds to the one in Step 2 of the proof of Theorem 5.3.3 to compensate for the lack of a discrete energy law. In contrast, the present argument here relies on the higher regularity given by strong solutions of the system (5.1.1)–(5.1.10).

The error estimates for Problem C concern only errors occurring due to Chorin's projection scheme for which results are given in Lemma 5.5.1. Since $\mathbf{f}_C \in C([0,T]; L^2(\Omega, \mathbb{R}^N))$, we immediately obtain with Lemma 5.5.1 the

Lemma 5.5.6. (Problem C) *The solution to Problem C satisfies the properties* $(P1)$ *and* $(P2)_1$*, provided time-steps* $k \leq k_0(t_J)$ *are chosen sufficiently small.*

The last step to complete the error analysis of Scheme B is

Lemma 5.5.7. (Problem D) *The solution to Problem D satisfies the properties* $(P1)$ *and* $(P2)_1$*, provided time-steps* $k \leq k_0(t_J)$ *are chosen sufficiently small.*

Proof. This proof is now done in more details. We introduce the shorthand notations

$$\mathbf{e}^j := \mathbf{u}_C^j - \mathbf{u}_D^j\,, \qquad \pi^j := p_C^j - p_D^j\,, \tag{5.5.36}$$

$$(\eta^{\pm})^j := (n^{\pm})_C^j - (n^{\pm})_D^j\,, \qquad \zeta^j := \psi_C^j - \psi_D^j\,, \tag{5.5.37}$$

which induce the following error equations

$$d_t\mathbf{e}^j - \Delta\mathbf{e}^j + \nabla\pi^{j-1} = \big((\eta^+)^j - (\eta^-)^j\big)\nabla\psi_C^{j-1} - \big((n^+)_D^j - (n^-)_D^j\big)\nabla\zeta^{j-1}\,, \tag{5.5.38}$$

$$\operatorname{div}\mathbf{e}^j - k\Delta\pi^j = 0\,, \tag{5.5.39}$$

$$\partial_{\mathbf{n}}\pi^j|_{\partial\Omega} = 0\,, \tag{5.5.40}$$

$$d_t(\eta^{\pm})^j - \Delta(\eta^{\pm})^j \mp \operatorname{div}\big((\eta^{\pm})^j\nabla\psi_C^{j-1}\big) \mp \operatorname{div}\big((n^{\pm})_D^j\nabla\zeta^{j-1}\big) = 0\,, \tag{5.5.41}$$

$$-\Delta\zeta^{j-1} = (\eta^+)^{j-1} - (\eta^-)^{j-1}\,. \tag{5.5.42}$$

Step 1: ($\mathbf{e}^j$ and $(\eta^{\pm})^j$ satisfy $(P2)_1$) We test 5.5.38) with $\mathbf{e}^j$, and the corresponding pressure equation (5.5.39) with π^j. The following two properties,

$$2(a-b,a) = |a|^2 - |b|^2 + |b-a|^2 \tag{5.5.43}$$

and

$$\begin{aligned} k(\nabla\pi^{j-1}, \nabla\pi^j) &= k\|\nabla\pi^j\|^2 - k^2(\nabla\pi^j, \nabla \mathrm{d}_t\pi^j) \\ &= k\|\nabla\pi^j\|^2 - k(\mathrm{d}_t\mathbf{e}^j, \nabla\pi^j) \\ &\geq \frac{k}{2}\big\{\|\nabla\pi^j\|^2 - \|\mathrm{d}_t\mathbf{e}^j\|^2\big\}\,, \end{aligned} \tag{5.5.44}$$

provide by repeating the techniques from Lemma 5.5.3 and 5.5.4 the estimate

$$\frac{1}{2}d_t\|\mathbf{e}^j\|^2 + \frac{1}{2}\|\nabla\mathbf{e}^j\|^2 + \frac{k}{2}\|\nabla\pi^j\|^2 \leq \text{(I)} + \text{(II)} \tag{5.5.45}$$

whith the right hand sides

$$\begin{aligned} \text{(I)} &:= \Big|\Big(\big\{(\eta^+)^j - (\eta^-)^j\big\}\nabla\psi_C^{j-1}, \mathbf{e}^j\Big)\Big| \leq C\left[\Big\|(n^+)_C^{j-1}\Big\|^2 + \Big\|(n^-)_C^{j-1}\Big\|^2\right]\|\mathbf{e}^j\|^2 \\ &\quad + \frac{1}{8}\left[\big\|(\eta^+)^j\big\|^2 + \big\|(\eta^-)^j\big\|^2 + \big\|\nabla(\eta^+)^j\big\|^2 + \big\|\nabla(\eta^-)^j\big\|^2\right] \\ \text{(II)} &:= \Big|\Big(\Big\{(n^+)_C^j - (\eta^+)^j - (n^-)_C^j + (\eta^-)^j\Big\}\nabla\zeta^{j-1}, \mathbf{e}^j\Big)\Big|\,. \end{aligned}$$

Similarly, we obtain by testing (5.5.41) with $(\eta^{\pm})^j$ the inequality

$$\frac{1}{2}d_t\|(\eta^{\pm})^j\|^2 + \frac{k}{2}\|d_t(\eta^{\pm})^j\|^2 + \frac{1}{2}\|\nabla(\eta^{\pm})^j\|^2 \leq \text{(I)} + \text{(II)} \tag{5.5.46}$$

where

$$\begin{aligned}
\text{(I)} &:= \Big|\Big((\eta^{\pm})^j \nabla\psi_C^{j-1}, \nabla(\eta^{\pm})^j\Big)\Big| \leq C\left[\left\|(n^+)_C^{j-1}\right\|^2 + \left\|(n^-)_C^{j-1}\right\|^2\right] \|\nabla(\eta^{\pm})^j\|^2 + \frac{1}{8}\left\|(\eta^{\pm})^j\right\|_{L^3}^2 \\
&\leq \left[\left\|(n^+)_C^{j-1}\right\|^2 + \left\|(n^-)_C^{j-1}\right\|^2\right] \|\nabla(\eta^{\pm})^j\|^2 + \frac{1}{8}\left[\|(\eta^{\pm})^j\|^2 + \|\nabla(\eta^{\pm})^j\|^2\right] \\
\text{(II)} &:= \Big|\Big(\Big\{(n^+)_C^j - (\eta^+)^j - (n^-)_C^j + (\eta^-)^j\Big\} \nabla\zeta^{j-1}, \nabla(\eta^{\pm})^j\Big)\Big| \,.
\end{aligned}$$

The term (II) in (5.5.45) may now be bounded as the term (III) in (5.5.33) for the lower index A instead of C and also the term (II) in (5.5.46) corresponds to the term (III) in (5.5.32), and we can repeat the same inductive argument as in Lemma 5.5.4.

