

Modeling, Analysis and Numerics in Electrohydrodynamics

Markus Schmuck

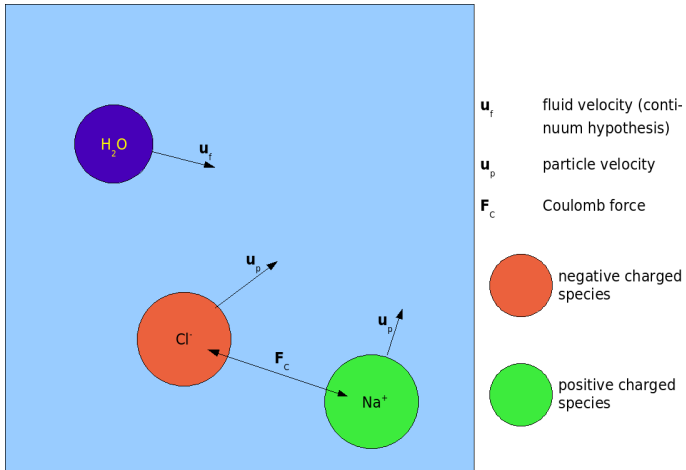
University Tübingen

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Outline

- 1 Continuous Model and Analytical Results
 - Analytical Results in $3D$
 - Approximation Goal
- 2 Finite Element Discretization
 - Van Roosbroeck part ($\mathbf{u} = 0$)
 - Results ($\mathbf{u} = 0$)
 - The whole EHD system ($\mathbf{u} \neq 0$)
 - Results ($\mathbf{u} \neq 0$)

Electrokinetics describes



Questions in Electrokinetics: (Modeling, Numerics)

- What happens at the solid/electrolyte interphase?
- Behavior of species in special geometries?



Goal: Construction/Optimization of innovative devices:

- separation devices, micro-/nano- mixers
- supercapacitors (electric vehicles)
- desalination devices

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Basic Continuous Model

Navier-Stokes equations:

$$\begin{aligned}\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \Delta \mathbf{u} + \nabla p &= -(n^+ - n^-) \nabla \psi & \text{in } \Omega_T \\ \operatorname{div} \mathbf{u} &= 0 & \text{in } \Omega_T\end{aligned}$$

Nernst-Planck-Poisson equations:

$$\partial_t n^\pm \mp \operatorname{div} (n^\pm \nabla \psi) - \Delta n^\pm + (\mathbf{u} \cdot \nabla) n^\pm = 0 \quad \text{in } \Omega_T$$

$$-\Delta \psi = n^+ - n^- \quad \text{in } \Omega_T$$

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The role of the energy and the entropy:

Energy in

- **Continuous Setting:** not required for (global) existence
- **Discrete Setting:** uniform bounds to study long-time asymptotics

Entropy in

- **Continuous Setting:** characterizes long-time asymptotics
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Results in 3D (Schmuck [07])

- **Existence of weak solutions:** Schauder's fixed point thm
- Existence of local strong solutions
- Characterizations of weak solutions:
(also for the pure van Roosbroeck equations)
 - $L^\infty(\Omega_T)$ -bound (Moser iteration)
 - (Lyapunov) entropy-law
 - Energy law
 - Non-negativity of n^\pm

Based on :

Gajewski/Gröger [86]; Bihler/Nadziedja [94]; Temam (book) [01]

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Approximation Goal

Discretization by affine finite elements:

Recover results from the continuous setting to the discrete world

Part II

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Energies and Characterizations not immediate:

Problems

• $\operatorname{div} \mathbf{u}_h \neq 0$



Tools

skew symmetry of $(\mathbf{u} \cdot \nabla \mathbf{u}, \mathbf{v})$

• No Moser-iteration



1) **M-matrix** \Rightarrow d.m.p

2) entropy provider S_ϵ

• log not linear



1) **perturbed entropy**,

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Approach:

- 1) energy based,
- 2) entropy based

2) **bases on** : Grün/Rumpf [00]; Barrett/Nürnberg [04];

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Two Discretization Strategies

Schemes:

$$(d_t(\mathcal{N}^\pm)^j, \Phi)_h + (\nabla(\mathcal{N}^\pm)^j, \nabla\Phi) \pm (R_\epsilon[(\mathcal{N}^\pm)^j] \nabla\psi^j, \nabla\Phi) = 0$$

$$(\nabla\psi^j, \nabla\Phi) = (P^j - N^j, \Phi)_h,$$

where

$$R_\epsilon[X] = \begin{cases} X & \text{energy based} \\ S_\epsilon(X) & \text{entropy based} \end{cases}$$

Remark: $S_\epsilon(\cdot)$ is a perturbation of the identity!

