Interface control of multi-phase flow

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joint work with L. Banas and A. Prohl

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Contents

Contents

The Model

- $\rho_0 = \rho_1 \chi_{\Omega_1} + \rho_2 \chi_{\Omega_2}$ mixture of two immiscible viscous incompressible fluids in a bounded domain in $\mathbb{R}^2$.
- Multi-phase flow evolution by Navier–Stokes Eq. (cf. [Lions, 1996])

$$(NSE) \begin{cases} \rho \boldsymbol{y}_t + \rho[\boldsymbol{y} \cdot \nabla]\boldsymbol{y} - \mu \Delta \boldsymbol{y} + \nabla p = \rho \boldsymbol{u}, & \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \rho_t + [\boldsymbol{y} \cdot \nabla]\rho = 0, & \rho(0) = \rho_0, \\ \operatorname{div} \boldsymbol{y} = 0 & + B.C. \end{cases}$$

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Minimize

"Shape" "Geometry" "Cost"

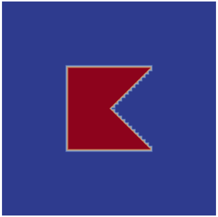
$$J(\rho, \boldsymbol{u}) = \int_0^T \int_\Omega |\rho(t) - \sigma|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t + \frac{\beta}{2} \int_0^T \mathcal{H}^1(S_\rho) \, \mathrm{d}t + \frac{\alpha}{2} \int_0^T \int_\Omega |\boldsymbol{u}|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t$$

subject to

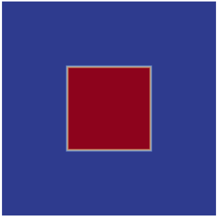
$$(NSE) \begin{cases} \rho \boldsymbol{y}_t + \rho[\boldsymbol{y} \cdot \nabla]\boldsymbol{y} - \mu \Delta \boldsymbol{y} + \nabla p = \rho \boldsymbol{u}, & \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \rho_t + [\boldsymbol{y} \cdot \nabla]\rho = 0, & \rho(0) = \rho_0, \\ \operatorname{div} \boldsymbol{y} = 0 & + B.C. \end{cases}$$

Evidence of the geometric functional

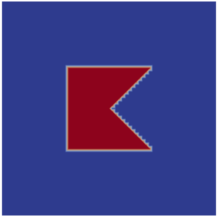
$\|\rho - \sigma\|^2_{L^2(\Omega_T)}$



Target σ



$$\|\rho - \sigma\|^2_{L^2(\Omega_T)} + \int_0^T \mathcal{H}^1(S_\rho)$$



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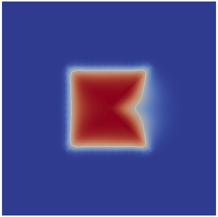

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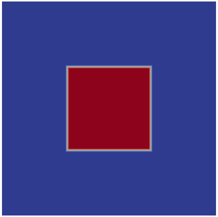

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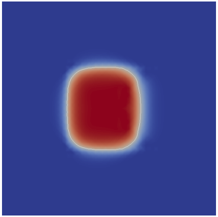

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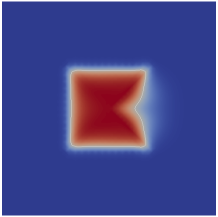

better corners

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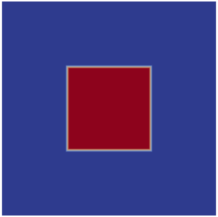