Step 2: (π^j enjoys property $(P2)_1$) The Step 1 and equation (5.5.12) enable the estimate

$$k\|\nabla\pi^j\| \leq \|\mathbf{e}^j\| \leq Ck\,, \tag{5.5.47}$$

and since $\pi^j = p_C^j - p_D^j$ and correspondingly for $(\eta^{\pm})^j$ and ζ^j controlled by (5.5.46), we obtain

$$\max_{0\leq j\leq J} \|\nabla p_D^{j-1}\|^2 + \|\nabla(n^{\pm})^{j-1}\|^2 + \|\psi_D^{j-1}\|_{H^2}^2 \leq C\,. \tag{5.5.48}$$

Hence, from equations (5.5.11), (5.5.48) and (5.5.45) we get further a priori bounds of the form

$$k\sum_{j=0}^{J}\big\{\|\Delta\mathbf{u}_D^j\|^2 + \|\mathrm{d}_t\mathbf{u}_D^j\|^2\big\} \leq C\,. \tag{5.5.49}$$

The error bound on the pressure function, as it is given in $(P2)_1$, we achieve by the estimate

(5.5.50)

$$\begin{aligned}
\|\pi^{j-1}\|_{H^{-1}} \leq \sup_{\chi\in H_0^1\cap H^2} \Bigg\{ \frac{1}{\|\chi\|_{H^2}} \bigg[\Big|\Big(d_t\mathbf{e}^j, \chi\Big)\Big| + \Big|\Big(\mathbf{e}^j, \Delta\chi\Big)\Big| \\
+ \Big|\Big(((\eta^+)^{j-1} - (\eta^-)^{j-1})\nabla\psi_C^{j-1}, \chi\Big)\Big| + \Big|\Big(((n^+)_C^{j-1} - (n^-)_C^{j-1})\nabla\zeta^{j-1}, \chi\Big)\Big| \bigg] \Bigg\}.
\end{aligned}$$

Then (5.5.45), (5.5.49), and Lemma 5.5.6 allow to control the right hand side of (5.5.50) in the following way

$$\begin{aligned}
&\leq C\Big\{\|d_t\mathbf{e}^j\| + \|\mathbf{e}^j\| + \Big[\|(\eta^+)^{j-1}\| + \|(\eta^-)^{j-1}\|\Big]\Big\}\|\nabla\psi_C^{j-1}\| \\
&\qquad + \Big[\|(n^+)_C^{j-1}\| + \|(n^-)_C^{j-1}\|\Big]\|\nabla\zeta^{j-1}\| \leq C\Big\{k + \|d_t\mathbf{e}^j\|\Big\}\,.
\end{aligned} \tag{5.5.51}$$

Hence, it leaves to control $\sum_{j=1}^{J}\|d_t\mathbf{e}^j\|^2$. For this purpose, we test () with $d_t\mathbf{e}^j$. First, observe the identity

$$\begin{aligned}
\Big(\nabla\pi^{j-1}, d_t\mathbf{e}^j\Big) &= k\Big(\nabla d_t\pi^j, \nabla\pi^{j-1}\Big) = -\frac{1}{2}\Big(\|\nabla\pi^{j-1}\|^2 - \|\nabla\pi^j\|^2 + \|\nabla\pi^j - \nabla\pi^{j-1}\|^2\Big) \\
&= \frac{k}{2}\Big\{d_t\|\nabla\pi^j\|^2 - k\|\nabla d_t\pi^j\|^2\Big\} \geq \frac{k}{2}d_t\|\nabla\pi^j\|^2 - \frac{1}{2}\|d_t\mathbf{e}^j\|^2\,,
\end{aligned} \tag{5.5.52}$$

where we used the equation (5.5.39), the identity (5.5.43) and in the last line again (5.5.39) tested with $\nabla d_t \pi^j$. Now, we test equation (5.5.38) with $d_t \mathbf{e}^j$ that results in

$$
\begin{aligned}
&\frac{1}{2}\|d_t\mathbf{e}^j\|^2 + \frac{1}{2}d_t\|\nabla\mathbf{e}^j\|^2 + k\frac{2}{5}\|d_t\nabla\mathbf{e}^j\|^2 + \frac{k}{2}d_t\|\nabla\pi^j\|^2 \leq \\
&\quad + C\|\psi_C^{j-1}\|_{H^2}^2\Big(\|(\eta^+)^j\|_{H^1}^2 + \|(\eta^-)^j\|_{H^1}^2\Big) \\
&\quad + C\Big[\|(n^+)_D^j\|_{H^1}^2 + \|(n^-)_D^j\|_{H^1}\Big]\Big(\|(\eta^+)^{j-1}\|^2 + \|(\eta^-)^{j-1}\|^2\Big)\,.
\end{aligned} \tag{5.5.53}
$$

Define π^0 by continuation of (5.5.39) as a solution of

$$
-\Delta\pi^0 = 0 \qquad \text{on } \Omega\,, \qquad \partial_{\mathbf{n}}\pi^0 = 0 \qquad \text{on } \partial\Omega\,,
$$

and hence $\pi^0 = 0$. To complete, we also test (5.5.13) with $d_t(\eta^\pm)^j$. Then we add the resulting estimate up with (5.5.53) to apply Gronwall's inequality at the end. This provides after summation over $0 \leq j \leq J$ the error controls

$$
k\sum_{j=1}^{J}\Big\{\|d_t\mathbf{e}^j\|^2 + \|d_t(\eta^\pm)^j\|^2\Big\} + \Big\{\|\nabla\mathbf{e}^J\|^2 + \|\nabla(\eta^\pm)^J\|^2\Big\} + \frac{k}{2}\|\nabla\pi^J\|^2 \leq Ck^{\frac{3}{2}}\,. \tag{5.5.54}
$$

Step 3: (Further a priori bounds for (P1)) With the estimate (5.5.54) in Step 2 we obtain directly with the a priori results stated in Lemma 5.5.6 the bounds

$$
\max_{1\leq j\leq J}\Big\{\|d_t\mathbf{u}_D^j\| + \|d_t(n^\pm)_D^j\| + \|\nabla p_D^j\|\Big\} \leq C\,. \tag{5.5.55}
$$

The latter bound (5.5.55) together with (5.5.11), and (5.5.54) enable the estimate

$$
\begin{aligned}
\|\Delta\mathbf{u}_D^j\| \leq{}& \|d_t\mathbf{u}_D^j\| + \|\nabla p_D^{j-1}\| + C\|\nabla\mathbf{u}_D^j\|\|\mathbf{u}_D^{j-1}\| \\
&+ \Big[\|(n^+)_D^j\|_{L^2} + \|(n^-)_D^j\|_{L^2}\Big]\|\psi_D^{j-1}\|_{H^1}\,.
\end{aligned}
$$

In the same way we can control $\Delta(n^\pm)_D^j$, such that we end up with

$$
\max_{0\leq j\leq J}\Big\{\|\mathbf{u}_D^j\|_{H^2} + \|(n^\pm)_D^j\|_{H^2}\Big\} \leq C\,.
$$

Step 4: (Optimal pressure bounds) Therefore we first apply d_t to (5.5.38) and then test the resulting equation with $\tau_j d_t e^j$, i.e.,

$$
\frac{1}{2}\tau_j d_t\|d_t\mathbf{e}^j\|^2 + \tau_j\|d_t\nabla\mathbf{e}^j\|^2 + k\tau_j\|d_t\nabla\pi^j\|^2 \leq \Big|F1 + F2\Big|\,, \tag{5.5.56}
$$

where we use the identity

$$
\begin{aligned}
\tau_j\Big(d_t\nabla\pi^j, d_t\mathbf{e}^j\Big) &= \frac{\tau_j}{k}\Big\{\Big(\nabla\pi^j, d_t\mathbf{e}^j\Big) - \Big(\nabla\pi^{j-1}, d_t\mathbf{e}^j\Big)\Big\} \\
&= \frac{\tau_j}{k}\Big\{k\Big(d_t\nabla\pi^j, \nabla\pi^j\Big) - k\Big(d_t\nabla\pi^j, \nabla\pi^{j-1}\Big)\Big\} = k\tau_j\|d_t\nabla\pi^j\|^2\,,
\end{aligned}
$$

which is obtained by testing equation (5.5.39) with $d_t\pi^j$. In the following, we control the nonlinear terms on the right hand side of (5.5.56). The two last terms originating from the

