



Controlling multiphase flow

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Introduction and Motivation

Analysis

Numerics



- ▶ $\rho_0 = \rho_1 \chi_{\Omega_1} + \rho_2 \chi_{\Omega_2}$ 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])

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


 ρ_0

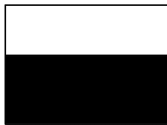


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$$\text{Minimize } J(\rho, \mathbf{u}) = \int_{\Omega_T} |\rho(t) - \sigma|^2 d\mathbf{x} dt + \frac{\alpha}{2} \int_{\Omega_T} |\mathbf{u}|^2 d\mathbf{x} dt$$

subject to

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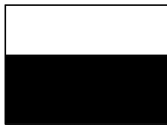
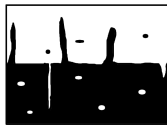


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 ρ_0

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



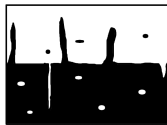
Add additional term to functional to minimize the interface area!
 ⇒ Geometric functional!

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

subject to

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 ρ_0

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

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



Applications

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

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].



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:** Not clear if **blue 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])

⇒ **Phase-field formulation**



Analytical problems and strategy

Minimize

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

subject to

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

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

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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.

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

- ▶ Use parabolic theory for regularity of ρ .
- ▶ Use [Lions, 1996] for regularity of \mathbf{y} .

Then direct application of Lagrange multiplier theorem. □



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



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- ▶ For $\varepsilon \searrow 0$, it is known (direct calculation) that $\rho_\varepsilon \rightarrow \rho$ in $L^2(L^2)$ and $\mathbf{y}_\varepsilon \rightarrow \mathbf{y}$ in $L^2(\mathbf{L}^2)$ (up to subsequences).



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- ▶ For $\delta \searrow 0$ (and no side constraints), it is known ([Braides, 1998]) that $J_\delta(\rho, \mathbf{u}) \xrightarrow{\Gamma} J(\rho, \mathbf{u})$ (Γ -convergence), i.e.,

1. For every sequence $(\rho_\delta, \mathbf{u}_\delta) \rightarrow (\rho, \mathbf{u})$ (for $\delta \rightarrow 0$) we have

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Open question: How to combine both results? How to choose $\delta = \delta(\varepsilon)$?



Optimality Conditions

$$0 = -\rho \mathbf{z}_t - \rho_t \mathbf{z} - \mu \Delta \mathbf{z} + \rho (\nabla \mathbf{y}) \cdot \mathbf{z} + \rho [\mathbf{y} \cdot \nabla] \mathbf{z} + (\nabla \rho \cdot \mathbf{y}) \mathbf{z} + \eta \nabla \rho,$$

$$0 = \lambda(\rho - \tilde{\rho}) - \beta \delta \Delta \rho + \frac{\beta}{8\delta} W'(\rho) + \mathbf{y}_t \cdot \mathbf{z} \\ - ([\mathbf{y} \cdot \nabla] \mathbf{y}) \cdot \mathbf{z} - \mathbf{u} \cdot \mathbf{z} - \eta_t - [\mathbf{y} \cdot \nabla] \eta - \varepsilon \Delta \eta_t,$$

$$0 = \alpha \mathbf{u} - \rho \mathbf{z},$$

$$0 = \rho \mathbf{y}_t - \rho [\mathbf{y} \cdot \nabla] \mathbf{y} - \mu(\rho) \Delta \mathbf{y} - \rho \mathbf{u},$$

$$0 = \rho_t + [\mathbf{y} \cdot \nabla] \rho - \varepsilon \Delta \rho.$$



Strategy for discretization

- ▶ Use **first discretize, then optimize** ansatz.
- ▶ Convergent and unconditionally stable scheme known for density dependent Navier–Stokes, cf. [Bañas 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)?



Numerical framework

- ▶ Density space R_h : standard piecewise linear FE space.
- ▶ Velocity/pressure space \mathbf{V}_h/M_h : standard inf-sup-stable FE spaces (e.g., Taylor–Hood, MINI).
- ▶ Time discretization: Implicit Euler.



