

**Project Description – Project Proposal: Dr. Dirk Peschka, Weierstrass Institute, Berlin**

# Mathematical modeling and simulation of substrate-flow interaction using generalized gradient flows

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## Project Description

### 1 State of the art and preliminary work

When considering bulk fluid flow, the main source of energy dissipation that is usually considered is the fluids *viscosity*. As soon as one takes into account the interaction of the fluid with a substrate, one needs to consider further mechanisms of *energy dissipation*: The generally accepted (linear) boundary condition at the fluid-substrate interface is the *Navier-slip* condition

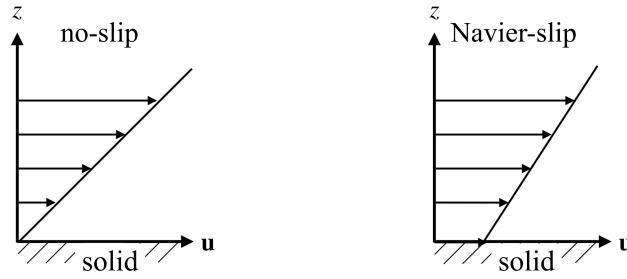
$$\mathbf{t} \cdot \boldsymbol{\tau} \mathbf{n} = -\mu_\Gamma \mathbf{u} \cdot \mathbf{t}. \quad (1)$$

It states that shear-stress  $\mathbf{t} \cdot \boldsymbol{\tau} \mathbf{n}$  and slip-velocity  $\mathbf{u} \cdot \mathbf{t}$  at the interface are proportional and thereby effectively assigns a certain amount of dissipation  $\frac{1}{2}\mu_\Gamma|\mathbf{u} \cdot \mathbf{t}|^2$  to that interface. Sending the corresponding friction coefficient  $\mu_\Gamma$  to infinity lets one recover the classical *no-slip* boundary condition, whereas for vanishing friction coefficient one recovers a *no-shear-stress* boundary condition. Additionally considering moving contact lines with no-slip condition, the impact of microscopic properties, e.g., surface roughness or chemical heterogeneities, on the dynamics at macroscopic scales becomes apparent but its description is complicated due to the appearance of singular stresses at the contact line. While the Navier-slip condition makes this singularity integrable, adding further *contact line dissipation* allows it to introduce models for *dynamic contact angles*. Obviously, the phenomena observed in reality, e.g., pattern formation, time-scales etc., can be drastically different depending on the magnitude of each of these contributions to the dissipation.

Taking into account additional physics in the substrate or on the interface can give these energetic contributions a concrete interpretation: *soft substrates* deform and have dissipation on their own; *surfactants* can move from bulk/surface (soluble/insoluble) liquid to the substrate and modify the surface energy; liquids can diffuse/flow into *porous substrates* and modify interface dissipation. In all of the above cases there is an intricate nonlinear interaction of flow and substrate physics. However, even without such a nonlinear coupling, the control of global and local surface energy and dissipation properties can be used to *control the flow* in a desired direction or to produce certain desired *dewetting patterns*. Hence, this motivates the goal of this proposal:

**Goal:** *The development of thermodynamically consistent models and numerical schemes for substrate-flow coupling and for control of flow based on energy-dissipation formulations for bulk, interfaces, and the contact line of the multiphysics system. The primary focus will be the embedding of dynamic contact angles into settings with strong substrate-flow coupling.*

The goal of the Priority Programme 2171 is to obtain a fundamental and deep understanding of the dewetting & wetting of flexible, adaptive and switchable substrates from an experimental and theoretical point-of-view. As this shall be restricted to simple liquids, this implies a simple relationship of stress  $\boldsymbol{\tau}$  and velocity  $\mathbf{u}$ , i.e.,  $\boldsymbol{\tau} = \boldsymbol{\tau}(\mathbb{D}\mathbf{u})$  where  $\mathbb{D}\mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top)$ . However, even for simple fluids the partial differential equations (PDE) for dewetting are highly nonlinear due to the fact that the Navier-Stokes problem is coupled to the motion of a time-dependent domain and thereby becomes a *free boundary problem*. Treating such a physical problem alone presents a couple of mathematical challenges. Furthermore, the strong coupling to substrate



**Figure 1:** Sketch of near-substrate flow profile (**left**) with no-slip and (**right**) Navier-slip.

dynamics requires a systematic method to introduce physical and mathematical feasible coupling mechanisms, *i.e.*, in the sense of *Onsager reciprocity* or *thermodynamic consistency* [1, 2, 3].

**Navier-Stokes Free Boundary Problem with Contact Lines:** For incompressible Newtonian fluids with viscosity  $\mu > 0$  the relation of velocity  $\mathbf{u}(t, \mathbf{x}) \in \mathbb{R}^d$  at time  $t$  in the domain  $\Omega(t) \subset \mathbb{R}^d$  and the stress tensor  $\boldsymbol{\tau}(\mathbf{u}) : \Omega \rightarrow \mathbb{R}^{d \times d}$  is given by

$$\boldsymbol{\tau}(\mathbf{u}) = 2\mu \mathbb{D}\mathbf{u}. \quad (2)$$

While  $\boldsymbol{\tau}(\mathbf{u})$  is the prototype tensor for bulk effects of simple viscous flows, the no-slip condition

$$\mathbf{u} = \mathbf{0} \quad \text{on} \quad \Gamma(t), \quad (3)$$

is assumed to be the prototype boundary condition at solid-fluid interfaces  $\Gamma$ . Balance of momentum and mass then lead to the Navier-Stokes equation in a time-dependent domain  $\Omega(t)$

$$\partial_t(\rho\mathbf{u}) + \mathbf{u} \cdot \nabla(\rho\mathbf{u}) = -\nabla p + \operatorname{div} \boldsymbol{\tau}(\mathbf{u}) + \mathbf{f}, \quad \nabla \cdot \mathbf{u} = 0, \quad (4)$$

where we seek the velocity  $\mathbf{u}(t, \cdot) : \Omega(t) \rightarrow \mathbb{R}^d$  and the pressure  $p(t, \cdot) : \Omega(t) \rightarrow \mathbb{R}$ . This partial differential equation is coupled with appropriate conditions at boundaries, interfaces, contact lines and provided with initial data  $\mathbf{u}(t = 0, \cdot) = \bar{\mathbf{u}}$  and  $\Omega(t = 0) = \bar{\Omega}$ . The domain  $\Omega(t)$  evolves according to a *kinematic condition*, which makes this PDE problem a free boundary problem. In a microfluidic setting the no-slip boundary condition (3) is often replaced by the Navier-slip condition in (1), where the friction coefficient  $\mu_\Gamma := \mu/b > 0$  is associated with the well-known *slip length*  $b$ , see also Fig. 1. In particular, for flows near a moving contact line  $\partial\Gamma(t)$ , the Navier-slip condition offers one out of various possible mechanism to remove the non-integrable stress singularity at a sliding contact line [4]. Influenced by physical and chemical interface properties such as hydrophobicity, surface roughness, coating or viscoelastic properties, different measuring techniques have found slip-lengths ranging from a few nanometers up to several micrometers, also indirectly visible by its impact on pattern formation processes. The validity of slip in microfluidic settings is undisputed nowadays [5]. Thin-film models with different magnitudes of dissipation  $\mu_\Gamma$  have been investigated in [6] and were extended to multiphase flows in [P1].