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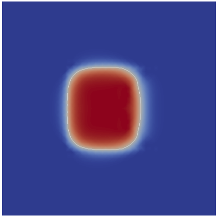
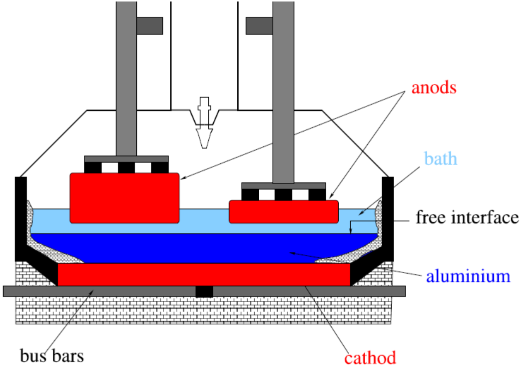


correct geometry

Application ([Gerbeau et al., 2006]): Aluminium production via electrolysis



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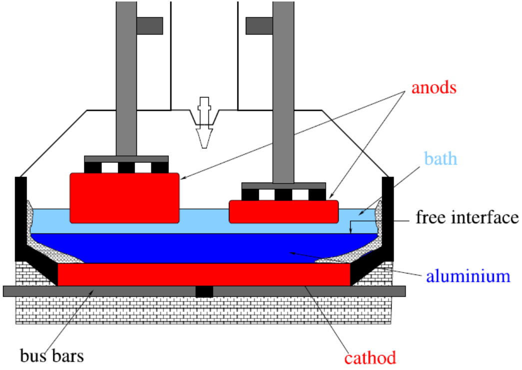

Anods shall not touch the interface!
$\Rightarrow$ Interface control

Goals

- Existence of optimum.
- (Necessary) first order optimality conditions.
- Numerical scheme with low order Finite Elements.
- Convergence of the numerical scheme.

Known result

- Optimization (analysis, no numerics) of L^2-functional (no geometric term) subject to Stokes equation, cf. [Kunisch and Lu, 2011].
- Convergent numerical scheme for equation (low regularity), cf. [Bańas and Prohl, 2010].

Contents

Analytical problems and strategy

Minimize

$$J(\rho, \boldsymbol{u}) = \int_0^T \int_\Omega |\rho(t) - \sigma|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t + \frac{\beta}{2} \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t + \frac{\alpha}{2} \int_0^T \int_\Omega |\boldsymbol{u}|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

subject to

$$(NSE) \begin{cases} \rho \boldsymbol{y}_t + \rho[\boldsymbol{y} \cdot \nabla]\boldsymbol{y} - \mu \Delta \boldsymbol{y} + \nabla p = \rho \boldsymbol{u}, & \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \rho_t + [\boldsymbol{y} \cdot \nabla]\rho = 0, & \rho(0) = \rho_0, \\ \operatorname{div} \boldsymbol{y} = 0 & + B.C. \end{cases}$$

- **Problem:** Not clear if red term is w.l.s.c., and not clear if corresponding Lagrange multiplier to mass equation exists and is a function.

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- **Solution:** Add artificial diffusion to equation and approximate Hausdorff measure ("Mortola-Modica", cf. [Braides, 1998])

Analytical problems and strategy

Minimize

$$J_{\delta}(\rho, \boldsymbol{u}) = \quad + \frac{\beta}{2}\left(\delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{\delta}\int_{\Omega_T} W(\rho)\right) + $$

subject to

$$(NSE_{\varepsilon})\begin{cases} \rho \boldsymbol{y}_t + \rho[\boldsymbol{y}\cdot\nabla]\boldsymbol{y} - \mu\Delta\boldsymbol{y} + \nabla p = \rho\boldsymbol{u}, & \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \rho_t + [\boldsymbol{y}\cdot\nabla]\rho - \varepsilon\Delta\rho = 0, & \rho(0) = \rho_0, \\ \operatorname{div} \boldsymbol{y} = 0 & + B.C. \end{cases}$$

($W \geq 0$ double Well functional with $W(\rho) = 0$ iff $\rho = \rho_1$ or $\rho = \rho_2$)

- **Solution:** Add artificial diffusion to equation and approximate Hausdorff measure ("Mortola-Modica", cf. [Braides, 1998])

Analytic results

Theorem (Existence)

For $\delta, \varepsilon > 0$, there exists at least one minimum and the corresponding Lagrange multipliers belong to some $L^p(\Omega_T)$ for $p > 1$.

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Proof.

Key are a priori estimates and regularity for $\boldsymbol{y}$ and ρ and Lagrange multiplier theorem. □

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Proof.