Coulomb force are again controlled by the same Hölder inequality, i.e.,

$$\begin{aligned}\Big|F1+F2\Big| &:= \Big|\Big(d_t\big((\eta^+)^j-(\eta^-)^j\big)\nabla\psi_C^{j-1},\tau_j d_t\mathbf{e}^j\Big)+\Big(\big((\eta^+)^{j-1}-(\eta^-)^{j-1}\big)\nabla d_t\psi_C^{j-1},\tau_j d_t\mathbf{e}^j\Big)\\ &\quad \Big(d_t\big((n^+)^j_C-(n^-)^j_C\big)\nabla\zeta^{j-1},\tau_j d_t\mathbf{e}^j\Big)+\Big(\big((n^+)^{j-1}_C-(n^-)^{j-1}_C\big)\nabla d_t\zeta^{j-1},\tau_j d_t\mathbf{e}^j\Big)\Big|\\ &\le C\tau_j\Big\{\|\psi_C^{j-1}\|^2_{H^2}\|d_t\mathbf{e}^j\|^2+\|\nabla d_t\psi_C^{j-1}\|^2\Big[\|(\eta^+)^{j-1}\|^2_{H^1}+\|(\eta^-)^{j-1}\|^2_{H^1}\Big]\Big\}\\ &\quad+\frac{1}{5}\tau_j\Big\{\|d_t(\eta^+)^j\|^2_{H^1}+\|d_t(\eta^-)^j\|^2_{H^1}+\|d_t\mathbf{e}^j\|^2+\|\nabla d_t\mathbf{e}^j\|^2\Big\}\\ &\quad+C\tau_j\Big\{\Big[\|d_t(n^+)^j_C\|^2_{H^1}+\|d_t(n^-)^j_C\|^2_{H^2}\Big]\|\zeta^{j-1}\|^2_{H^2}\\ &\qquad+\Big[\|(n^+)^{j-1}_C\|^2_{H^2}+\|(n^-)^{j-1}_C\|^2_{H^2}\Big]\|\nabla d_t\zeta^{j-1}\|^2\Big\}+\frac{1}{5}\tau_j\|\nabla d_t\mathbf{e}^j\|^2\,.\end{aligned}$$

In the same way we control $\tau_j\|d_t(\eta^{\pm})^j\|$ and sum up the resulting estimate with (5.5.56) to obtain with Gronwall's inequality the required pressure bound.

Still we have to establish the a priori bounds $k\sum_{j=1}^J\|d_t\xi_i^j\|^2\le C$, $i\in\{1,3,4\}$. But since the arguments correspond to the verification of (5.5.56) by omitting time-weights, we skip the elaboration of this argument. □

5.5.4 Spatial Discretization of Scheme B, Corollary 5.3.8

We first reformulate the Scheme B for $(\mathbf{v}^j,q^j,(\phi^{\pm})^j,(\psi)^j)\in H^1_0(\Omega,\mathbb{R}^N)\times\big[H^1(\Omega)\cap L^2_0(\Omega)\big]\times[H^1(\Omega)]^2\times H^2(\Omega)$ for the purely temporal discretization in the context of strong solutions as

$$\begin{aligned}&\Big(\mathrm{d}_t\mathbf{u}^j,\mathbf{v}\Big)+\Big(\nabla\mathbf{u}^j,\nabla\mathbf{v}\Big)+\Big((\mathbf{u}^{j-1}\cdot\nabla)\mathbf{u}^j,\mathbf{v}\Big)+\frac{1}{2}\Big((\operatorname{div}\mathbf{u}^{j-1})\mathbf{u}^j,\mathbf{v}\Big)\\ &\qquad-\Big(p^j,\operatorname{div}\mathbf{v}\Big)=-\Big(\big((n^+)^j-(n^-)^j\big)\nabla\psi^{j-1},\mathbf{v}\Big),\\ &\Big(\operatorname{div}\mathbf{u}^j,\,q\Big)+k\Big(\nabla p^j,\nabla q\Big)=0\,,\\ &\Big(\mathrm{d}_t(n^{\pm})^j,\phi^{\pm}\Big)+\Big(\nabla(n^{\pm})^j,\nabla\phi^{\pm}\Big)\pm\Big((n^{\pm})^j\nabla\psi^{j-1},\nabla\phi^{\pm}\Big)-\Big(\mathbf{u}^{j-1}(n^{\pm})^j,\nabla\phi^{\pm}\Big)=0\,,\\ &\Big(\nabla\psi^{j-1},\nabla\phi\Big)=\Big(n^+)^{j-1}-(n^-)^{j-1},\phi\Big)\,,\end{aligned}$$

from which we subtract the conforming finite element version of Scheme B for

$$(\mathbf{V},Q,\Phi^{\pm},\Phi)\in\mathbf{V}_h\times M_h\times[Y_h]^3$$

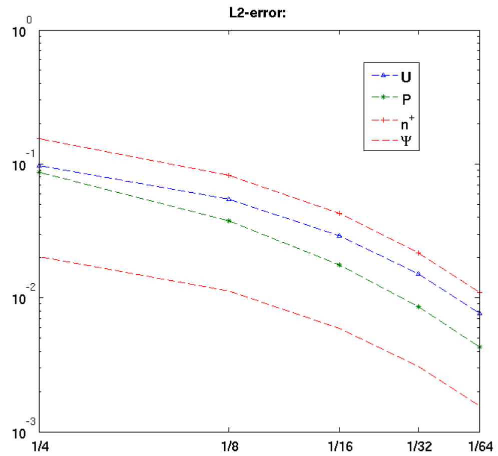
rewritten as

(5.5.57)

$$\begin{aligned}&\Big(\mathrm{d}_t\mathbf{U}^j,\mathbf{V}\Big)+\Big(\nabla\mathbf{U}^j,\nabla\mathbf{V}\Big)+\Big((\mathbf{U}^{j-1}\cdot\nabla)\mathbf{U}^j,\mathbf{V}\Big)+\frac{1}{2}\Big((\operatorname{div}\mathbf{U}^{j-1})\mathbf{U}^j,\mathbf{V}\Big)\\ &\qquad-\Big(\Pi^j,\operatorname{div}\mathbf{V}\Big)=-\Big(\big((N^+)^j-(N^-)^j\big)\nabla\Psi^{j-1},\mathbf{V}\Big),\\ &\Big(\operatorname{div}\mathbf{U}^j,\,Q\Big)+k\Big(\nabla\Pi^j,\nabla Q\Big)=0\,,\\ &\Big(d_t(N^{\pm})^j,\Phi^{\pm}\Big)+\Big(\nabla(N^{\pm})^j,\nabla\Phi^{\pm}\Big)\pm\Big((N^{\pm})^j\nabla\Psi^{j-1},\nabla\Phi^{\pm}\Big)-\Big(\mathbf{U}^{j-1}(N^{\pm})^j,\nabla\Phi^{\pm}\Big)=0\,,\\ &\Big(\nabla\Psi^{j-1},\nabla\Phi\Big)=\Big(\big((N^+)^{j-1}-(N^-)^{j-1}\big),\Phi\Big)\,.\end{aligned}$$

The result then follows from standard error estimates that base on corresponding stability arguments as provided in the proof of Lemma 5.5.7.

Remark 5.5.8. The finite element spaces chosen in the above space discretization (5.5.57) of Scheme B does not have to satisfy the compatibility condition (5.2.6) as for Scheme A.