Free boundary problems become more complex when considering moving contact lines. Interfacial tensions between solid-vapor  $\gamma_{SV}$ , solid-liquid  $\gamma_{SL}$  and liquid-vapor  $\gamma$  lead to equilibrium contact angles  $\vartheta = \vartheta_e$  determined by the famous Young-Dupré equation

$$\gamma(\cos(\vartheta_e) - 1) = S \quad \text{at} \quad \partial\Gamma(t), \quad (5)$$

with spreading coefficient  $S = \gamma_{SV} - (\gamma_{SL} + \gamma)$  on rigid substrates or by the Neumann triangle construction when considering soft elastic or liquid substrates. The physics becomes even more

involved for contact lines moving over *physically realistic nonideal surfaces*, e.g., which are not perfectly smooth, rigid or chemically homogeneous. While molecular kinetic models are useful to understand the microscopic origins of contact line motion, this proposal employs hydrodynamic descriptions with sharp interfaces. Primarily for liquid-liquid-solid junctions rolling motion was observed and thermodynamic descriptions have been developed, e.g., [7, 8], but the focus here is on sliding motion and stick-slip. For sliding contact lines, models with contact angle hysteresis/stick-slip and empirical laws for contact line dynamics are discussed in the literature, e.g., see [9, 10]. In the Young-Dupré equation (5) the spreading coefficient needs to be replaced using the Cassie-Baxter relation with the homogenized coefficient  $\bar{S}$  [11].

However, the corresponding equilibrium angle might never be attained. Due to pinning at microscopic defects, the contact line is stationary for contact angles  $\vartheta_r < \vartheta < \vartheta_a$  and only starts to advance or recede beyond these values. Models for smooth contact line dynamics without hysteresis are often based on empirical laws and microscopic theories. For instance, assuming an energy-dissipation balance truncated at a microscopic length scale  $\ell$  and with a macroscopic length scale  $L$  away from the contact line, the theory by Cox and Voinov predicts  $\vartheta^3 - \vartheta_e^3 = \pm 9 \text{Ca} \ln(L/\ell)$ , where the Capillary number  $\text{Ca} = \mu U / \gamma$  depends on dynamic viscosity  $\mu$ , surface tension  $\gamma$  and contact line velocity  $U$  [12]. Another contact line model by Ruschak and Hayes produces a similar law, which, however, was derived from a molecular-kinetic model of wetting using dissipation at the contact line [13]. Most models considered in the literature are of the form  $W(\vartheta, \vartheta_e) = \pm \text{Ca}$  with power-law dependence on angles and  $W(\vartheta_e, \vartheta_e) = 0$ . Using such a dynamic contact angle, one can make predictions for dewetting rates of complex systems, e.g., liquid dewetting, droplet spreading or gravity-driven droplet motion. On the continuum level, an energetic approach to such phenomena can be achieved using variational structures, e.g., see [14], where the corresponding contact line model is

$$\gamma(\cos \vartheta_e - \cos \vartheta) = \mu_\gamma \boldsymbol{\nu}_x \cdot \mathbf{u}_x. \quad (6)$$

**Thermodynamics, Gradient Flows, and the Role of Dissipation:** Nowadays, variational principles are widely used to model complex physical systems with partial differential equations derived from purely energetic arguments, see e.g. [15, 3]. General variational approaches for complex fluids often rely on a classification of dissipative or nondissipative kinematics, e.g., see [16, 17, 18]. For wetting and dewetting flows flows on rigid substrates such formulations have amplified the physical and mathematical understanding of the corresponding free boundary problems [19]. The GENERIC<sup>1</sup> framework of reversible and irreversible processes proposed by Öttinger and Grmela [17] is an advanced variational structure that has been used extensively to model complex fluids, e.g., nonlinear viscoelastic polymers. This construction has been formalized to model a number of thermodynamical processes with convection and diffusion, e.g., [20] and [P2] and transferred to simulations, e.g., see [21].

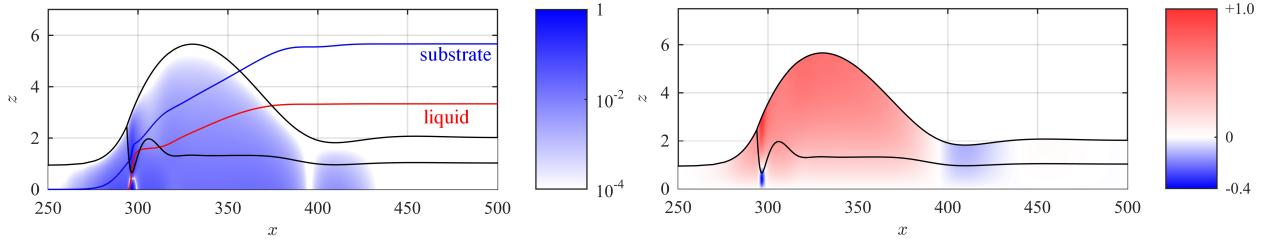
To define a gradient flow, let  $q \in Q$  be a generalized state with velocities  $\dot{q} \in V$ . Then its evolution, driven by a thermodynamic potential  $\mathcal{E} : Q \rightarrow \mathbb{R}$  such as the free energy, is given by

$$\dot{q}(t) = -\nabla_g \mathcal{E}(q(t)), \quad (7a)$$

where the gradient with respect to the positive symmetric bilinear form  $g_q : V \times V \rightarrow \mathbb{R}$  is defined  $g_q(\nabla_g \mathcal{E}(q), v) = \langle D\mathcal{E}(q), v \rangle$  for all  $v \in V$  and functional derivative  $D\mathcal{E}(q) \in V^*$ . The decay of the (free) energy  $\frac{d}{dt} \mathcal{E}(q(t)) \equiv \langle D\mathcal{E}(q), \dot{q} \rangle = -g_q(\dot{q}, \dot{q}) \leq 0$  holds by construction using (7a).

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<sup>1</sup>an acronym for General Equations for Non-Equilibrium Reversible Irreversible Coupling



**Figure 2:** Dewetting from soft substrate [P4] (**left**) log-scale local dissipation and (**right**) corresponding local velocity.

Defining  $\mathcal{D}(v) = g_q(v, v)$  we can state an evolution equation that is formally equivalent to (7a):

$$\dot{q} = \operatorname{argmin}_{v \in V} \left( \frac{1}{2} \mathcal{D}(v) + \langle D\mathcal{E}, v \rangle \right). \quad (7b)$$

In the context of fluid flows, this is the Helmholtz-Rayleigh dissipation principle for the dissipation functional  $\mathcal{D} : V \rightarrow \mathbb{R}$  where the velocity corresponds to the flow field  $\dot{q} \simeq \mathbf{u}$  and correspondingly  $v \simeq \mathbf{v}$ . For Newtonian fluids the bulk dissipation is  $\mathcal{D}_{\text{bulk}}(\mathbf{v}) = \int_{\Omega} 2\mu \mathbb{D}\mathbf{v} : \mathbb{D}\mathbf{v} \, dx$  and in [P3] it was demonstrated that a formal gradient structure can be established based on a further decomposition of the total dissipation into contributions  $\mathcal{D} = \mathcal{D}_{\text{bulk}} + \mathcal{D}_{\text{bound}} + \mathcal{D}_{\text{cl}}$ , where

$$\mathcal{D}_{\text{bound}} = \int_{\Gamma \subset \partial\Omega} W_{\text{bound}}(\mathbf{u}) \, da, \quad \mathcal{D}_{\text{cl}} = \int_{\partial\Gamma} W_{\text{cl}}(\mathbf{u}) \, d\ell, \quad (8)$$

and allows it to designate some of the effective substrate-flow interaction into dissipative mechanism. Modeling of dissipation has been extensively discussed for the Navier-slip condition [5] encoded in the boundary term  $W_{\text{bound}}$ , but a detailed study of contact line dynamics based on the dissipation  $W_{\text{cl}}$  is still elusive.

