Controlling multiphase flow

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1. Introduction and Motivation

Let $0 < T < \infty$. Find $\bar{\rho} : \Omega_T \to \mathbb{R}$ and $\bar{\boldsymbol{y}}, \bar{\boldsymbol{u}} : \Omega_T \to \mathbb{R}^2$ as a minimum of

$$G(\rho, \boldsymbol{u}) := \int_0^T \left\{ \beta \mathcal{H}^1(S_\rho) + \frac{\lambda}{2} \int_\Omega |\rho - \tilde{\rho}|^2 \,\mathrm{d}\boldsymbol{x} + \frac{\alpha}{2} \int_\Omega |\boldsymbol{u}|^2 \,\mathrm{d}\boldsymbol{x} \right\} \mathrm{d}t \tag{1}$$

subject to the density dependent Navier–Stokes equation,

$$\partial_t \rho + [\boldsymbol{y} \cdot \nabla] \rho = 0, \tag{2a}$$
$$\rho \partial_t \boldsymbol{y} + \rho [\boldsymbol{y} \cdot \nabla] \boldsymbol{y} - \operatorname{div}(\mu(\rho) \nabla \boldsymbol{y}) + \nabla p = \rho \boldsymbol{u}, \tag{2b}$$
$$\operatorname{div} \boldsymbol{y} = 0, \tag{2c}$$

together with the initial and boundary conditions

$$\rho(t=0) = \rho_0, \qquad \boldsymbol{y}(t=0) = \boldsymbol{y}_0, \qquad \boldsymbol{y} = 0 \text{ on } (0,T] \times \Omega.$$

Here, $\tilde{\rho} : \Omega_T \to \mathbb{R}$ is fixed and S_ρ denotes the jump set of ρ.

- The problem involves the geometric perimeter problem, and the density dependent Navier–Stokes equation. A related work is [3], which uses a L^2-functional as well as a linear version of (2).
- We use a phase–field approximation (Mortola–Modica) to approximate the perimeter functional, and a regularization of (2a).

Practical motivation: Control aluminium production ([2]), where the magneto-hydrodynamical two-phase flow describes theoretical behavoir, and a control of the interface is needed.

Assumptions:

- $\Omega \subseteq \mathbb{R}^2$ bounded, open, convex and polyhedral.
- $\rho_0 := \rho_1 \chi_{\Omega_1} + \rho_2 \chi_{\Omega_2}$ with $\Omega_1 \cap \Omega_2 = \varnothing$ and $0 < \rho_1 < \rho_2 < \infty$.
- $\boldsymbol{y}_0 \in \boldsymbol{L}^2(\Omega)$ with $\operatorname{div} \boldsymbol{y}_0 = 0$.
- $\mu(\rho) = \bar{\mu}\rho$ with $\bar{\mu} > 0$.

Problems: A solution ρ of (2a) is only in $L^\infty(L^\infty)$ ([4]), in general not more regular.

- The *jump set* S_ρ is *not defined* for $\rho \in L^\infty$.
- Due to the *low regularity* of ρ, it is not clear if a *Lagrange multiplier* exists or if the Lagrange multiplier is a function $\Omega_T \to \mathbb{R}$.

Solution:

- Require initial data $\boldsymbol{y}_0 \in \boldsymbol{H}^1_0(\Omega)$ with $\operatorname{div} \boldsymbol{y}_0 = 0$ and $\rho_0 \in H^1(\Omega)$ with $0 < \rho_1 \le \rho_0 \le \rho_2$. The smoothing of ρ_0 can be done by a mollifier at a scale $\varepsilon > 0$.
- Add artificial diffusion $-\varepsilon \Delta \rho$ to (2a) with a small $\varepsilon > 0$, i.e., replace (2) by

$$\partial_t \rho + [\boldsymbol{y} \cdot \nabla] \rho - \varepsilon \Delta \rho = 0, \tag{3a}$$
$$\rho \partial_t \boldsymbol{y} + \rho [\boldsymbol{y} \cdot \nabla] \boldsymbol{y} - \operatorname{div}(\mu(\rho) \nabla \boldsymbol{y}) + \nabla p = \rho \boldsymbol{u}, \tag{3b}$$
$$\operatorname{div} \boldsymbol{y} = 0, \tag{3c}$$

together with the boundary conditions $\boldsymbol{y} = 0$ on $\partial\Omega$ and $\rho = \rho_1$ on $\partial\Omega$, as well as the initial conditions $\boldsymbol{y}(t=0) = \boldsymbol{y}_0 \in \boldsymbol{H}^1_0(\Omega)$ and $\rho(t=0) = \rho_0 \in H^1_0(\Omega)$.

