Control of Interface Evolution in Multi-Phase Fluid Flows

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joint work with: Ľ. Baňas (Edinburgh) and A. Prohl (Tübingen)

Numerical Methods for Two-phase Flow
Stuttgart, 2012-11-30

Outline

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" "Topology" "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

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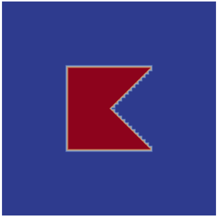
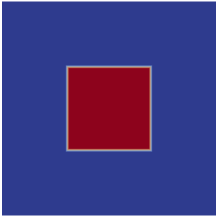
Evidence of the geometric functional

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

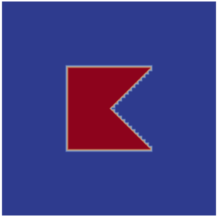


Target σ



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

$+ \int_0^T \mathcal{H}^1(S_\rho)$



Evidence of the geometric functional

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

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

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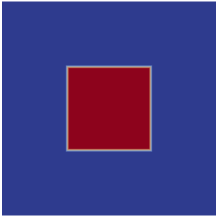

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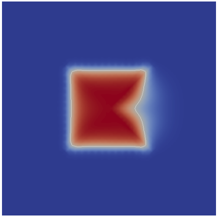
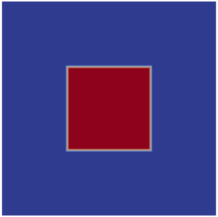
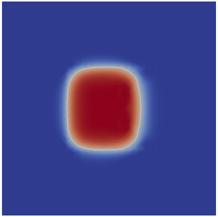


better corners

Target σ



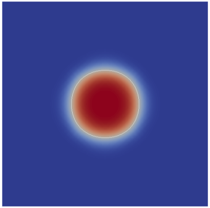
$\|\rho - \sigma\|^2_{L^2(\Omega_T)} + \int_0^T \mathcal{H}^1(S_\rho)$



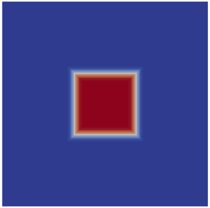
correct topology

Another example

$$\int_0^T \mathcal{H}^1(S_\rho)$$



Initial value ρ_0
Target σ



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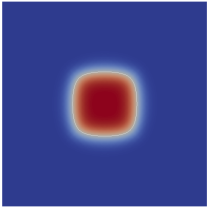

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$$\int_0^T \mathcal{H}^1(S_\rho)$$

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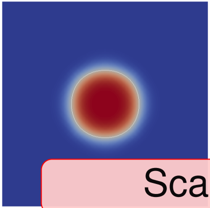
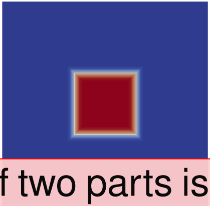
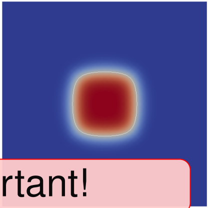
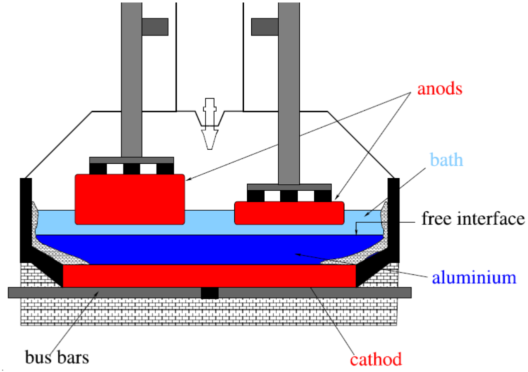






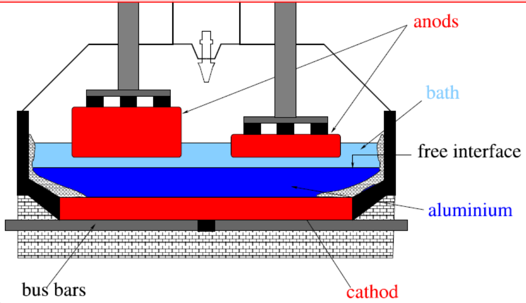
Scaling of two parts is important!

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



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

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



Goals

- Existence of optimum
- 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. [Baňas and Prohl, 2010].