**Coupling Flow via Interfaces with Substrates:** However, variational approaches are also highly useful when considering strongly and nonlinear coupled PDE problem. In a previous study on dewetting from liquid substrates, we showed that explicitly considering the substrate dissipation produces a much deeper understanding of the underlying physical mechanisms [P4], see also Fig. 2. These results were based on an earlier work [P5], where we showed that the gradient flow structure is even useful for the design of complex coupled numerical algorithms with moving contact lines. In this work we developed a gradient flow based algorithm for a thin-film flow dewetting from soft (liquid) substrate [P5], *i.e.*,

$$\partial_t \begin{pmatrix} h_\ell \\ h_s \end{pmatrix} - \nabla \cdot \mathbb{M} \nabla \begin{pmatrix} \pi_\ell \\ \pi_s \end{pmatrix} = 0, \quad \text{wetted area } \omega, \quad (9)$$

$$\partial_t h_s - \nabla \cdot m \nabla \pi_s = 0, \quad \text{dewetted area } \mathbb{R}^{d-1} \setminus \omega, \quad (10)$$

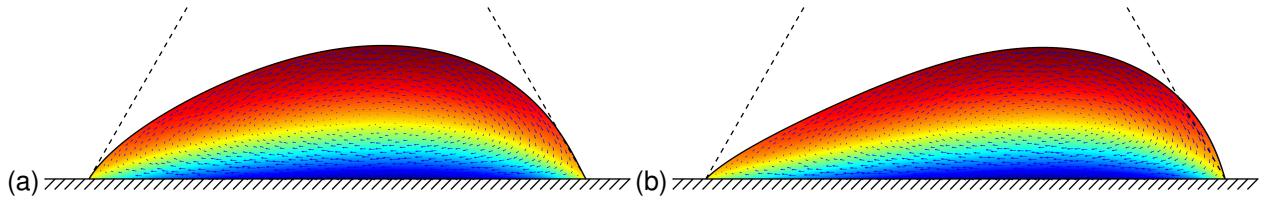
where  $h_s$  encodes the substrate film thickness,  $h_\ell$  is the liquid film thickness as shown in the black lines in Fig. 2, and  $\pi_i$  are the generalized pressures. The main challenge was the construction of a monolithic time-discretization, which features a force balance (Neumann triangle) at the moving contact line  $\partial\omega$  enforced and a corresponding ALE scheme. The corresponding Stokes flow is based on the dissipation

$$\mathcal{D}(\mathbf{u}_s, \mathbf{u}_\ell) = \int_{\Omega_s} 2\mu_s |\mathbb{D}\mathbf{u}_s|^2 \, dx + \int_{\Omega_\ell} 2\mu_\ell |\mathbb{D}\mathbf{u}_\ell|^2 \, dx + \int_{\Gamma} \mu_\Gamma |\mathbf{u}_s - \mathbf{u}_\ell|^2 \, da, \quad (11)$$

and a corresponding solution for  $\mu_\Gamma \rightarrow \infty$  is shown in Fig. 4. Both, Stokes and thin-film are solved

using a finite-element method (FEM) and required the construction of discrete spaces with discontinuous solutions at interfaces/contact lines. Considering the quantitative agreement obtained in [22] and [P4] the thin-film model delivers a prediction in terms of a more efficient/reduced problem formulation. In [P1] we also showed that with finite  $\mu_\Gamma$  corresponding Navier-slip conditions in a multilayer setup can be systematically enforced and a mathematical analysis of stationary solutions was performed in [P6]. In a recent work [23] on multiphase flows (dense suspensions) we worked on the dissipation modeling for suspension flows based on a flow-map concept. This concept is particularly important for complex liquids, but can be easily extended to the problems studied in the Priority Programme: While the fluid behavior is simple and  $W_{\text{bulk}}$  is basically Newtonian, the substrate interaction should be rather complex, possibly leading to complicated interaction mechanisms encoded in boundary and contact line dissipation.

**Numerical Methods for Free Boundary Problems with Contact Lines:** Fluid flows with moving domains are modeled either using diffuse or sharp interface representations. This proposal will focus on the latter and use interface-tracking and ALE methods<sup>2</sup> with conforming finite-elements. This approach has the advantage that it allows a finer control over solutions near contact lines and near interfaces but is problematic for handling topological transitions. For diffuse interface models, on the other hand, topological transitions are unproblematic [24] but require spatial adaptivity to ensure the correct behavior for vanishing layer width.



**Figure 3:** Numerical solution of Stokes flow for 2D sliding droplet with gravity in  $+x$  direction (a) with equilibrium angle  $\vartheta = \vartheta_e$  indicated by dashed lines and (b) with smooth dynamic contact angle as in (6) and flow field (arrows  $\sim \mathbf{u}(t, \mathbf{x}) - \bar{\mathbf{u}}$  in comoving frame; shading  $\sim \mathbf{u}(t, \mathbf{x})$  in Eulerian frame) with advancing and receding contact angle.

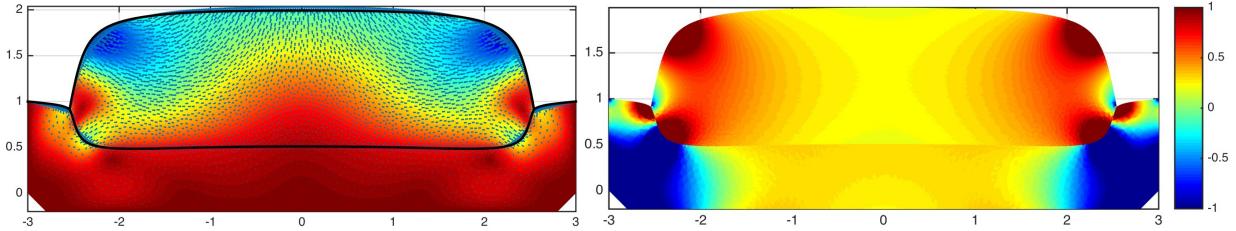
We will couple ALE methods to gradient flow based models, where the fluid dynamics is strongly coupled to the substrate. Therefore, the main ingredient is a flow map  $\mathbf{X}_t : \bar{\Omega} \rightarrow \mathbb{R}^d$  mapping the reference domain  $\bar{\Omega} = \Omega(t=0)$  to its later state  $\Omega(t) \subset \mathbb{R}^d$ . The corresponding flow field is  $\mathbf{u} = (\partial_t \mathbf{X}_t) \circ \mathbf{X}_t^{-1}$ . Numerical algorithms for fluid flow with moving domains usually solve for  $\mathbf{X}_t$ , where a single step of the time-discretization with flow maps is solved in a spatially fixed frame and one can linearize  $\mathbf{X}_{t_0 \rightarrow t_0 + \Delta t}(\mathbf{x}) = \mathbf{X}_{t_0 + \Delta t} \circ \mathbf{X}_{t_0}^{-1}(\mathbf{x}) \approx \mathbf{x} + (\Delta t)\mathbf{u}(t_0, \mathbf{x})$ . In the literature also higher-order ALE schemes are discussed, e.g. [25]. The spatial discretization of the Stokes free boundary problem for an incompressible fluid uses inf-sup stable isoparametric mixed finite-element pairs, most commonly  $P_2/P_1$  or  $P_2^{\text{bubble}}/P_1^{\text{disc}}$  [26]. The weak formulation of the Stokes problem is a saddle-point problem of the form: Find  $(\mathbf{u}, p) \in (H_0^1(\Omega))^d \times L^2(\Omega) = W$  such that  $a(\mathbf{u}, \mathbf{v}) + (-\nabla p, \mathbf{v})_{L^2} + (q, \nabla \cdot \mathbf{u})_{L^2} = f(\mathbf{v})$  for all  $(\mathbf{v}, q) \in W$ . If the flow is driven by surface energy  $\mathcal{E}_{\text{surf}} = \gamma |\Gamma_f|$ , then we get  $f(\mathbf{v}) = \langle -D\mathcal{E}_{\text{surf}}, \mathbf{v} \rangle$  and obtain the weak form [P3]