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Explanations to the Schemes:

Fully implicit Scheme:

⇒ Necessary for energy and entropy properties

Consequence:

⇒ In practice a linearization required

Tool:

⇒ Banach's fixed point theorem (constructive proof for the energy based strategy)

⇒ fully practical algorithm

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Energy based approach \Rightarrow perturbed Entropy

Problems:

- $\ln \mathcal{N}^\pm$ not allowed test fct. \Rightarrow linear interpolation
 $\mathcal{I}_h[\ln(\mathcal{N}^\pm + \delta)]$

- $(\mathcal{N}^\pm \nabla \Psi, \nabla \mathcal{I}_h[\ln(\mathcal{N}^\pm + \delta)]) \neq (\nabla \Psi, \nabla \mathcal{N}^\pm)$
“=” is desired, since $(\nabla \Psi, \nabla(\mathcal{N}^+ - \mathcal{N}^-)) = \|\mathcal{N}^+ - \mathcal{N}^-\|^2$

Idea: Use the interpolation error

$$\mathcal{I}_h[\ln(\mathcal{N}^\pm + \delta)] = (\mathcal{I}_h[\ln(\mathcal{N}^\pm + \delta)] - \ln(\mathcal{N}^\pm + \delta)) + \ln(\mathcal{N}^\pm + \delta)$$

\Rightarrow perturbation term depending on δ , more regular initial data and the mesh coupling $k < C h^2$

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- **Idea:** Imitate the **continuous situation** :

$$\left(n^\pm \nabla \psi, \nabla \ln n^\pm \right) = \left(\nabla \psi, \nabla n^\pm \right)$$

- **Tool:** Define $S_\epsilon(\mathcal{N}^\pm)$ such that

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Summary of Results (Prohl/Schmuck [07])

- Existence and convergence
- Mass conservation for \mathcal{N}^\pm
- Energy law
- 1) perturbed versus 2) unperturbed entropy law
- 1) Maximum principle versus 2) nothing
- 1) Non-negativity versus 2) quasi-non-negativity

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Topic of the remaining part:

Extend the energy based strategy to the whole
electrohydrodynamic system

Energy based Scheme:

Let $\mathbf{F}_C^j := ((\mathcal{N}^+)^j - (\mathcal{N}^-)^j) \nabla \Psi^j$, and $(\mathbf{V}, \Phi, Q) \in \mathbf{X}_h \times Y_h \times M_h$

$$\begin{aligned} & (d_t \mathbf{U}^j, \mathbf{V}) + (\nabla \mathbf{U}^j, \nabla \mathbf{V}) + \sigma (\nabla d_t \mathbf{U}^j, \nabla \mathbf{V}) + ((\mathbf{U}^{j-1} \cdot \nabla) \mathbf{U}^j, \mathbf{V}) \\ & + \frac{1}{2} ((\operatorname{div} \mathbf{U}^{j-1}) \mathbf{U}^j, \mathbf{V}) - (\Pi^j, \operatorname{div} \mathbf{V}) = (-\mathbf{F}_C^j, \mathbf{V}) \\ & (\operatorname{div} \mathbf{U}^j, Q) = 0 \end{aligned}$$

$$\begin{aligned} & (d_t (\mathcal{N}^\pm)^j, \Phi)_h + (\nabla (\mathcal{N}^\pm)^j, \nabla \Phi) \\ & \pm ((\mathcal{N}^\pm)^j \nabla \Psi^j, \nabla \Phi) + (\mathbf{U}^j (\mathcal{N}^\pm)^j, \nabla \Phi) = 0 \end{aligned}$$

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