Controlling Sliding Droplets with Optimal Contact Angle Distributions and a Phase Field Model

Henning Bonart[1,*], **Christian Kahle**[2], and **Jens-Uwe Repke**[1]

[1] TU Berlin, Fachgebiet Dynamik und Betrieb technischer Anlagen, Straße des 17. Juni 135, 10623 Berlin, Germany

[2] TUM, Zentrum Mathematik, Boltzmannstraße 3, 85748 Garching b. München, Germany

We consider the optimal control of a droplet on a solid by means of the static contact angle between the contact line and the solid. The droplet is described by a thermodynamically consistent phase field model from [Abels et al., Math. Mod. Meth. Appl. Sc., 22(3), 2012] together with boundary data for the moving contact line from [Qian et al., J. Fluid Mech., 564, 2006]. We state an energy stable time discrete scheme for the forward problem based on known results, and pose an optimal control problem with tracking type objective.

1 Introduction

We are concerned with optimal control of droplets where the static contact angle between solid and droplet serves as a control variable. As a mathematical model we consider the Navier–Stokes Cahn–Hilliard equations with a moving contact line model. The bulk model is the thermodynamically consistent model from [1], while the boundary data are taken from [2] and contain generalized Navier boundary conditions for the Navier–Stokes equation together with dynamically advected boundary conditions for the moving contact angle. In this model the two phases forming the contact line are described by a phase field function φ together with a chemical potential μ. The velocity field is denoted by v together with a pressure field p.

2 The time discrete forward model

We consider the following time discrete system and refer to [3] for more details. Let $\Omega \subset \mathbb{R}^n$ with boundary $\partial\Omega$ and $t_0 < t_1 < \ldots < t_{m-1} < t_m < \ldots t_M$ be an equidistant subdivision of the time interval $[0, T]$ with $t_m - t_{m-1} =: \tau$. Moreover, let φ_0 and v_0 be given. For $m = 1, \ldots, M$ we solve the following system of equations

$$\frac{1}{\tau}\left(\frac{\rho^m + \rho^{m-1}}{2}v^m - \rho^{m-1}v^{m-1}, w\right) + a(k^{m-1}, v^m, w) + (2\eta^{m-1}Dv^m, Dw) - (\operatorname{div} w, p^m)$$
$$+ (\varphi^{m-1}\nabla\mu^m, w) - (g\rho^{m-1}, w) + (l^{m-1}v_{tan}^m + rB^m\nabla\varphi^{m-1}, w)_{\partial\Omega} = 0, \tag{1}$$
$$-(\operatorname{div} v^m, q) = 0, \tag{2}$$
$$\frac{1}{\tau}(\varphi^m - \varphi^{m-1}, \Psi) - (v^{m-1} - \tau(\rho^{m-1})^{-1}\varphi^{m-1}\nabla\mu^m, \varphi^{m-1}\nabla\Psi) + b(\nabla\mu^m, \nabla\Psi) = 0, \tag{3}$$
$$\sigma\epsilon(\nabla\varphi^m, \nabla\Phi) + \frac{\sigma}{\epsilon}(W'(\varphi^{m-1}) + S_W(\varphi^m - \varphi^{m-1}), \Phi) - (\mu^m, \Phi)$$
$$+ \left(rB^m + \gamma'(\varphi^{m-1}) + S_\gamma(\varphi^m - \varphi^{m-1}), \Phi\right)_{\partial\Omega} = 0, \tag{4}$$

where w, q, Ψ, and Φ are suitable test functions. We abbreviate $(u, v) := \int_\Omega uv$ and $(u, v)_{\partial\Omega} := \int_{\partial\Omega} uv$. Here $l^{m-1} := l(\varphi^{m-1})$, $\rho^{m-1} := \rho(\varphi^{m-1})$, and $\eta^{m-1} := \eta(\varphi^{m-1})$, denote the evaluations of given functions l, representing the slip length, ρ, representing the density, and η, representing the viscosity. Further abbreviations are $k^{m-1} := \rho^{m-1}v^{m-1} - b\frac{\partial\rho}{\partial\varphi}(\varphi^{m-1})\nabla\mu^{m-1}$, $B^m := \left(\frac{1}{\tau}(\varphi^m - \varphi^{m-1}) + v^m \cdot \nabla\varphi^{m-1}\right)$, and $a(u, v, w) = \frac{1}{2}\left(\int_\Omega(u \cdot \nabla)v \cdot w\, dx - \int_\Omega(u \cdot \nabla)w \cdot v\, dx\right)$. The tangential part of v^m is denoted v_{tan}^m.

Further constant parameters are the gravitational acceleration g, the mobility b, the scaled surface tension $\sigma = c_W\sigma_{12}$, where c_W is a scaling constant depending on the free energy potential $W = \frac{1}{4}(1 - \varphi^2)^2$ and σ_{12} denotes the surface tension between the two phases, the interfacial thickness parameter ϵ, and a relaxation parameter r.