$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} 2\mu \mathbb{D}\mathbf{u} : \mathbb{D}\mathbf{v} \, dx, \quad f(\mathbf{v}) = - \int_{\Gamma_f} \gamma \operatorname{div}_{\Gamma}(\mathbf{v}) \, da = \int_{\Gamma_f} \gamma \kappa \nu \cdot \mathbf{v} \, da. \quad (12)$$

This indicates how the weak formulation of the problem, including boundary and interface conditions, naturally emerge from energy functionals. Typical numerical issues which arise in such an ALE framework are that the time-discretization suggests a (semi)implicit treatment of the cur-

<sup>2</sup>Acronym for Arbitrary Lagrangian Eulerian referring to methods, where the frame of reference is between Lagrangian (material) and Eulerian (current) point-of-view.

vature, that higher regularity requires to unravel the dependence of dissipation  $\mathcal{D}$  and energy  $\mathcal{E}$  on the state  $\mathbf{X}_t$ , that moving the triangulation according to  $T_k(t) = \mathbf{X}_t(T_k(0))$  has an impact on mesh quality, and that one should avoid spurious velocities. For multiphase flows a common strategy is to enrich the  $L^2$  pressure space approximated by  $P_1$  finite-element functions with an element-wise discontinuous part in  $P_1^{\text{disc}}$ , that is able to absorb the pressure-jump as shown in Fig. 4. For the simulation of bilayer dewetting a related methodology was also used in [P7]. The resulting speed of convergence depends on both the choice of the FE space and on the resolution of the interface.



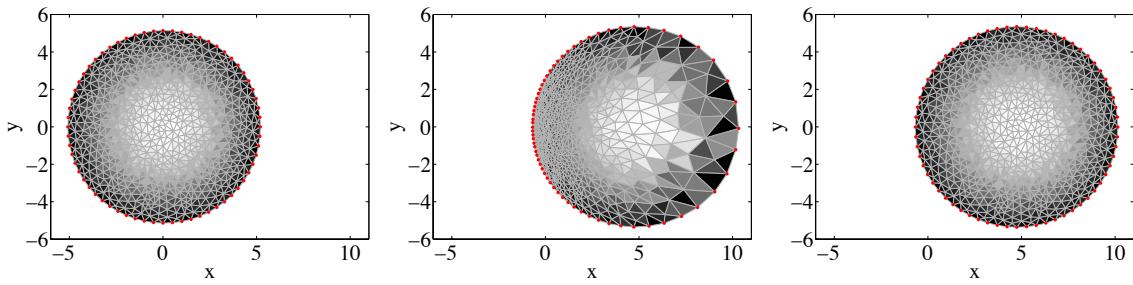
**Figure 4:** Droplet for  $\Omega(t) \subset \mathbb{R}^2$  on a liquid substrate showing (**left**) direction and magnitude of the flow field  $\mathbf{u}$  and the free interfaces and (**right**) the discontinuous pressure with resolved jumps across internal interfaces.

Another problem of ALE methods is caused by the moving mesh, which can become anisotropic or corrupted or develop mathematical & numerical singularities when approaching a topological transition, e.g., corresponding to merging and splitting droplets during film rupture or pinch-off. This is usually addressed using spatial and temporal adaptivity and sophisticated ALE methods to improve the mesh motion [27]. A similar ALE strategy was also used in the  $d = 3$  thin-film setting in [P8] to maintain mesh quality for a longer time, e.g., see Fig. 5.

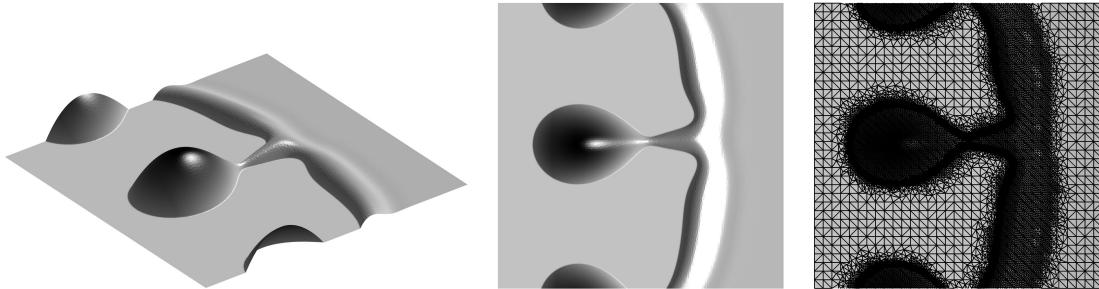
Thin-film models are reduced models that are easier to analyze and solve. Often, they give qualitative explanation for physical mechanisms [O1] or even quantitative predictions [P4]. Assume the time-dependent domain  $\Omega(t) = \{\mathbf{x} \equiv (x, z) \in \mathbb{R}^{d-1} \times \mathbb{R}_{\geq 0} : 0 < z < h(t, x)\} \subset \mathbb{R}^d$  is parametrized using  $h(t, x) \geq 0$  and  $|\nabla h| \ll 1$ , then the Stokes equation on a planar solid surface can be reduced [28] to a thin-film type equation of the form

$$\partial_t h - \nabla_x \cdot (m(h) \nabla_x \pi) = 0, \quad \pi = \frac{\delta}{\delta h} \mathcal{E}(h), \quad \mathcal{E}(h) = \int_{\mathbb{R}^{d-1}} \frac{1}{2} |\nabla h|^2 dx + V(h). \quad (13)$$

with degenerate mobility  $m(h)$ . The thin-film framework is powerful, since it can describe many wetting and dewetting flows quantitatively, e.g., [29] and [P9] and [P4], while maintaining the mathematical complexity of the a free boundary problem [30]. Considerable work was devoted to the study of global solutions, where  $h$  is nonnegative and defined on the entire domain and where algorithms ensure these properties [31, 32]. However, as also suggested by analytical results in [30] and introduced as a numerical algorithm in [P8], the problem should be interpreted as a free boundary problem, where the support set  $\omega(t) = \{x \in \mathbb{R}^{d-1} : h(t, x) > 0\}$  depends on time and evolves due to a kinematic condition. We call corresponding solutions  $(h, \omega)$  of the thin-film equation also **supported solutions**. Alternative approaches regularize the energy by replacing  $V$  by a *precursor potential*  $V_\delta(h) = \int (-S) W(h/\delta) dx$  where  $W(h) = 1 + (m-n)^{-1}(mh^{-n} - nh^{-m})$  and thereby remove the nonsmoothness of  $V(h) = (-S)|\omega|$ . While the degeneracy of  $m(h) \sim h^\sigma$  ( $0 < \sigma < 3$ ) in (13) is sufficient to ensure nonnegativity of  $h$  [33], these intermolecular potentials  $V(h)$  are often also used to enforce positivity of solutions [34]. Numerical solutions of the regularized problem require local spatial adaptivity as shown in Fig. 6. However, it appears that only supported solutions allow the systematic inclusion of contact line physics and in particular of dynamic contact angles into a long-wave framework [P3].