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

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- **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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- **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.
- **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

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

($W \geq 0$ 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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Key are a priori estimates and regularity for $\boldsymbol{y}$ and ρ and Lagrange multiplier theorem. □

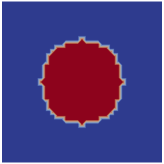
Passing to the limit for $\varepsilon, \delta \to 0$?

Necessary condition for convergence of the whole system is

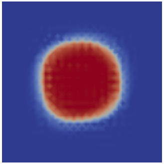
$$\delta \approx \varepsilon.$$

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

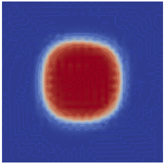
$$\min \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{\delta} \int_{\Omega_T} W(\rho) \quad \text{s.t.} \quad (NSE_\varepsilon).$$



$\rho(t = 0)$



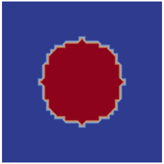
$\rho(t = 0.25)$



$\rho(t = 0.5)$

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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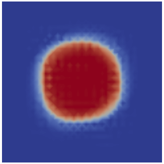

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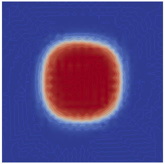

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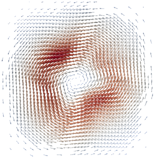
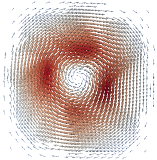
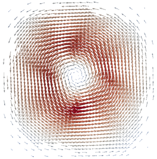


$\boldsymbol{y}(t = 0.05)$



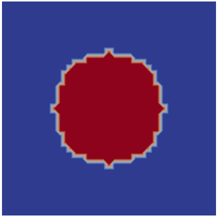
$\boldsymbol{y}(t = 0.15)$



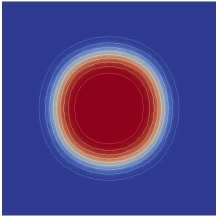
$\boldsymbol{y}(t = 0.35)$

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

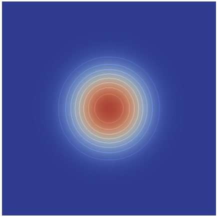
$$\min \; \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{\delta} \int_{\Omega_T} W(\rho) \quad \text{s.t.} \quad (NSE_\varepsilon).$$



$\rho(t = 0)$



$\rho(t = 0.5)$
moderate ε



$\rho(t = 0.5)$
big ε

Optimality Conditions

$$\mathbf{0} = \frac{1}{2}\eta\nabla\rho - \frac{1}{2}\rho\nabla\eta - \frac{1}{2}\rho_t \boldsymbol{z} - \rho\boldsymbol{z}_t + \frac{1}{2}\rho\nabla\boldsymbol{y}\boldsymbol{z} - \frac{1}{2}[\nabla\rho\cdot\boldsymbol{y}]\boldsymbol{z}$$
$$- \rho[\boldsymbol{y}\cdot\nabla]\boldsymbol{z} - \frac{1}{2}\rho\nabla\boldsymbol{z}\boldsymbol{y} - \mu\Delta\boldsymbol{z} - \nabla q,$$
$$0 = \operatorname{div}\boldsymbol{z}, \operatorname{div}\boldsymbol{y}$$
$$0 = \lambda(\rho - \tilde{\rho}) - \beta\delta\Delta\rho + \frac{\beta}{8\delta}W'(\rho) - \eta_t - [\boldsymbol{y}\cdot\nabla]\eta + \varepsilon\Delta\eta_t$$
$$+ \frac{1}{2}\boldsymbol{z}\cdot\boldsymbol{y}_t - \frac{1}{2}\boldsymbol{y}\cdot\boldsymbol{z}_t + \frac{1}{2}[\boldsymbol{y}\cdot\nabla]\boldsymbol{y}\cdot\boldsymbol{z} - \boldsymbol{u}\cdot\boldsymbol{z} - \frac{1}{2}[\boldsymbol{y}\cdot\nabla]\boldsymbol{z}\cdot\boldsymbol{y},$$
$$\mathbf{0} = \alpha\boldsymbol{u} - \rho\boldsymbol{z},$$
$$\mathbf{0} = \rho\boldsymbol{y}_t - \rho[\boldsymbol{y}\cdot\nabla]\boldsymbol{y} - \mu\Delta\boldsymbol{y} - \rho\boldsymbol{u} + \nabla p,$$
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$\boldsymbol{z}(T) = \mathbf{0}$, $\eta(T) = 0$ + B.C.