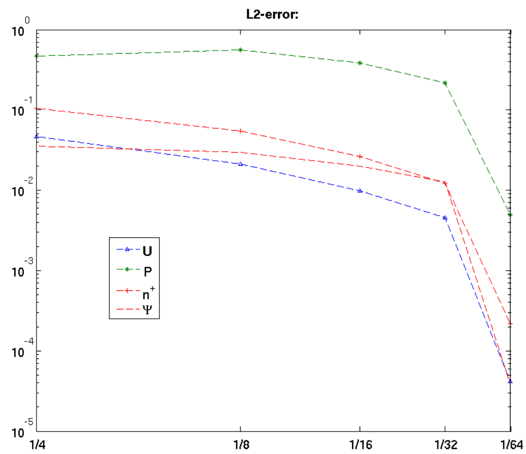


Figure 5.6.1: L^2**-Convergence:** Scheme A (left) and Scheme B (right) for different mesh sizes.

5.6 Computational Studies

The Section 5.6.1 studies the convergence behavior of the two Schemes A and B. In the next four sections, we relax step by step the academic assumptions to be able to distinguish the effects originating by the system itself from the external ones which we pose by boundary conditions. These steps allow us to recover the pure influence of the quasi-electrostatic forces as a driving force to the fluid. The computational demand of the fixed point iterations used in the Algorithm A_1 is for the Examples 1 and 2 at most three iterations, and for the Examples 3 and 5 up to six iterations. The comparison of Algorithm A_1 with Scheme B indicates through all computations that the time-splitting Scheme B requires only half of the computational time than Algorithm A_1. Especially, if small time scales are needed to obtain more accurate results, then the fixed point iterations consume a significant amount of CPU-time. Therefore, it is reasonable to only use Scheme A_1, if physical relevant properties such as non-negativity, discrete maximum principle, energy and entropy characterizations have necessarily to be preserved.

5.6.1 L^2-Convergence

The L^2-convergence behavior of iterates belonging to the Schemes A and B is studied in this section. Let $\Omega = [0,1]^2$. We consider the exact solutions

$$u_1(x,y,t) = -t\cos(\pi x)\sin(\pi y)\,, \qquad u_2(x,y,t) = t\sin(\pi x)\cos(\pi y) \tag{5.6.1}$$

$$p(x,y,t) = -\frac{1}{4}\Big(\cos(2\pi x) + \cos(2\pi y)\Big) \tag{5.6.2}$$

$$\psi(x,y,t) = \frac{t}{\pi^2}\Big(\cos(\pi x) - \sin(\pi y)\Big) \tag{5.6.3}$$

$$n^+(x,y,t) = t\cos(\pi x)\,, \qquad n^-(x,y,t) = t\sin(\pi y) \tag{5.6.4}$$

for the system (5.1.1)–(5.1.10). The convergence results for the time discretization $k = 0.001$ and the space discretizations $h = 0.25, 0.125, 0.0625, 0.03125, 0.0156$ are shown by a double logarithmic plot in Figure 5.6.1. The snapshot on the right hand side of Figure 5.6.1 indicates that the asymptotic regime is reached for a mesh-size smaller than $h = 0.0312$.

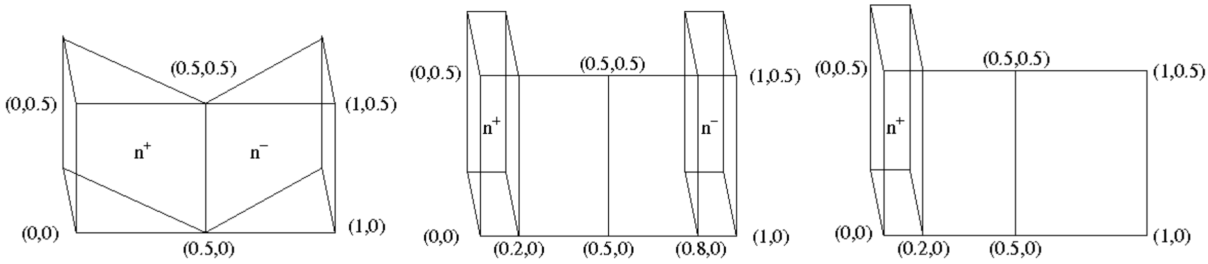


Figure 5.6.2: **Domain Geometries and Initial Configurations** of the positive and negative charges for the Academic Example 1 (left), Example 2 (middle), and Example 3 and 4 (right).

5.6.2 Academic Example 1

The only driving force originates from the initial concentrations of positive n^+ and negative n^- charges for which the initial configuration is depicted in Figure 5.6.2. In applications, the concentration differences originate between the interface of the electrolyte and the solid surfaces. The atomic structure of the solid induces counter ions stemming from the electrolyte on the solid surface. This movement of the ions around the solid particle is called electroosmosis. Hence we consider the system (5.1.1)–(5.1.10) for the initial data

$$\begin{aligned} u_1(x,y,0) &= 0\,, \qquad u_2(x,y,0) = 0\,, \\ n^+(x,y,0) &= \begin{cases} 1-2x & \text{if } 0 \le x \le 0.5\,, \\ 0 & \text{else}\,, \end{cases} \qquad n^-(x,y,0) = \begin{cases} 0 & \text{if } 0 \le x \le 0.5\,, \\ 2(x-0.5) & \text{else}\,, \end{cases} \end{aligned}$$

and vanishing Neumann boundary conditions as required in Definition 5.3.1. Such assumptions for Scheme A and B result in the energy and entropy behavior plotted in Figure 5.6.3, where

$$H_\delta[P,N] := \int_\Omega F_\delta(P) + F_\delta(N)\ d\mathbf{x}\,,$$

for $F_\delta(x) := x\,\log(x+\delta)$ and $\delta \ge 0$. In the Examples 2, 3 and 4, we use $\delta = 0,00001$. The characteristic plots of both, energy and entropy show an asymptotic ($t \to \infty$) exponential decay of almost the same rate. Moreover, the entropy curve shows that the system is mainly active in the first 0.3 seconds. We choose $h = 0.0312$, $k = 0.0015$ on the time interval $[0, 0.3]$. Some snapshots for the velocity $\mathbf{U}^j$, the positive concentration P^j and the pressure Π^j of Example 2 are given in Figure 5.6.7.

5.6.3 Academic Example 2

We investigate the influence of L^∞-initial data. More precisely, the only difference to the Example 1 is that we change initial concentrations presented on the left hand side of Figure 5.6.2 to the situation depicted in the middle. One recognizes slightly smaller values of the energy for the Schemes A and B in Figure 5.6.4. Such a behavior seems to arise because of the smaller mass $M^+ := \|n^+\|_{L^1}$ in Example 2 where $M^+ = 0.1$ compared to $M^+ = 0.375$ in Example 1. Conversely, the entropy is larger for rough initial data for both Schemes A and B. Here, the entropy functional is regularized for $\delta = 0.0001$.
In Figure 5.6.7, we provide some snapshots for the most interesting values obtained for the mesh parameters $h = 0.0312$, $k = 0.00015$ on a time interval $[0, 0.3]$.