**Figure 5:** Harmonic ALE mesh motion (**left**) starting point at  $t = 0$  and (**middle**) at final position  $t = 14$  transport purely in normal direction deteriorates the mesh but (**right**) with artificial tangential velocity mesh is preserved.



**Figure 6:** Dewetting thin film with regularized energy  $\mathcal{E}_\delta$  (**left**) 3D view of the function  $h(t, x)$  (**middle**) top view and (**right**) top view with locally refined mesh.

**Summary:** Variational methods based on dissipative processes have become an important tool for modeling of complex fluids. But also for simple fluids with complex coupling to substrate dynamics variational methods are essential for coupling of PDEs across interfaces in a consistent manner and to derive advanced models for dynamic contact lines. The author of this proposal has developed several novel theoretical frameworks to model, analyse, and simulate *nonlinearly coupled PDEs* and *free boundary problems*, in particular in the context of thin films.

## 1.1 Project-related publications

### 1.1.1 Articles published by outlets with scientific quality assurance, book publications, and works accepted for publication but not yet published.

- [P1] S. Jachalski, D. Peschka, A. Münch, and B. Wagner, “Impact of interfacial slip on the stability of liquid two-layer polymer films,” *J. Eng. Math.*, vol. 86, 2014.
- [P2] A. Mielke, D. Peschka, N. Rotundo, and M. Thomas, “On some extension of energy-drift-diffusion models: Gradient structure for optoelectronic models of semiconductors,” *Prog. Ind. Math. at ECMI 2016*, vol. 26, 2017.
- [P3] D. Peschka, “Variational approach to contact line dynamics for thin films,” *Phys. Fluids*, vol. 30, 2018.
- [P4] D. Peschka, S. Bommer, S. Jachalski, R. Seemann, and B. Wagner, “Impact of energy dissipation on interface shapes and on rates for dewetting from liquid substrates,” *Sci. Reports*, vol. 8, 2018.
- [P5] R. Huth, S. Jachalski, G. Kitavtsev, and D. Peschka, “Gradient flow perspective on thin-film bilayer flows,” *J. Eng. Math.*, vol. 94, 2015.
- [P6] S. Jachalski, R. Huth, G. Kitavtsev, D. Peschka, and B. Wagner, “Stationary solutions of liquid two-layer thin-film models,” *SIAM J. on Appl. Math.*, vol. 73, 2013.
- [P7] S. Jachalski, D. Peschka, S. Bommer, R. Seemann, and B. Wagner, “Structure formation in thin liquid-liquid films,” in *Transport Processes at Fluidic Interfaces*, Springer, 2017.

- [P8] D. Peschka, "Thin-film free boundary problems for partial wetting," *J. Comput. Phys.*, vol. 295, 2015.
- [P9] S. Bommer, F. Cartellier, S. Jachalski, D. Peschka, R. Seemann, and B. Wagner, "Droplets on liquids and their journey into equilibrium," *The Eur. Phys. J. E*, vol. 36, Aug 2013.

### 1.1.2 Other publications

- [O1] D. Peschka, S. Haefner, K. Jacobs, A. Münch, and B. Wagner, "Signatures of slip in dewetting polymer films," *WIAS preprint No. 2538*, 2018.

## 2 Objectives and work programme

### 2.1 Anticipated total duration of the project

The work programme is composed for a duration of three years starting October 1st, 2019.

### 2.2 Objectives

In this work the proposer's existing results for modeling and simulation using ALE formulations for flows on substrates with dynamic contact angles will be extended to hysteretic motion. The main approach that will be employed is the modeling of dissipative effects in the substrate, on interfaces, and at contact lines. In the long-wave approximation, a framework for the strongly coupled evolution of substrate/interface species and Newtonian bulk flow will be developed. In particular, existing state-of-art results will be extended to include dynamic contact lines using the concept of *supported solutions*. This framework will then be transferred to applications in other projects of the Priority Programme: Pattern formation in dewetting flows, flows over porous substrates, surfactant transport, and the modeling of soft substrates. The common main focus will be the extension to variational formulations with strong coupling of flow and substrate physics.

### 2.3 Work programme incl. proposed research methods

**WP1:** Development of advanced theoretical and numerical methods for long-wave modelling with moving contact lines as the basis for multiphysics models to be used within the SPP.

**Planned Cooperation:** Prof. Axel Voigt (internal, Dresden), Prof. Arnold Reusken (internal, Aachen) Prof. Holger Stark (internal, Berlin), Prof. Uwe Thiele (internal, Münster), Prof. Luca Heltai (external, SISSA, Trieste, Italy).

**Task WP1-1:** *Develop macroscopic long-wave theory and models with moving contact lines to 2D/3D flows with contact angle dynamics with smooth and hysteretic behaviour. (3 months)*

**Description WP1-1:** While the modeling basis for the long-wave theory with contact lines has been described in [P3], the extension to a variational framework including hysteretic contact line motion remains open, even for Stokes flows. Therefore, we will devise different dissipation mechanisms at contact lines, which create physically realistic models for dynamic contact angles, e.g., see [35, 9]. To achieve this task, the strategy of this proposal within the SPP will be two-fold: Firstly, as a proof-of-principle a 2D Stokes flow/thin-film flow solver, which implements contact line dynamics with hysteresis based on generalized gradient flows, will be developed. This will require to solve the nonsmooth convex minimization problem

$$\min_{\mathbf{v} \in V} \left( \frac{1}{2} \mathcal{D}(\mathbf{v}) + \mathcal{J}(\mathbf{v}) + \langle D\mathcal{E}, \mathbf{v} \rangle \right), \quad (14)$$

which transforms the original PDE formulation into a subdifferential inclusion for the nonsmooth contribution to the dissipation  $\mathcal{J}$  and can be solved by relaxation, augmented Lagrangian techniques, or dualization. Similar methods are popular for flows of Bingham fluids, e.g. cf. [36],

and should be adaptable to this situation. In this task, different methods to solve the nonsmooth problem will be investigated. Furthermore, the formal thin-film reduction will be performed and the corresponding variational structure will be investigated. It will be examined if the resulting problem also has a generalized gradient flow structure, *i.e.*, it can also be written as a nonsmooth (convex) minimization problem. The identification of such a structure will later be useful for the development of advanced numerical methods. Methods for the convex nonsmooth optimization (the generalized gradient flow (14)) will be discussed with M. Hintermüller and T. Surowiec.