The contact line energy $\gamma(\varphi)$ is given by $\gamma(\varphi) = \frac{1}{2}(\sigma_{s1} + \sigma_{s2}) + \sigma\cos\theta_s\vartheta(\varphi)$, where ϑ satisfies $\vartheta(-1) = -\frac{1}{2}$ and $\vartheta(1) = \frac{1}{2}$ such that $\gamma(-1) = \sigma_{s2}$ and $\gamma(1) = \sigma_{s1}$ holds by Young's law, where $\sigma_{s1/s2}$ denote the surface tension between solid and phase 1, respectively phase 2, and ϑ_s denotes the static contact angle.

The existence of a solution to (1)–(4) follows by Galerkin approach and Brouwer's fixpoint theorem, following [4].

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* Corresponding author: e-mail henning.bonart@tu-berlin.de, phone +49 (0)30 314 23418

PAMM · Proc. Appl. Math. Mech. 2019;**19**:e201900223.   www.gamm-proceedings.com

https://doi.org/10.1002/pamm.201900223   © 2020 The Authors *Proceedings in Applied Mathematics & Mechanics* published by Wiley-VCH Verlag GmbH & Co. KGaA Weinheim

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3 The optimal control problem

In the following we identify $u^m(x) := \cos(\theta_s(t_m, x))$, $m = 1, \ldots, M$, as control variable that can be chosen freely in space and time on some portion $\Gamma_c \subset \partial\Omega$ to influence the distribution of φ. Notice that this especially means, that the static contact angle can be chosen arbitrarily in space and time. In practice physical and manufacturing constraints apply. On $\partial\Omega \setminus \Gamma_c$ we use a given static contact angle. Let $\varphi_d(t, x)$ denote a desired distribution of the droplet over space in time.

We consider the following optimization problem.

$$\min_{u \in (L^2(\Gamma_c))^M} \frac{\tau}{2} \sum_{m=1}^{M} \int_{\Omega} |\varphi^m - \varphi_d(t_m)|^2$$

such that $(1) - (4)$ with $\cos(\theta_s) =: u^m$

$$\cos(\theta_{\min}) \leq u^m \leq \cos(\theta_{\max}).$$

Here $\theta_{\min}$ and $\theta_{\max}$ are given minimum and maximum static contact angles.
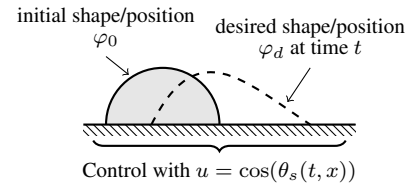

Fig. 1: Setup of the optimal control problem.

4 Numerical results

For a numerical realization we discretize (1)–(4) in space using piecewise quadratic finite elements for v and piecewise linear elements for φ, μ, and p. These are provided by the finite element library FEniCS [5] together with the linear algebra package PETSc [6]. The adjoint and the gradient are derived by automatic differentiation using dolfin-adjoint [7]. The software IPOPT [8] is applied for the solution of the optimization problem. As a test example, we consider a single droplet on a flat surface, see Figure 1. The top row in Figure 2 shows the desired shape and position of the droplet for specific time intervals. We specify an asymmetric φ_d which changes three times over the optimization horizon. The second row shows the calculated shape of the droplet whereas the third row shows the optimal distribution of θ_s.
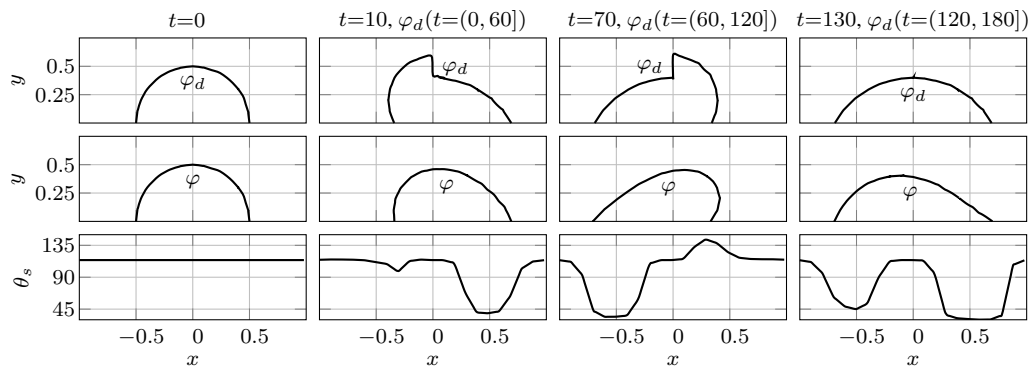

Fig. 2: Desired and calculated shapes and positions of the droplet φ_d respectively φ (top and second row) together with the optimal contact angle distributions (bottom row) at four different instances of time.

This is a first prove of concept that the static contact angle can be used to control a droplet. An investigation of the influence of the droplet properties on the optimal contact angle distribution and the ability to reach the objective is subject to future work.

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