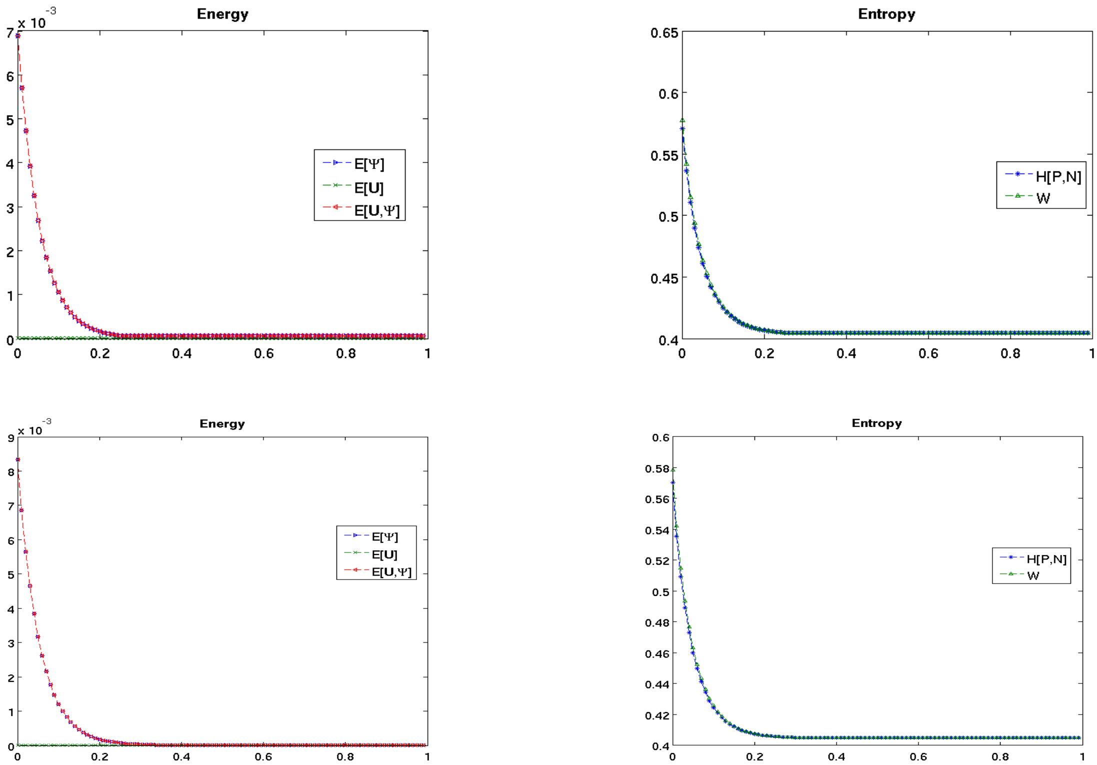


Figure 5.6.3: **Example 1:** 1st line: Energy (left) and Entropy (right) for the Scheme A ($h = 0.03125$, $k = 0.01$). 2nd line: corresponding results for Scheme B.

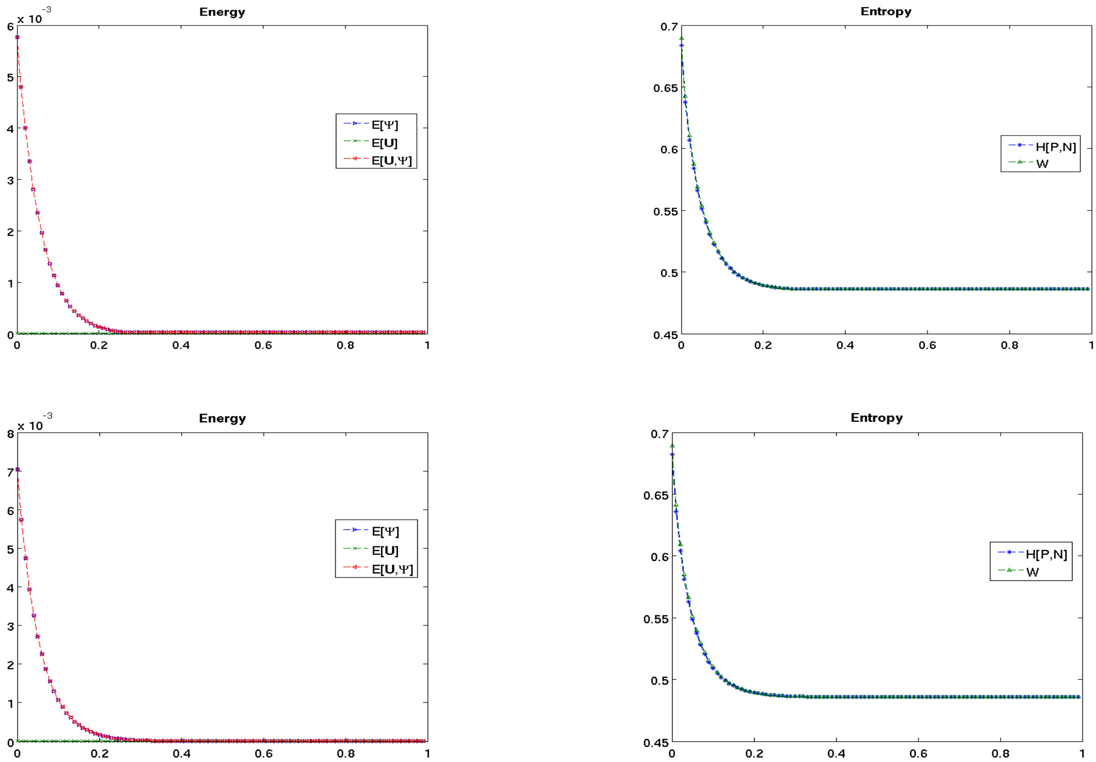


Figure 5.6.4: **Example 2:** 1st line: energy (left) and entropy (right) for the Scheme A and $h = 0.03125$, $k = 0.01$. 2nd line: represents corresponding results for Scheme B in the same order.

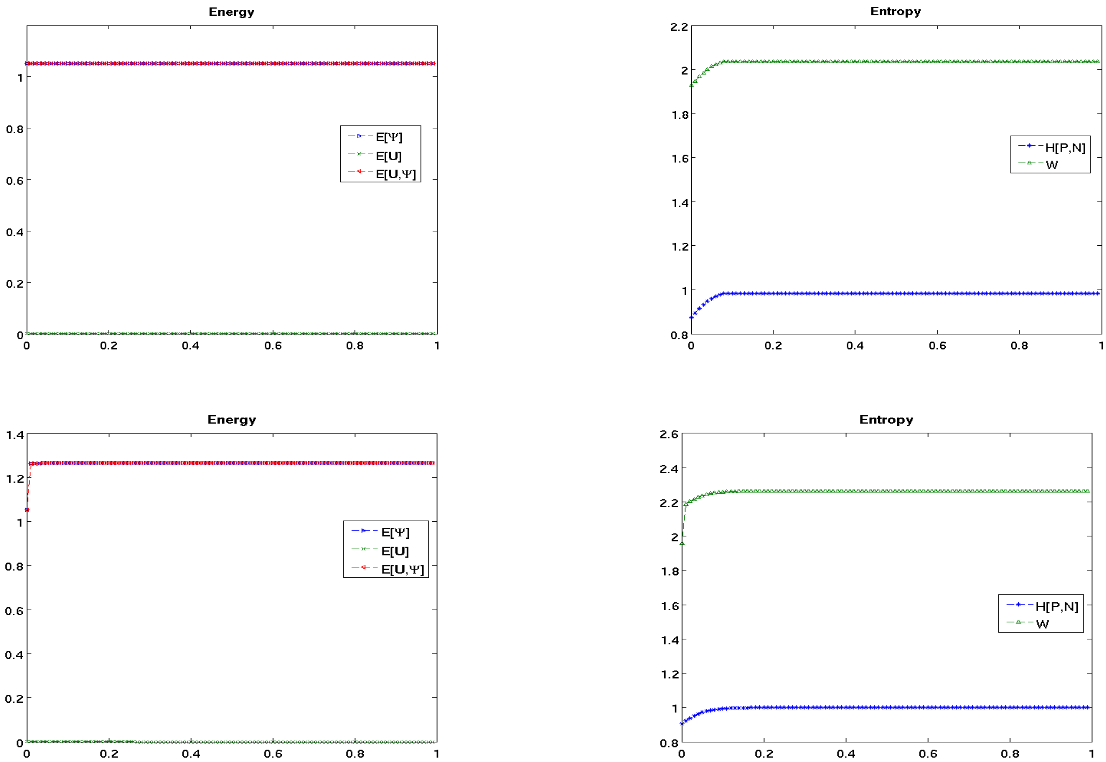


Figure 5.6.5: **Example 3:** 1st line: energy (left) and entropy (right) computed for $h = 0.03125$, $k = 0.01$, and $\delta = 0.00001$ for Scheme A. 2nd line: corresponding values for Scheme B.