**Task WP1-2:** *Develop finite-element based tools to solve these problems using higher-order methods in space and time with sharp-interface ALE methods. (6 months)*

**Description WP1-2:** The first goal of the task WP1-2 is to develop the numerical tools for WP1-1, which then serve as the basis for the remaining tasks, where the dissipative substrate-flow coupling will be implemented. In two spatial dimensions, this amounts to generalizing the numerical code published alongside [P3] to deal with hysteresis in the sense of (14). As the corresponding numerical algorithm is devised to be versatile and simple, it is intended to provide it to a software pool within the SPP, which can be used to advance and discuss numerical methods for contact line motion (and to teach to PhD students). This is also relevant, since nonsmooth PDE settings are not commonly used in the physics community. This implies, in particular, that several strategies for solving the nonsmooth (convex) minimization problem will be also presented and compared numerically. The second goal is to extend these methods to higher dimensions, similar to the methods presented in [P8]. Therefore, the plan of WP1-2 is to include the corresponding algorithm into the FEM library deal.II (<https://dealii.org>), which is work in progress with Luca Heltai, one of the maintainers of this library. The deal.II library provides various mapped finite elements, which therefore allows to develop higher-order methods for problems with moving domains. Some preliminary work in this direction has already become part of deal.II version 9.0.0. The main ingredients to be developed for this purpose is an efficient ALE mesh motion strategy, where maps and the problem finite-element formulation are adjusted to produce a higher-order (isoparametric) PDE formulation.

**Task WP1-3:** *Develop a benchmark for free boundary problem with dynamic contact angles to numerical predictions of other groups within the SPP. (1 month)*

**Description WP1-3:** Within the SPP, several numerical approaches to solve flow problems with free boundaries and contact lines are envisioned, *e.g.*, Arnold Reusken (level set based unfitted finite-element method), Holger Stark (boundary element method), Axel Voigt (phase field methods), and the ALE approach of this proposal (for Stokes and thin-films). The goal of WP1-3 is to define models and benchmarks suited for model validation for all these approaches and including dynamic contact angles. As the work of this proposal is more focussed on thin-films, the corresponding numerical method will be extended to encode the full surface energy, which will give rise to the full mean-curvature instead of the Laplacian in the thin-film equation. In the energetic-variational approach this directly generalizes the dynamic contact angle to the corresponding full evolution law. With Uwe Thiele we will compare supported thin-film solutions (and Stokes) with solutions from precursor approaches (full curvature). As part of the preliminary work, also a 2D Taylor-Hood based solver for the Stokes free boundary problem was developed and contains a dynamic contact angle implementation. It is envisioned to extend this work to a full 3D Stokes solver with isoparametric P2-FEM using an ALE-based mesh motion algorithm.

**WP2:** Extension of the long-wave toolbox to a unified theoretical framework of coupled multiphase reactive transport with moving contact lines, where constituents are defined separately in the fluid, in the substrate, on interfaces, or at contact lines.

**Planned Cooperation:** Prof. Uwe Thiele (internal, Münster), Dr. Georgy Kitavtsev (external, Oxford)

**Task WP2-1:** Extension of the existing framework for mass exchange of bulk and interface to mass exchange across (and affecting) contact lines. (4 months)

**Description WP2-1:** The goal of this work package is to develop a general framework for multiphase transport with moving contact lines, where different means of substrate coupling will be investigated, e.g. cf. [37, 38, 39]. In order to be able to highlight the subtleties of the intended approach, in the following a more detailed account of the modeling approach for this task will be given. A long-wave binary mixtures flow with bulk-concentration  $0 \leq \theta \leq 1$  and film height  $h \geq 0$  involves the vector of transported quantities<sup>3</sup>  $\mathbf{c} = (h, w)$  such that

$$\partial_t \mathbf{c} - \nabla \cdot \left( \mathbb{M}(\mathbf{c}) \nabla \frac{\delta \tilde{E}}{\delta \mathbf{c}} \right) = -\mathbb{G}(\mathbf{c}) \frac{\delta \tilde{E}}{\delta \mathbf{c}}. \quad (15)$$

where  $w = h\theta$  and we have additional boundary conditions. From the modeling point-of-view one can write the energy either  $\tilde{E}(\mathbf{c})$  or  $E(h, \theta)$  and derivatives of  $E$  transform as

$$\pi_h := \frac{\delta}{\delta h} \tilde{E} = \left( \frac{\delta}{\delta h} - \frac{\theta}{h} \frac{\delta}{\delta \theta} \right) E, \quad \pi_w := \frac{\delta}{\delta w} \tilde{E} = \frac{1}{h} \frac{\delta}{\delta \theta} E.$$

A large class of energies, which are important for this type of problem, are of the form

$$E(h, \theta) = \int_a^b \frac{1}{2} |\nabla h|^2 + s(\theta) + h f(h, \theta; x) + \frac{1}{2} \gamma h |\nabla \theta|^2 dx,$$

and  $\mathbb{G}, \mathbb{M} \in \mathbb{R}^{2 \times 2}$  above in (15) are symmetric positive semidefinite. A detailed account of the interpretation of the different *bulk contributions* can be found in [40, 41]. If one considers reaction of the constituents  $\theta$  and  $1 - \theta$  with total volume being conserved and a decomposition into convective and diffusional transport, the following choice is found often

$$\mathbb{G}(\mathbf{c}) = \begin{pmatrix} 0 & 0 \\ 0 & g(h, \theta) \end{pmatrix}, \quad \mathbb{M}(\mathbf{c}) = m(h, \theta) \begin{pmatrix} 1 & \theta \\ \theta & \theta^2 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & d(h, \theta) \end{pmatrix}.$$

so that the only unknown material laws are the scalar functions  $s, f$  and  $g, m, d \geq 0$ . This bulk Onsager structure is well-known [42]. In the SPP, I will consider general classes of mobility matrices  $\mathbb{M}$ , e.g., to facilitate surfactant transport or transport into porous substrates [43]. Also, we will consider *supported solutions*, i.e., we seek the contact line positions  $a(t) < b(t)$  such that  $h(t, \cdot) > 0$  on  $(a(t), b(t))$  and  $h(t, a(t)) = h(t, b(t)) = 0$ . Additionally, for the SPP the inclusion of (sharp) contact line dynamics is important and not considered in the literature. Therefore, in addition to the statement of (15) (with boundary conditions) it is postulated that energy is dissipated according to the balance

$$\frac{d}{dt} \tilde{E}(\mathbf{c}(t)) = -D(\dot{\mathbf{c}}) := - \sum_{i,j=1}^2 \left[ \int_a^b \mathbb{M}_{ij} \nabla \pi_i \nabla \pi_j + \mathbb{G}_{ij} \pi_i \pi_j dx + \int_{\partial[a,b]} \mathbb{R}_{ij} \pi_i \pi_j \right] \leq 0.$$

<sup>3</sup>**Note:** Conventionally one would use transport equations for  $c_1 = \theta$  and  $c_2 = 1 - \theta$ . However, instead we write transport equation for  $\theta$  (total amount of  $c_1$ ) and  $h$  (total volume  $c_1 + c_2$ ).

with a new contribution  $\mathbb{R}(\mathbf{c})$  at the contact line. In order for the total volume to be conserved, we define this contact line reaction term by

$$\mathbb{R}(\mathbf{c}) = \begin{pmatrix} 0 & 0 \\ 0 & r(\mathbf{c}) \end{pmatrix},$$

which is constructed using  $r(\mathbf{c}) \geq 0$  and more general choices of  $\mathbb{R}(\mathbf{c})$  are possible (symmetric, positive semidefinite). In addition to (15), this creates another boundary reaction-term in the  $\theta$ -transport equation. The kinematic condition corresponding to  $h(t, a) = h(t, b) = 0$  is

$$\dot{h} + \dot{a} \cdot \nabla h = 0 \quad \text{and} \quad \dot{h} + \dot{b} \cdot \nabla h = 0, \quad (16)$$

at  $x = a$  and  $x = b$ , respectively. Evaluating (15) and the energy-dissipation balance above produces the multiphase flow equations with mass transport at the contact line. While many works consider Onsager structures for bulk processes, the proposed work will extend this approach and consider dissipation on interfaces and at contact lines, so that flow-substrate coupling can be introduced in a systematic manner. For the application within the SPP, this approach will be further extended in several aspects: the solution vector  $\mathbf{c}$  will include quantities (densities, energies, etc.) defined outside the fluid support  $(a, b)$  and defined in the substrate; further state-dependent dissipation terms at the contact line will be added to include contact angle dynamics. The gradient flow approach constructed here is somewhat similar to the approach used for liquid substrates [P5] but extended due to the concept of reactive flow presented above.