Key are a priori estimates and regularity for $\boldsymbol{y}$ and ρ and Lagrange multiplier theorem. $\square$

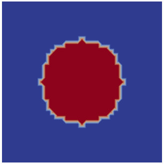
Passing to the limit for $\varepsilon, \delta \to 0$?

Necessary condition for convergence of the whole system is

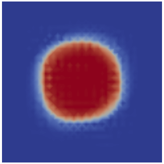
$$\delta \approx \varepsilon.$$

Case $\varepsilon \ll \delta$: parasitic currents

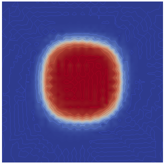
$$\min \; \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{\delta} \int_{\Omega_T} W(\rho) \quad \text{s.t.} \quad (NSE_\varepsilon).$$



$\rho(t = 0)$



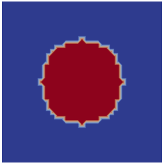
$\rho(t = 0.25)$



$\rho(t = 0.5)$

Case $\varepsilon \ll \delta$: parasitic currents

$$\min \; \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{\delta} \int_{\Omega_T} W(\rho) \quad \text{s.t.} \quad (NSE_\varepsilon).$$



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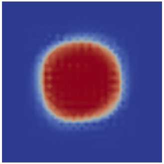

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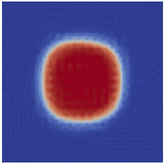

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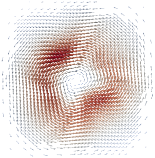
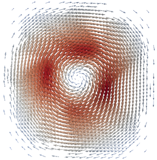
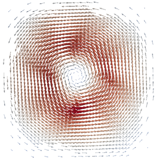


$\boldsymbol{y}(t = 0.05)$



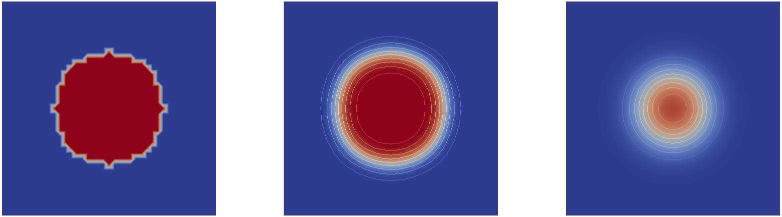
$\boldsymbol{y}(t = 0.15)$



$\boldsymbol{y}(t = 0.35)$

Case $\varepsilon \gg \delta$: massive diffusion

$$\min \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{\delta} \int_{\Omega_T} W(\rho) \quad \text{s.t.} \quad (NSE_\varepsilon).$$



$\rho(t = 0)$ | $\rho(t = 0.5)$ moderate ε | $\rho(t = 0.5)$ big ε

Contents

Strategy

Strategy for the discretization

- Fix $\delta, \varepsilon > 0$.
- Use “first discretize, then optimize” ansatz with convergent and unconditionally stable scheme, cf. [Bañas and Prohl, 2010].
- Show existence of discrete optimum, derive discrete optimality conditions.

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$$\sup_{t\in[0,T]} \left[\|\nabla\boldsymbol{\mathcal{Y}}(t)\|^2 + \|\nabla\mathcal{R}(t)\|^2\right] + \int_0^T \|\Delta_h\boldsymbol{\mathcal{Y}}(t)\|^2 + \|\Delta_h\mathcal{R}(t)\|^2 + \|d_t\boldsymbol{\mathcal{Y}}(t)\|^2 + \|d_t\nabla\mathcal{R}(t)\|^2 \,\mathrm{d}t \leq C.$$

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- $\Rightarrow$ Bounds for dual variables, but. . .