5.6.4 Academic Example 3

We neglect the negative concentrations by setting $n_0^- \equiv 0$. In order not to be inconsistent with the given vanishing Neumann boundary conditions for ψ, we change them below. Such a configuration is motivated to recover the pure influence of an external electrical field as driving force. For such a situation, the existence of contrary charged species would unnecessarily disturb our configuration with compensating effects. Hence, in difference to Example 2, we consider the initial concentration of positively charged species as depicted in Figure 5.6.2 on one hand, and on the other hand we set for the electrical potential the Dirichlet boundary conditions

$$\psi(x,y,t) = \begin{cases} 1 & \text{for } (x,y) \in \{0\} \times [0,0.5] \\ 0 & \text{for } (x,y) \in \{1\} \times [0,0.5] \end{cases}, \tag{5.6.5}$$

and for the remaining part of the boundary we set $\partial_{\mathbf{n}}\psi = 0$.
As in the examples before, we compute the energy and the entropy for the rather coarse mesh parameters $k = 0.01$ and $h = 0.0312$. Again, we regularize the entropy functional by the parameter $\delta = 0.00001$. The resulting screenshots are given in Figure 5.6.5. The influence of the new boundary conditions acting as external forces results in non-dissipative energy and entropy values.

5.6.5 Academic Example 4

Conversely to Example 3, the channel is already streamed by a certain fluid. Hence we are interested in how a previously defined amount of positively charged species n^+ with an initial

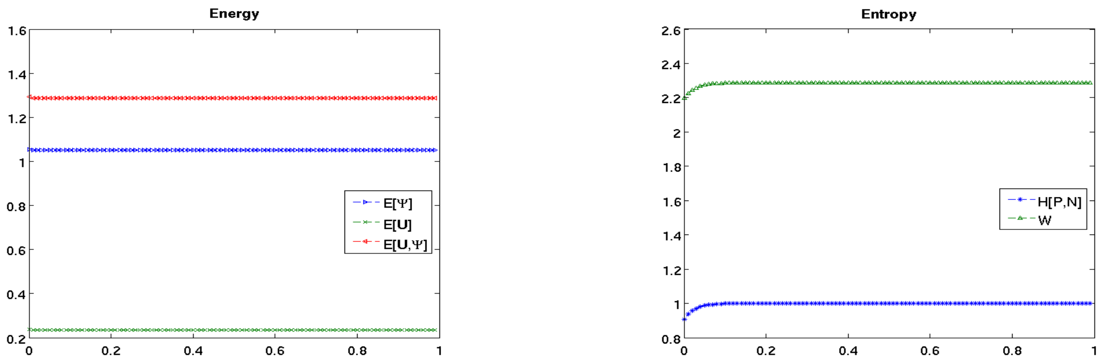


Figure 5.6.6: **Example 4:** The energy (left) and entropy (right) computed for $h = 0.03125$, $k = 0.01$ and $\delta = 0.00001$. In this example we obtain corresponding results for Scheme A and B.

rectangular geometry given by the right picture in Figure 5.6.2 evolves starting from the right hand side of the channel. Therefore, the fluid velocity satisfies the initial conditions

$$u_1(x,y,0) = 1 \quad \text{on } \Omega \setminus \Big\{\{0\}\times[0,1]\cup\{1\}\times[0,1]\Big\}, \tag{5.6.6}$$

$$u_2(x,y,0) = 0 \quad \text{on } \Omega, \tag{5.6.7}$$

and the boundary conditions

$$u_1(x,y,t) = \begin{cases} 1 & \text{for } (x,y)\in\{0\}\times(0,0.5)\cup\{1\}\times(0,0.5), \\ 0 & \text{else} \end{cases}, \tag{5.6.8}$$

$$u_2(x,y,t) = 0 \quad \text{on } \partial\Omega. \tag{5.6.9}$$

Again, we compute the energy and entropy for the rough mesh parameters $k = 0.01$ and $h = 0.0312$. Further we regularize the logarithms in the entropy with $\delta = 0.00001$. The plots are given in Figure 5.6.6. If compared to Example 3, the resulting energy and entropy values are higher, as expected due to the strong influence of the constant streaming fluid. Hence the energy $E(\mathbf{U}^j)$ is now remarkably away from zero. An interesting consequence of the streaming fluid is that the energy density of the electric field $E(\Psi^j)$ decreases in such a way that the total energy $E(\mathbf{U},\Psi)$ remains on the same value as in Example 3.