The goal of the task WP2-1 is to extend the variational framework to reactive mass transport starting with the binary case, where the particular novelty will be the coupling of mass transport to sharp contact lines and including nontrivial contact line dynamics. Formal asymptotics similar to [44] will show if the mathematical model, *i.e.*, in particular the contact line dynamics, is admissible. Since also similar Stokes models for binary mixtures exist, *e.g.*, [45], we will also perform the long-wave approximation in order to find regimes with possibly novel transport laws  $\mathbb{M}(\mathbf{c})$  in the strongly coupled cases where  $\theta \rightarrow \theta_{\text{crit}} \leq 1$ . In particular for multiphase flows of (non-colloidal) suspensions there is active research in the direction of understanding jamming transitions, normal pressures, and shear induced migration [46, 47, 48], which is also an interesting application of the strong-coupling, *e.g.*, influence of suspension density on dewetting in Fig. 9. Similar models also play a role in cell-motility problems [44]. In order to couple the fluid flow to an elastic deformable substrate, we will consider the inclusion of algebraic equation into the gradient flow. This is similar to the role of the electrostatic potential in the gradient flow construction for the van Roosbroeck system for charge transport in semiconductors, which is presented in [P2].

The discussion of the bulk-thermodynamics for the reactive transport framework with contact lines is planned to be in cooperation with Uwe Thiele, with a particular focus also on mixtures and surfactant flows. The related application to cell-motility problems will be investigated with Georgy Kitavtsev.

**Task WP2-2:** Develop a general numerical finite-element based framework for fluid-substrate coupling with moving contact lines. (4 months)

**Description WP2-2:** The bulk part of the degenerate parabolic equation is rather standard to implement [34, 49] or [O1]. While the mathematical long-wave theory for the corresponding problem with moving contact lines has been developed in the last years [30, 50], the construction of corresponding versatile numerical algorithms was done in [P8, P3] and [51]. For the topic of surfactant transport and substrate interaction the work by Karapetsas et al. [52] is a notable mention for coupled systems. However, in the proposer's understanding the numerical approach in

that paper lacks the necessary versatility, which the gradient flow approach based on functionals supplied in [P5] delivers.

Therefore, the goal of WP2-2 is to develop a toolbox of FE methods needed to solve problems similar to [P5], where different types of substrate dissipation mechanisms are coupled to contact line dynamics. Possible routes for implementation of the coupling are:

- (mapped) finite-elements for multiphysics problems: degrees of freedom on subdomains; jumps across interfaces; PDEs on interfaces; Lagrange multipliers,
- (classical) numerical strategies for coupling in multiphysics problems: Mortar elements; Lagrange multipliers; domain decomposition; time-splitting,
- time-discretization schemes: explicit/implicit; higher-order; stabilization,
- advance ALE methods from WP1 to flow-substrate coupling (rigid vs elastic substrates).

This toolbox development is also explorative, since the choice of method will certainly depend on the type of considered coupling. While for liquid substrates as considered in [P5] the strong coupling required to solve the fully coupled system in a monolithic way, for fluid-structure interaction problems also splitting or iterative methods can be feasible, e.g., see for Stokes flow [53, 54].

### WP3: Transfer of the developed methodologies within the SPP and externally.

**Planned Cooperation:** Prof. B. Rapp/Dr. D. Helmer (internal, Karlsruhe Institute of Technology), Prof. U. Thiele (internal, Münster), Dr. M. Brinkmann (internal, Saarbrücken), Prof. R. Seemann/Prof. B. Wagner (internal, Saarbrücken & Berlin), Prof. Karin Jacobs (external, Saarbrücken), Prof. Alexander Mielke (external, Berlin)

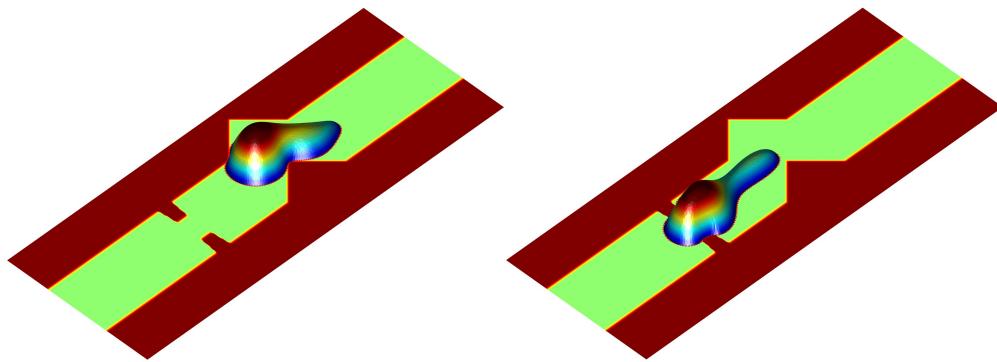
#### Task WP3-1: Control and pattern formation of fluid flow by effective, heterogeneous, and switchable substrates. (6 months)

**Description WP3-1:** The goal of the task to apply the previously developed simulation tools to the experimental situations considered in the SPP. Therefore, the algorithms developed in WP1 and the model framework considered in WP2 will be extended to account for heterogeneous (in space) and switchable (in time) substrate properties. In general, wetting and dewetting of (chemically) heterogeneous substrates with precursor approaches is well studied [55, 56, 57] and is also confirmed experimentally, e.g. [58]. An example for dewetting from a heterogeneous substrate with supported solutions is shown in Fig. 7, where the spreading coefficient is inhomogeneous, so that it is energetically favorable to cover the green instead of the red areas. The corresponding surface energy is

$$E_{\text{surf}}(h) = \int_{\omega} \frac{1}{2} |\nabla h|^2 + f(h, x) dx, \quad (17)$$

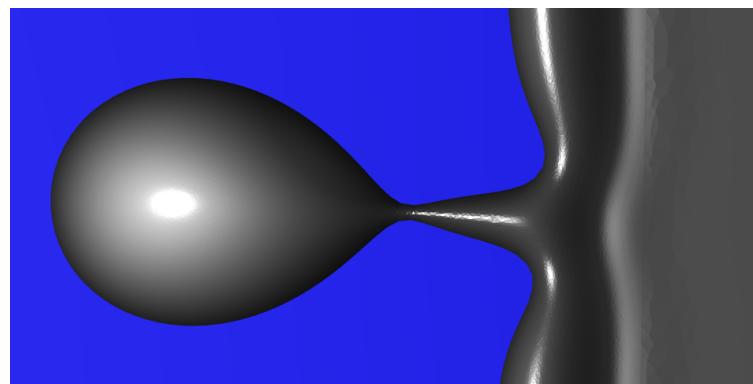
where  $f(h, x) \geq 0$  encodes space-dependent surface (and bulk) energy. In this example a gravity-type force is additionally used to move the droplet over the energetic texture. The advantage of the proposed approach is that within the energetic gradient formulation such a modification is straight-forward to implement. Other properties which will be changed to control of fluid flow are: *modification of magnitude and mechanism for substrate-flow interface condition, anisotropy of substrate-flow slip, oscillating surface energy (roughness and microstructure) and chemically textured surfaces* as shown above. These interface properties can depend on space (heterogeneous) and time (switchable).