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

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

Comments

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



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Comments

First line becomes skew symmetric.



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

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

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Comments

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

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



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Comments

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

⇒ **M-matrix property for first line**

⇒ **lower bound for R^n**



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Comments

Assume: $R_h \cap L_0^2 \subseteq M_h$
 \Rightarrow Upper bound for R^n



Lemma (Bounds for primal variables)

There exists a solution $\{(R^n, \mathbf{Y}^n, P^n)\}$ of the discrete equation with the property

$$0 < \rho_1 \leq R^n \leq \rho_2 < \infty$$

and for the time interpolant of the solution $(\mathcal{R}, \mathcal{Y}, \mathcal{P})$ there is a constant $C = C(\varepsilon, \delta, T)$ independent of k, h with

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



Discrete Optimality Conditions

$$\begin{aligned}
 0 = & \frac{1}{2} E^n \nabla R^n - \frac{1}{2} R^n \nabla E^n - \frac{1}{2} d_t R^n \mathbf{Z}^n - R^n d_t \mathbf{Z}^{n+1} + \frac{1}{2} R^n \nabla \mathbf{Y}^{n+1} \cdot \mathbf{Z}^{n+1} \\
 & + \frac{1}{2} R^n \nabla \mathbf{Z}^{n+1} \cdot \mathbf{Y}^{n+1} - \frac{1}{2} (\nabla R^{n-1} \cdot \mathbf{Y}^{n-1}) \mathbf{Z}^n - \frac{1}{2} R^{n-1} \operatorname{div} \mathbf{Y}^{n-1} \mathbf{Z}^n \\
 & - \frac{1}{2} [R^{n-1} \mathbf{Y}^{n-1} \cdot \nabla] \mathbf{Z}^n - \mu \Delta_h \mathbf{Z}^n - \nabla Q^n,
 \end{aligned}$$

$$0 = -\operatorname{div} \mathbf{Z}^n,$$

$$\begin{aligned}
 0 = & -d_t E^{n+1} - [\mathbf{Y}^n \cdot \nabla] E^n - \frac{1}{2} (\operatorname{div} \mathbf{Y}^n) E^n + \varepsilon d_t \Delta_h E^{n+1} + \frac{1}{2} d_t \mathbf{Y}^{n+1} \cdot \mathbf{Z}^{n+1} \\
 & - \frac{1}{2} \mathbf{Y}^n \cdot d_t \mathbf{Z}^{n+1} + \frac{1}{2} [\mathbf{Y}^n \cdot \nabla] \mathbf{Y}^{n+1} \cdot \mathbf{Z}^{n+1} - \mathbf{U}^{n+1} \cdot \mathbf{Z}^{n+1} \\
 & - \frac{1}{2} [\mathbf{Y}^n \cdot \nabla] \mathbf{Z}^{n+1} \cdot \mathbf{Y}^{n+1} + \lambda (R^n - \tilde{\rho}(t_n)) - \beta \delta \Delta_h R^n + \frac{\beta}{8\delta} W'(R^n),
 \end{aligned}$$

$$0 = \alpha \mathbf{U}^n - R^{n-1} \mathbf{Z}^n.$$



Lemma (Bounds for dual variables)

By the Lagrange multiplier theorem, there exist Lagrange multipliers $(\mathcal{Z}, Q, \mathcal{E})$ and there exists a constant $C = C(\varepsilon, \delta, T)$ independent of k, h with

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



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Proof.

Simultaneously test discrete optimality system with \mathbf{Z}^n , R^n and $d_t \mathbf{Z}^{n+1}$. □



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Theorem (Convergence)

There exist $\mathbf{y}, \rho, \rho; \mathbf{z}, \mathbf{q}, \eta; \mathbf{u} : \Omega_T \rightarrow \mathbb{R}^{(2)}$, 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.



Done

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

Outlook

- ▶ What happens for $\varepsilon, \delta \rightarrow 0$?
- ▶ Implementation.
- ▶ Compare model with corresponding graph formulation.



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THANK YOU FOR YOUR ATTENTION!



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