- Replace Hausdorff-measure term in (1) by phase-field approximation, i.e., for a small $\delta > 0$ we replace G by

$$J_\delta(\rho, \boldsymbol{u}) := \frac{\beta}{2} \int_0^T \int_\Omega \left\{ \delta |\nabla \rho|^2 + \frac{1}{\delta} (\rho - \rho_1)^2 (\rho - \rho_2)^2 \right\} \mathrm{d}\boldsymbol{x}\,\mathrm{d}t + \frac{\lambda}{2} \int_0^T \int_\Omega |\rho - \tilde{\rho}|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t + \frac{\alpha}{2} \int_0^T \int_\Omega |\boldsymbol{u}|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \tag{4}$$

2. Analysis

Lemma 1. *For $\boldsymbol{u} \in L^2(\boldsymbol{L}^2)$, there exists a solution $(\boldsymbol{y}, \rho) \in L^2(\boldsymbol{H}^2) \cap H^1(\boldsymbol{L}^2) \times L^4(\boldsymbol{W}^{2,4}) \cap W^{1,4}(\boldsymbol{L}^4)$ with estimates depending on $\boldsymbol{u}$, ε, and T.*

Problem 2. *Let $\varepsilon, \delta > 0$. Minimize* (4) *subject to* (3)*.*

Theorem 3. *There exists a solution $(\boldsymbol{y}, \rho, \boldsymbol{u}) \in L^2(\boldsymbol{H}^2) \cap H^1(\boldsymbol{L}^2) \times L^4(\boldsymbol{W}^{2,4}) \cap W^{1,4}(\boldsymbol{L}^4) \times L^2(\boldsymbol{L}^2)$ of Problem 2. There exist corresponding Lagrange multiplier which can be considered as functions in some $L^p(\Omega_T)$.*

Proof. Existence of a minimum follows from standard technique. Existence of Lagrange multipliers follows from the Lagrange multiplier theorem and Lemma 1. □

3. Numerics

- $\mathcal{T}_h$ quasi-uniform triangulation of Ω with $h := \max_{T \in \mathcal{T}_h} \operatorname{diam} T$, and

$$X^\ell_h := \left\{ x_h \in \mathcal{C}^0(\bar{\Omega}) : \; x_h\big|_T \in P_\ell(T) \quad \forall T \in \mathcal{T}_h \right\}.$$

Triangulation must be strongly acute. This is needed in order to have non-negativity for the discrete density.

- We take $R_h := X^1_h$ for the approximation of the density ρ, and $\boldsymbol{V}_h$ and M_h as a Taylor–Hood finite element pair for the velocity $\boldsymbol{y}$ and the pressure p.
- Compatibility is required (see [1]), i.e.,

$$R_h \cap L^2_0 \subseteq M_h. \tag{5}$$

This is needed to have pointwise upper bounds for the discrete density.

- Let $t_n := nk$ with $k = \frac{T}{N}$. Piecewise affine time interpolants of e.g. $\{v^n\}$ will be denoted by $\mathcal{V}$, and the discrete time derivative will be denoted by d_t.

Discrete version of (3)**:** Let $\gamma > 0$. For $1 \le n \le N$ find $(\boldsymbol{y}^n, p^n, \rho^n) \in \boldsymbol{V}_h \times M_h \times R_h$ such that for all $(\boldsymbol{z}, \pi, \eta) \in \boldsymbol{V}_h \times M_h \times R_h$

$$(d_t \rho^n, \eta) + \varepsilon (\nabla \rho^n, \nabla \eta) + ([\boldsymbol{y}^n \cdot \nabla] \rho^n, \eta) + \frac{1}{2} (\rho^n \operatorname{div} \boldsymbol{y}^n, \eta) = 0, \tag{6a}$$
$$\frac{1}{2}(\rho^{n-1} d_t \boldsymbol{y}^n, \boldsymbol{z}) + \frac{1}{2}(d_t(\rho^n \boldsymbol{y}^n), \boldsymbol{z}) + \mu(\nabla \boldsymbol{y}^n, \nabla \boldsymbol{z}) + \frac{1}{2}([\rho^{n-1} \boldsymbol{y}^{n-1} \cdot \nabla] \boldsymbol{y}^n, \boldsymbol{z}) - \frac{1}{2}([\rho^{n-1} \boldsymbol{y}^{n-1} \cdot \nabla] \boldsymbol{z}, \boldsymbol{y}^n) + \gamma h^\gamma (\nabla d_t \boldsymbol{y}^n, \nabla \boldsymbol{z}) + (\nabla p^n, \boldsymbol{z}) - (\rho^{n-1} \boldsymbol{u}^n, \boldsymbol{z}) = 0, \tag{6b}$$
$$(\operatorname{div} \boldsymbol{y}^n, \pi) = 0. \tag{6c}$$

- In [5], the following identity was originally used for a discretization of (3b):

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

This reformulation and the blue term are needed to have energy estimates.

- The purple term is needed to control $d_t \boldsymbol{\mathcal{Y}}$. This regularity is needed in order to pass to the limit in the discrete optimality conditions.

Theorem 4. *There exists a solution $\{(\rho^n, \boldsymbol{y}^n, p^n)\}$ of* (6) *with the property*

$$0 < \rho_1 \le \rho^n \le \rho_2 < \infty$$

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

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

Theorem 5. *For a corresponding discrete functional of* (4)*, the discrete optimization problem subject to* (6)*, has at least one solution and there exist corresponding Lagrange multipliers.*

Theorem 6. *The time interpolants $(\mathcal{R}, \boldsymbol{\mathcal{Y}}, \mathcal{P})$ and the time interpolants of the corresponding Lagrange multipliers converge to a solution of the optimality system from Theorem 3.*

4. Outlook and open questions

- Relative scalings of ε and δ for $\varepsilon, \delta \to 0$? Γ-convergence of (4) towards (1) involving corresponding constraints?
- What is an effecient and convergent way to implement the problem?

References

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