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Strategy for the discrization

- Use “first discretize, then optimize” ansatz.
- Convergent and unconditionally stable scheme known for density depedend Navier–Stokes, cf. [Baňas and Prohl, 2010].
- Due to strong coupling of primal and dual variables in the adjoint equation, we need bounds on higher bounds of the primal variables.
- Here: Fix $\delta, \varepsilon > 0$. **Still open**: Interplay between δ, ε and numerical parameters (time step size *k* and grid size *h*)?

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Numerical framework

- Density space R_h: standard piecewise linear FE space.
- Velocity/pressure space $\boldsymbol{V}_h/M_h$: standard inf-sup-stable FE spaces (e.g., Taylor–Hood).
- Control $\boldsymbol{u}$ is automatically discretized by means of the other variables.

Find $(\boldsymbol{Y}^n, P^n, R^n) \in \boldsymbol{V}_h \times M_h \times R_h$ such that for all $(\boldsymbol{Z}, \Pi, E) \in \boldsymbol{V}_h \times M_h \times R_h$:

$$
\begin{aligned}
(d_t R^n, E) + \varepsilon(d_t \nabla R^n, \nabla E) + ([\boldsymbol{Y}^n \cdot \nabla] R^n, E) + \frac{1}{2}(R^n \operatorname{div} \boldsymbol{Y}^n, E) &= 0, \\
\frac{1}{2}(R^{n-1} d_t \boldsymbol{Y}^n, \boldsymbol{Z}) + \frac{1}{2}(d_t(R^n \boldsymbol{Y}^n), \boldsymbol{Z}) + \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Y}^n, \boldsymbol{Z}) & \\
- \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Z}, \boldsymbol{Y}^n) + \mu(\nabla \boldsymbol{Y}^n, \nabla \boldsymbol{Z}) + (\nabla P^n, \boldsymbol{Z}) &= (R^{n-1} \boldsymbol{U}^n, \boldsymbol{Z}), \\
(\operatorname{div} \boldsymbol{Y}^n, \Pi) &= 0.
\end{aligned}
$$

Comments

Scheme is modification of scheme in [Baňas and Prohl, 2010].

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Comments

First line becomes skew symmetric.

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$$\frac{1}{2}(R^{n-1} d_t \boldsymbol{Y}^n, \boldsymbol{Z}) + \frac{1}{2}(d_t(R^n \boldsymbol{Y}^n), \boldsymbol{Z}) + \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Y}^n, \boldsymbol{Z})$$
$$- \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Z}, \boldsymbol{Y}^n) + \mu(\nabla \boldsymbol{Y}^n, \nabla \boldsymbol{Z}) + (\nabla P^n, \boldsymbol{Z}) = (R^{n-1} \boldsymbol{U}^n, \boldsymbol{Z}),$$

$$(\operatorname{div} \boldsymbol{Y}^n, \Pi) = 0.$$

Comments

Second line becomes skew symmetric as (cf. [Liu and Walkington, 2007])

$$\rho(\boldsymbol{y}_t + [\boldsymbol{y} \cdot \nabla] \boldsymbol{y}) = \frac{1}{2}\Big(\rho \boldsymbol{y}_t + \rho[\boldsymbol{y} \cdot \nabla] \boldsymbol{y} + (\rho \boldsymbol{y})_t + \operatorname{div}(\rho \boldsymbol{y} \otimes \boldsymbol{y})\Big).$$

Find $(\boldsymbol{Y}^n, P^n, R^n) \in \boldsymbol{V}_h \times M_h \times R_h$ such that for all $(\boldsymbol{Z}, \Pi, E) \in \boldsymbol{V}_h \times M_h \times R_h$:

$$(d_t R^n, E) + \varepsilon(d_t \nabla R^n, \nabla E) + ([\boldsymbol{Y}^n \cdot \nabla] R^n, E) + \frac{1}{2}(R^n \operatorname{div} \boldsymbol{Y}^n, E) = 0,$$

$$\frac{1}{2}(R^{n-1} d_t \boldsymbol{Y}^n, \boldsymbol{Z}) + \frac{1}{2}(d_t(R^n \boldsymbol{Y}^n), \boldsymbol{Z}) + \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Y}^n, \boldsymbol{Z}) - \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Z}, \boldsymbol{Y}^n) + \mu(\nabla \boldsymbol{Y}^n, \nabla \boldsymbol{Z}) + (\nabla P^n, \boldsymbol{Z}) = (R^{n-1} \boldsymbol{U}^n, \boldsymbol{Z}),$$

$$(\operatorname{div} \boldsymbol{Y}^n, \Pi) = 0.$$

Comments

Assume: Triangulation is strongly acute (iff angles of interior edges are bdd away from 90°)