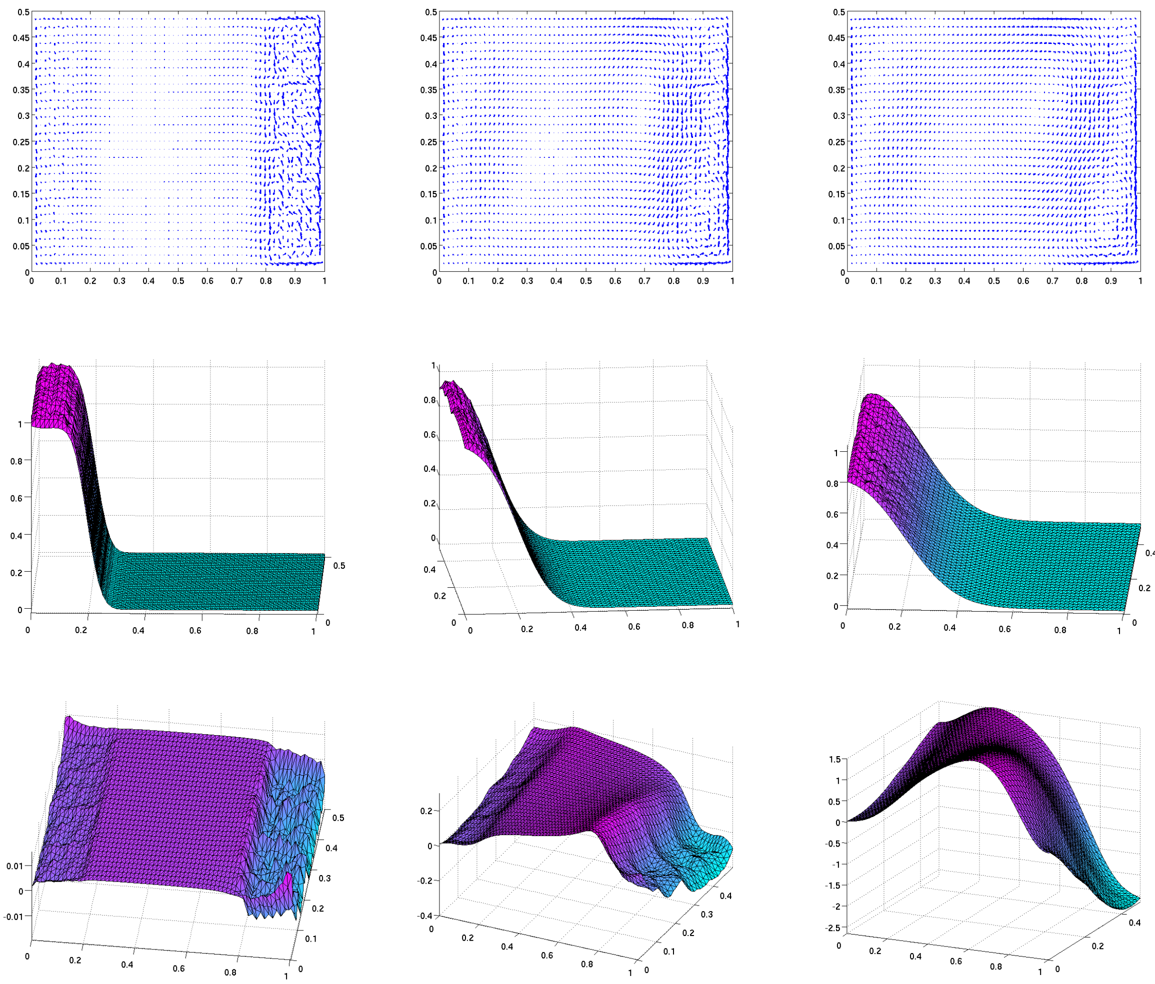


Figure 5.6.7: **Snapshots for Example 2:** 1st line: fluid velocities $\mathbf{U}^j$ for the times $t_{30} = 0.005$, $t_{200} = 0.03$, $t_{450} = 0.07$. 2nd line: corresponding concentration $(N^+)^j$. 3rd line: pressure Π^j for time steps $t_1 = 0.0002$, $t_{30} = 0.005$, $t_{450} = 0.07$. Moreover, Π^1 shows a shock whose size depends on the temporal discretization k. This shock is a result of the switch-on character of Example 2. The pictures for Scheme A and B are similar. ($h = 0.0312$, $k = 0.00015$)

Bibliography

[1] R. A. Adams, J. J. F. Fournier, Sobolev Spaces, Elsevier, 2003.

[2] P.M. Adler, *Porous Media: Geometry and Transports*, Boston: Butterworth-Heinemann, 1992.

[3] A.M. Anile, N. Nikiforakis, V. Romano, G. Russo, *Discretization of semiconductor device problems. II. Handbook of numerical analysis. Vol. XIII*, Handb. Numer. Anal. **XIII**, pp. 443–522 (2005).

[4] D.N. Arnold, F. Brezzi, M. Fortin, *A stable finite element for the Stokes equations*, Calcolo **23**, pp. 337–344, (1984).

[5] A. Arnold, P. Markowich, G. Toscani, *On large time asymptotics for drift-diffusion Poisson systems*, Transp. Theory Statist. Phys. **291**, pp. 571–581 (2000).

[6] J.W. Barrett, J.F. Blowey, *Finite element approximation of a nonlinear cross-diffusion population model*, Numer. Math. **98**, pp. 195–221 (2004).

[7] J.W. Barrett, R. Nürnberg, *Finite-element approximation of a nonlinear degenerate parabolic system describing bacterial pattern formation*, Interfaces Free Boundaries **4**, pp. 277–307 (2002).

[8] G.K. Batchelor, *An Introduction to Fluid Dynamics*, Cambr. Univ. Press., 1967.

[9] M.Z. Bazant, K. Thornton, A. Adjari, Phys. Rev. E, **70**, 021506, (2004).

[10] Balbuena, P.B, and Wang, Y., *LITHIUM-ION BATTERIES, Solid-Electrolyte Interphase*, Imperial Collage Press, 2004.

[11] Bazant, M. Z., Thornton, K., and Ajdari, A., *Diffuse-charge dynamics in electrochemical systems*, Phys Rev E, **70**, 2004.

[12] Biler, P., and Brandolese, L., *Global Existence versus blow up for some models of interacting particles*, Colloq. Math. (to appear).

[13] P. Biler, J. Dolbeault, *Long time behavior of solutions to Nernst-Planck and Debye-Hückel drift-diffusion systems*, Ann. Henri Poincare **1**, pp. 461–472 (2000).

[14] P. Biler, W. Hebisch, T. Nadzieja, *The Debye system: existence and large time behaviour of solutions*, Nonl. Anal., Theory, Meht. & Applications **23**, pp. 1189–1209 (1994).

[15] Blanchet, A., Dolbeault, J., Perthame, B., *Two-Dimensional Keller-Segel Model: Optimal Critical Mass and Qualitative Properties of the Solutions*, EJDE, **44**, 1-33, 2006.

[16] S.C. Brenner, L. Scott, *The Mathematical Theory of Finite Element Methods*, 2nd ed. 2002.

[17] F. Brezzi, L. Marini, S. Micheletti, P. Pietra, R. Sacco, S. Wang, *Discretization of semiconductor device problems. I. Handbook of numerical analysis. Vol. XIII*, Handb. Numer. Anal. **XIII**, pp. 317–441 (2005).

[18] Castellanos, A., *Electrohydrodynamics*, Springer, 1998.

[19] Castellanos, A., Ramos, A., Gonzalez, A., Green, N.G., and Morgan, H., *Electrohydrodynamics and dielectrophoresis in microsystems: scaling laws*, J. Phys. D: Appl. Phys., **36**, 2584-2597, 2003.

[20] C. Chainais-Hillairet, F. Filbet, *Asymptotic behavior of a finite volume scheme for the transient drift-diffusion model*, IMA J. Numer. Anal. (2007).

[21] C. Chainais-Hillairet, J.-G. Liu, Y.-J. Peng, *Finite volume scheme for multi-dimensional drift-diffusion equations and convergence analysis*, M2AN **37**, pp. 319–338 (2003).

[22] A. Chorin, *On the convergence of discrete approximations of the Navier-Stokes Equations*, Math. Com. 23, pp. 341–353 (1969).

[23] P.G. Ciarlet, P.A. Raviart, *Maximum principle and uniform convergence for the finite element method*, Comput. Methods Appl. Mech. Engrg., 2, pp. 1-67, (1992).

[24] Corrias L., Perthame B., Zaag H., *Global Solutions of Some Chemotaxis and Angiogenesis Systems in High Space Dimensions*, Milan j. math., **72**, 1-28, 2004.

[25] M. Crouzeix, V. Thomee, *The stability in L^p and W_p^1 of the L^2-projection onto Finite element Function Spaces*, Math. Comp. **48**, pp. 521–532 (1987).

[26] Enikov, E. T., and Seo, G. S., *Analysis of water and proton fluxes in ion-exchange polymer-metal composite (IPMC) actuators subjected to large external potentials*, Sensors and Actuators, **122**, 264-272, 2005.

[27] Enikov, E. T., and Nelson, B. J., *Electrotransport and deformation model of ion exchange membrane based actuators*, Smart Structures and Materials, Vol. 3987, 2000.

[28] Evans, L. C., *Partial Differential Equations,* AMS, 2002.

[29] W. Fang, K. Ito, *Global solutions of the time-dependent drift-diffusion semiconductor equations*, J. Diff. Eqn.s **123**, pp. 523–566 (1995).

[30] W. Fang, K. Ito, *On the time-dependent drift-diffusion model for semiconductors*, J. Diff. Eqn.s **117**, pp. 245–280 (1995).

[31] W. Fang, K. Ito, *Asymptotic behavior of the drift-diffusion semiconductor equations*, J. Diff. Eqn.s **123**, pp. 567–587 (1995).