(Continuous) adjoint equation

$$\mathbf{0} = -\rho \boldsymbol{z}_t - \nabla q - \mu \Delta \boldsymbol{z} - {}^1\!/\!_2 \rho \nabla \eta + \text{further terms}$$
$$0 = J_\rho(\rho, \boldsymbol{u}) - \eta_t - \varepsilon \Delta \eta - {}^1\!/\!_2 \boldsymbol{y} \cdot \boldsymbol{z}_t + \text{further terms}$$

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- Test first line with $\boldsymbol{z}$ $\Rightarrow$ Problem with red Term

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- Test second line with η $\Rightarrow$ Problem with red Term

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- Test first line with $\boldsymbol{z} \Rightarrow$ Problem with red Term
- Test second line with $\eta \Rightarrow$ Problem with red Term
- Have (L integrable in time):

$$-d_t\|\eta\|^2 - d_t\|\boldsymbol{z}\|^2 + \|\nabla \boldsymbol{z}\|^2 + \varepsilon\|\nabla\eta\|^2 \leq \text{small}\|\boldsymbol{z}_t\|^2 + L(t)\left(\|\eta\|^2 + \|\boldsymbol{z}\|^2\right). \tag{A}$$

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- Test first line with $\boldsymbol{z}_t$, get

$$-d_t\|\nabla \boldsymbol{z}\|^2 + \|\boldsymbol{z}_t\|^2 \leq \text{number}\|\nabla \eta\|^2 + L(t)\left(\|\eta\|^2 + \|\boldsymbol{z}\|^2 + \|\nabla \boldsymbol{z}\|^2\right). \quad \text{(B)}$$

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- Consider

$$\text{big number} \cdot (A) + (B)$$

and use Gronwall.

Main result

Theorem (Stability)

1. The discrete states, adjoints and controls are uniformly (in $h, k > 0$) bounded in some norms.
2. These functions converge to some weak limit functions in these norms (up to subsequences).

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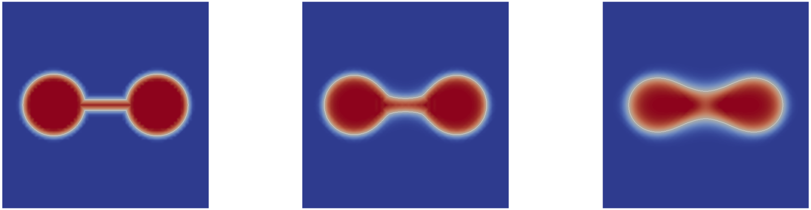
Theorem (Convergence)

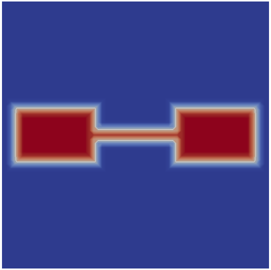
The limit functions solve the original fully continuous optimality system.

$$\min \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t$$



$\rho(t = 0)$ $\rho(t = 0.15)$ $\rho(t = 1)$

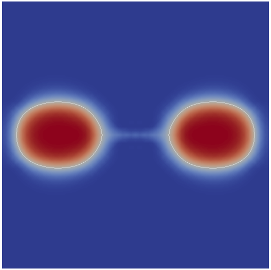
$$\min \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t$$



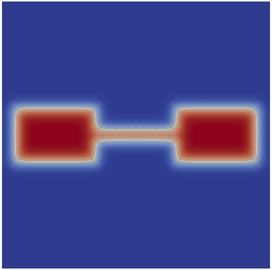
$\rho(t = 0)$

$$\min \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t$$

Control $u \equiv 0$



$\rho(t = 1)$



$\rho(t = 1)$

Summary

Done

- New geometric functional considered with PDE constraints: Evidence, existence and optimality conditions for $\delta, \varepsilon > 0$.
- Rigorous convergence analysis with unconditionally stable scheme for $\delta, \varepsilon > 0$.
- Implementation for $\delta, \varepsilon > 0$.

Outlook

- What happens for $\varepsilon, \delta \to 0$? Proofs?
- Interplay between δ, ε and numerical parameters (time step size *k* and grid size *h*)?
- Surface tension instead of geometric functional?
- Other models (sharp interface, thin film, etc.)?

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Thank you for your attention!

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