$\Rightarrow$ M-matrix property for mass equation $\Rightarrow$ lower bound for R^n

Lemma (Bounds for primal variables)

There exists a solution $\{(R^n, \boldsymbol{Y}^n, P^n)\}$ and a constant $C = C(\varepsilon, \delta, T)$ with

$$0 < \rho_1 \leq R^n \leq C < \infty.$$

The time interpolants $(\mathcal{R}, \boldsymbol{\mathcal{Y}}, \mathcal{P})$ hold

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

Lemma (Bounds for primal and dual variables)

There exists a solution $\{(R^n, \boldsymbol{Y}^n, P^n)\}$ and a constant $C = C(\varepsilon, \delta, T)$ with

$$0 < \rho_1 \leq R^n \leq C < \infty.$$

The time interpolants $(\mathcal{R}, \boldsymbol{\mathcal{Y}}, \mathcal{P})$ hold

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

Moreover, there exist Lagrange multipliers $(\boldsymbol{\mathcal{Z}}, \mathcal{Q}, \mathcal{E})$ such that

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

Main result

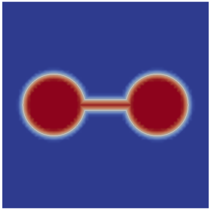
Theorem (Convergence)

There exist $\boldsymbol{y}, p, \rho; \boldsymbol{z}, q, \eta; \boldsymbol{u} : \Omega_T \to \mathbb{R}^{(2)}$, such that the solutions of the fully discrete optimality system converge to them in some norms (up to subsequences). The limit functions solve the original fully continuous optimality system.

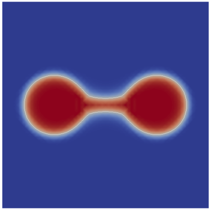
Proof.

Use bounds from last slide. □

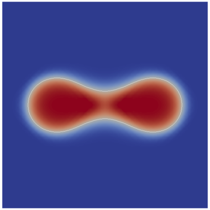
$$\min \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t\,.$$



$\rho(t = 0)$

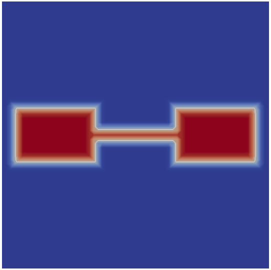


$\rho(t = 0.15)$



$\rho(t = 1)$

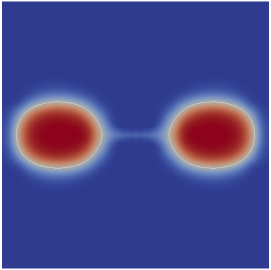
$$\min \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t$$



$\rho(t = 0)$

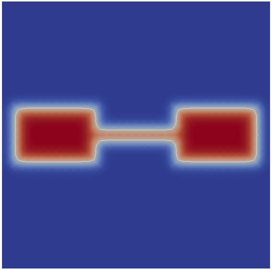
$$\min \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t$$

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



$\rho(t = 1)$

Control $u \equiv 0$



$\rho(t = 1)$

Done

- Existence for optimization of geometric functional for $\delta, \varepsilon > 0$.
- Optimality conditions for $\delta, \varepsilon > 0$.
- Discretization of optimality conditions.
- Convergence analysis with unconditionally stable scheme.

Outlook

- What happens for $\varepsilon, \delta \to 0$?
- Comparison with different models (sharp interface, thin film, etc.)
- Surface tension?

Done

- Existence for optimization of geometric functional for $\delta, \varepsilon > 0$.
- Optimality conditions for $\delta, \varepsilon > 0$.
- Discretization optimality conditions
- Convergence analysis with unconditionally stable scheme.

Thank you for your attention!

Outlook

- What happens for $\varepsilon, \delta \to 0$?
- Comparison with different models (sharp interface, thin film, etc.)
- Surface tension?

References I

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