[32] H. Gajewski, K. Gröger, *On the basic equations for carrier transport in semiconductors*, J. Math. Anal. Appl. **113**, pp. 12–35 (1986).

[33] H. Gajewski, K. Gärtner, *On the Discretization of van Roosbroeck's Equations with Magnetic Field*, Z. angew. Math. Mech., **76**, pp. 247–264 (1996).

[34] Gilbarg, D., and Trudinger, N. S., *Elliptic Partial Differential Equations of Second Order*, Springer, 2001.

[35] P. Grisvard, *Elliptic Problems in Nonsmooth Domains*, Pitman Advanced Publishing Program, Boston, 1985.

[36] G. Grün, M. Rumpf, *Nonnegativity preserving convergent schemes for the thin film equation*, J. Math. Anal. Appl. **87**, pp. 113– 152 (2000).

[37] R. J. Hunter, *Foundations of Colloidal Science*, Oxford University Press, 2000.

[38] J.G. Heywood, R. Rannacher, *Finite element approximation of the non-stationary Navier-Stokes problem I: Regularity of solutions and second-order error estimates for spatial discretization*, SIAM J. Numer. Anal. **19**, pp. 275–311 (1982).

[39] J.W. Jerome, *Analysis of charge transport*, Springer, Berlin (1996).

[40] Jerome, J. W., *Analytical Approaches to Charge Transport in a Moving Medium*, Transport Theory and Statistical Physics, **31**, 333–366, 2002.

[41] A. Jüngel, Y.J. Peng, *A discretization scheme for a quasi-hydrodynamic semiconductor model*, Math. Mod. Meth. Appl. Sci. **7**, pp. 935–955 (1997).

[42] M.S. Kilic, M.Z. Bazant, A. Adjari, *Steric effects in the dynamics of electrolytes at large applied voltages. II. Modified Poisson-Nernst-Planck equations*, Phys. Rev. E, **75**, 021503, (2007).

[43] Koch, Ch., *Biophysics of Computation, Information Processing in Single Neurons*, Oxford Univ. Pr., 2004.

[44] Kim, K., Nakayama, Y., and Yamamoto, R., *Direct Numerical Simulations of Electrophoresis of Charged Colloids*, PRL, **96**, 2006.

[45] Kodama, H., Takeshita, K., Araki, T., and Tanaka, H., *Fluid particle dynamics simulation of charged colloidal supsensions*, J. Phys.: Condens. Matter, **16**, 2004.

[46] S. Korotiv, M. Krizek, P. Neittaanmäki, *Weakened Acute Type Condition for Tetrahedral Triangulations and the Discrete Maximum Prinicple*, Math. Comp., **70**, pp. 107–119 (2001).

[47] Ladyzhenskaya, O. A., Solonnikov, V. A., Ural'ceva, N. N., *Linear and Quasi Linear Elliptic Equations of Parabolic Type*, Vol. 23, Trans. Math. Monograhps 23, American Mathematical Society, Providence, RI, 1968.

[48] Lions, J.-L., *Quelques méthodes de résolution des problèmes aux limites non linéaires.* Dunod, Paris, 1968.

[49] Lions J.L., and Magenes E., *Nonhomogeneous Boundary Value Problems and Applications*, Springer, New York, 1972.

[50] P. L. Lions, *Mathematical Topics in Fluid Mechanics, Volume 1, Incompressible Models,* Oxford University Press, 1996.

[51] M. Luskin, R. Rannacher, *On the smoothing property of the Galerkin method for parabolic equations*, SIAM J. Numer. Anal. **19**, pp. 93–113 (1981).

[52] B.B. Mandelbrot, *The Fractal Geometry of Nature*, San Francisco: W.H. Freeman, 1982.

[53] P.A. Markovitch, *The stationary semiconductor device equations*, Springer, Wien (1986).

[54] P.A. Markovitch, C.A. Ringhofer, C. Schmeiser, *Semiconductor equations*, Springer, Wien (1990).

[55] Moser, J., *A New Proof of de Giorgi's Theorem Concerning the Regularity Problem for Elliptic Differential Equations*, Comm. pure a. appl. math., **8**, 457-468, 1960.

[56] Newman, J., and Thomas-Alyea, K., E., *Electrochemical Systems, Third Edition*, Wiley & Sons, 2004.

[57] L. Nirenberg, *On elliptic partial differential equations*, Annali della Scoula Norm. Sup. Pisa, **13**, 115–162, (1959).

[58] R.H. Nochetto, C. Verdi, *Convergence past singularities for a fully discrete approximation of curvature-driven interfaces*

[59] M.F. Perutz, *The hemoglobin molecule*, Sci. Amer. **211**, 64–76, (1964).

[60] R. F. Probstein, *Physiochemical Hydrodynamics*, *An introduction*, John Wiley and Sons, INC., 1994.

[61] A. Prohl, *Projection and Quasi- Compressibility Methods for Solving the Incompressible Navier-Stokes Equations*, Teubner, 1997.

[62] A. Prohl, M. Schmuck, *Convergent Discretizations for the Nernst-Planck-Poisson System*, accepted by Num. Math., preprint: `http://na.uni-tuebingen.de/preprints`, (2007).

[63] A. Prohl, M. Schmuck, *One reliable and one efficient scheme for the Navier-Stokes-Nernst-Planck-Poisson system*, preprint, downloadable from: `http://na.uni-tuebingen.de/preprints`, (2008).

[64] J. Rauch, *Partial Differential Equations*, Springer, New York, 1988.

[65] R. Roubicek, *Incompressible ionized fluid mixtures*, Cont. Mech. Thermodyn., pp. 429-440, (2006).

[66] Roubicek, T., *Incompressible ionized fluid mixtures*, Continuum Mech. Thermodyn., Springer, 429-440, 2006.

[67] Roubicek, T., *Incompressible Ionized Non-Newtonian Fluid Mixtures*, SIAM J. Math. Anal., **39**, 863-890, (2007).

[68] Shahinpoor, M., and Kim, K. J., *Ionic polymer-metal composites: I. Fundamentals*, Smart Mater. Struct., **10**, 819-833, 2001.

[69] Shahinpoor, M., and Kim, K. J., *Ionic polymer-metal composites: III. Modeling and simulation as biomimetic sensors, actuators, transducers, and artificial muscles*, Smart Mater. Struct. **13**, 1362-1388, 2004.

[70] L. Stryer, *Biochemistry*, 3rd ed., New York:W.H. Freeman, 1988.

[71] M. Schmuck, *Analysis of the Navier-Stokes-Nernst-Planck-Poisson System*, accepted by M3AS, preprint: `http://na.uni-tuebingen.de/preprints`, (2007).

[72] R.E. Showalter, *Monotone operators in Banach space and nonlinear partial differential equations*, AMS (1997).

[73] J.H. Spurk, N. Aksel, *Strömungslehre*, 6th ed., 2006.

[74] Temam, R., *Navier-Stokes equations and Nonlinear Functional Analysis*, SIAM, 1995.

[75] R. Temam, *Navier-Stokes equations – theory and numerical analysis*, AMS Chelsea Publishing, Providence, Rhode Island, reprinted version (2001).

[76] D.A. Weitz, M. Oliveria, *Fractal structures formed by kinetic aggregation of aqueous gold colloids*, Phys. Rev. Letters, **52**,1433–1436, (1984).

[77] T.A. Witten, M.E. Cates. *Tenuous structures from disorderly growth processes*, Science, **232**, 1607–1612, (1986).

[78] F.M. White, *Fluid Mechanics*, 2nd ed., McGraw-Hill, 1999.

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