Consistent Finite Elements for Optimal Control Problems in Computational Fluid Dynamics

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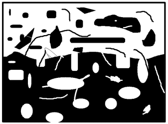
Contents

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

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



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Minimize

$$J(\rho, \mathbf{u}) = \int_{\Omega_T} |\rho(t) - \sigma|^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}t + \frac{\alpha}{2} \int_{\Omega_T} |\mathbf{u}|^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

subject to

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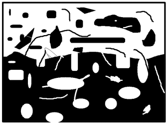

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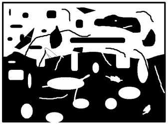

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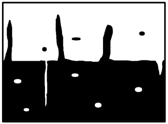

$\rho(t)$ **BAD**

Add additional term to functional to minimize the interface area!
$\Rightarrow$ Geometric functional!
Minimize

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

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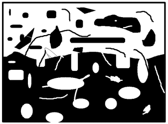

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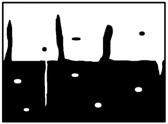

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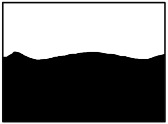

$\rho(t)$ **GOOD**

Applications

- Air-water dynamics (air bubbles, water drops)
- Aluminium production (Al_2 and Al_2O_3)

Goals

- Multi-phase flow in connection with optimal control

Analytical

- Existence of optimum
- Optimality conditions
- Convergence analysis

Practical

- Implementation
- Handle topological changes (interface can merge or break)
- Treatment of interfaces in discrete scheme

Known result: Optimization of L^2-functional (no geometric term) subject to Stokes equation, cf. [Kunisch and Lu, 2011].

Analytical problems and strategy

Minimize

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

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- **Problem for Existence:** Blue term is only w.l.s.c. on $SBV(\Omega)$. Not clear if $\rho(t) \in SBV(\Omega)$ for a.e. t.
- **Solution:** Add artificial diffusion to equation and approximate Hausdorff measure ("Mortola-Modica", cf. [Braides, 1998])

$\Rightarrow$ **Phase-field formulation**

Analytical problems and strategy

Minimize

$$\int_{\Omega_T} |\rho(t)-\sigma|^2 + \frac{\alpha}{2}\int_{\Omega_T} |\mathbf{u}|^2 + \frac{\beta}{2}\left(\delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{4\delta}\int_{\Omega_T} W(\rho)\right)$$

subject to

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

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Theorem (K.)

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.

Lot of technical calculations. Key are a priori estimates and regularity:

- Use parabolic theory for regularity of ρ.
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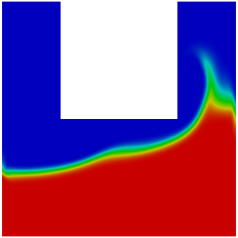
- **Ongoing:** Consistent Finite Element approach and convergence analysis
- **Goal:** What happens for $\varepsilon, \delta \to 0$?

Contents

Direct implementation of (NSE).

- $\mathbb{Q}_1$-elements, $h = 1/128$
- implicit Euler, $\Delta t = 0.005$
- strong oszillations due to discontinuity of density



Implementation of (NSE_ε) with $\varepsilon = 1e - 4$.

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No uniform thickness due to diffusion term!

Level set formulation and reinitialization

Idea (by [Osher and Sethian, 1988]): Introduce a smooth level set function ϕ.

- Sign of ϕ stands for the component; $\phi = 0$ is the interface.
- ϕ_0 signed distance function to interace.

Write $\rho_\varepsilon(\phi) = \rho_1 + (\rho_2 - \rho_1)H_\varepsilon(\phi)$ (H_ε smoothed Heaviside function) and solve

$$\begin{cases} \phi_t + [\mathbf{y} \cdot \nabla]\phi = 0, & \phi(0) = \phi_0 \\ \mathbf{y}_t + [\mathbf{y} \cdot \nabla]\mathbf{y} - \frac{1}{\rho_\varepsilon(\phi)}\mu\Delta\mathbf{y} + \frac{1}{\rho_\varepsilon(\phi)}\nabla p = \mathbf{g} + \mathbf{u}, & \mathbf{y}(0) = \mathbf{y}_0 \\ \operatorname{div}\mathbf{y} = 0 & + B.C. \end{cases}$$

- **Remark:** We keep a uniform thickness $\mathcal{O}(\varepsilon)$, if $|\nabla\phi| = 1$.
- **Problem:** ϕ does not remain distance function for long time computations!

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Idea (by [Sussman et al., 1994]): At some time step, solve auxiliary evolution problem (Reinitialization!), where stationary solutions have $|\nabla\phi| = 1$.

- Evolution starts at interface.
- **Problem**: Zero-level changes at reinitialization at discrete level $\Rightarrow$ mass loss.
- **Question**: At which time should this be done?

How does reinitialization affect the optimization algorithm?

- Compare reduction in the error rate of cost functional and control in each Newton-step on fixed mesh
- Numerical example, where exact control is known.

$$J(\rho, \mathbf{u}) = \frac{1}{2} \int_{\Omega} |\rho(T = 1) - \sigma|^2 \, \mathrm{d}\mathbf{x} \to \text{min!}$$

k- N.-It	$J(\rho^k, \mathbf{u}^k)$	$\lvert\mathbf{u}_{\text{ref}} - \mathbf{u}^k\rvert$
0	1.2e-3	20
1	3.1e-8	1.0e-1
2	6.1e-16	1.4e-5
3	7.3e-26	4.1e-11

Table: without reinitialization

k- N.-It	$J(\rho^k, \mathbf{u}^k)$	$\lvert\mathbf{u}_{\text{ref}} - \mathbf{u}^k\rvert$
0	8.3e-4	20
1	5.4e-6	1.6e 0
2	4.0e-8	1.4e-1
3	3.2e-10	1.3e-2
4	2.8e-12	1.2e-3
5	1.8e-14	9.9e-5
6	1.4e-16	8.4e-6
7	1.1e-18	7.6e-7

Table: reinitialization after 10 timesteps

- Reduced convergence order if reinitialization is used, **but**
- Reinitialization is neccesary for long time computations **and**
- Reinitialization is not included in optimality conditions.

Done

- Existence for optimization of geometric functional (with $\delta > 0$) s.t. NSE_ε for $\delta, \varepsilon > 0$.
- Optimality conditions for the above problem.
- Implementation for multi-phase flow including optimization.
- Implementation of reinitialization.
- First tests

Outlook

- Numerical analysis: Stability and convergence of phase-field formulation.
- Compare model with corresponding graph formulation.
- Conservation of zero-level during reinitialization (for level set method).
- Resultion of diffuse interface: Adaptivity!

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THANK YOU FOR YOUR ATTENTION!

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