With respect to the experiments provided by the groups within the SPP, this should provide effective and viable routes for free surface flow control and the proposed methods should be able to effectively describe the intended physical behavior of moving contact lines. In cooperation with Bastian Rapp & Dorothea Helmer I plan to perform a joint simulation/experimental description



**Figure 7:** Supported droplet (shading=height) driven over a chemically heterogeneous substrate landscape.

of droplets moving over patterned/functionalized surface [59, 60]. The droplet motion (height and contact line) will be monitored using a high-speed camera and compared with the simulation results. The goal of this study is to indirectly identify/verify physical parameters such as interface slip and dynamic contact angle. Even for homogeneous substrates, the magnitude of the dissipation mechanism can drastically influence the observed pattern formation process, e.g. cf. [O1] for a systematic study concerning the magnitude of Navier-slip. With the development of the theoretical and numerical framework for dynamic contact angles in WP1, a similar study for dewetting films and the created patterns will be performed in this proposal and compared with experimental results from the group of Karin Jacobs, e.g. cf. [61] & [O1]. For preliminary result of such a simulation with sharp contact lines but with equilibrium contact angles is shown in Fig. 8. Concerning the quasi-static evolution of gravity-driven droplets I will work with Martin Brinkmann to investigate the impact of different (gradient formulations) for dynamic contact angle on observed droplet and join the approaches of [62] and [P3].



**Figure 8:** Droplet pinch-off from a dewetting liquid computed using supported solutions (blue=outside support).

**Task WP3-2: Models for flows over and into porous substrates (4 months).**

**Description WP3-2:** On the full hydrodynamic level, the substrate-flow interaction with a porous substrate is well-known and described by the Stokes-Darcy equation [37]. The numerical strategy to couple these equations, for example, was investigated in [63] and its impact on the spreading dynamics has been studied in [38]. In particular in relation with the previous task WP3-1, we will study how transport of fluid into the porous substrate impacts the interface properties (interface energies, Navier-slip, hysteresis) and how this can be observed in the corresponding dynamic behavior of the spreading/dewetting process. Additionally, valuable information about the coupled flow will be extracted, if the flow in the porous substrate can be at least partially observed experimentally, e.g., velocity of internal liquid front. In cooperation with Bastian Rapp & Dorothea

Helmer we also plan to investigate the transport of fluid into a porous substrate, e.g. produced as in [64]. In the experiment, fluorescently marked water will be introduced into a porous polymer and the spreading of the water on the substrate and into the substrate will be tracked by fluorescence microscopy in 2D and by confocal microscopy in 3D to provide experimental insight on spreading dynamics. We will compare with models and simulations developed within this proposal to study if such models are useful for predicting substrate properties such as pore sizes from spreading data by applying a fitting theoretical model. With Martin Brinkmann I will investigate the dynamics and wetting of flows on elastic posts and the flow into these porous structures. Depending their characteristic length scale and wetting properties, we claim that dynamical transitions between Cassie-Baxter-like and Wenzel-like states can be observed, which we will then describe in thermodynamic consistent manner. Following experimental evidence, we will particularly focus on investigating hysteretic behavior in the substrate dynamics.

Assume a porous/heterogeneous substrate gives rise to a microscopically oscillating surface energy where  $f_\varepsilon(h, x) = g(x/\varepsilon)$  with a 1-periodic function  $g : [0, 1]^d \rightarrow \mathbb{R}^+$ . Upon homogenization the energy converges to the mean spreading coefficient  $f_\varepsilon(h, x) \rightarrow \int_{[0,1]^d} g(y) dy \in \mathbb{R}$  as  $\varepsilon \rightarrow 0$ , while the limit for the (sharp interface) evolution is still an open problem. While for models with precursor pinning has been observed [56], the behavior of the moving contact line should be investigated in more detail (numerically and mathematically). There are hints how hysteresis can emerge from such a limit mathematically [65], which will be investigated with Alexander Mielke.

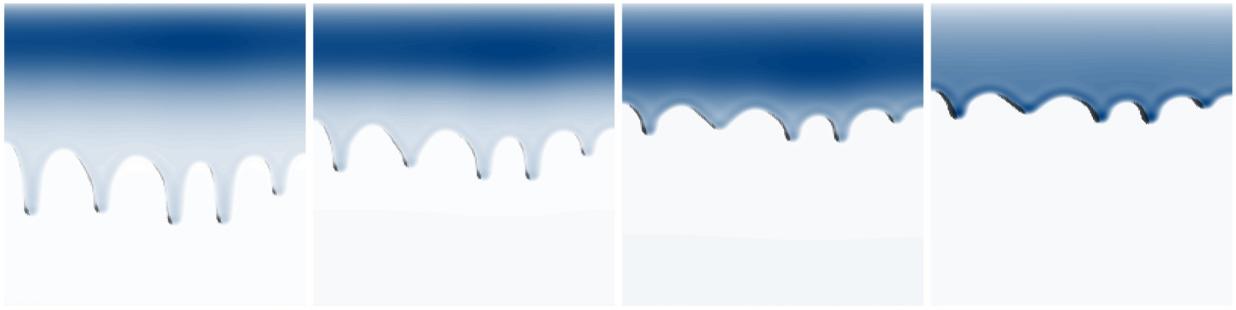
#### **Task WP3-3:** *Model surfactant transport (soluble and insoluble) (4 months).*

**Description WP3-3:** A natural physical setting corresponding to WP2 is the study of surfactant dynamics for soluble and insoluble surfactants distributed on surfaces, substrate-liquid interface, and in the liquid bulk. For an overview concerning surfactant assisted spreading we refer to Matar & Craster [66]. Corresponding models have been analysed in [67] and phase-field variants considered in [68]. A 1D thin-film model with moving contact lines and surfactants has been considered in [52]. However, the advantage of a gradient flow formulation with moving contact lines, which the current proposal is concerned with, is that all natural boundary conditions are derived from energy or dissipation functionals. Onsager structures for the flow with surfactants have been studied in [40] and their hydrodynamical stability investigated in [69].

In the SPP, the first part of the task WP3-3 I will focus on the theoretical derivation and formalization of a gradient flow structure for a surfactant transport model with moving contact lines and nontrivial contact angle dynamics. This will be studied in a joint effort with Uwe Thiele, who will investigate similar models from the perspective of bulk/interface substrate-flow coupling with adaptive brushes. The theoretical contributions are complementary with my focus on generalized gradient flows with moving contact lines (supported solutions with hysteresis), where Uwe Thiele's focus is on Onsager-structures with adaptive brushes. The development of corresponding advanced numerical algorithms should allow a rich discussion and creation of benchmark studies within the SPP. Jointly, Georgy Kitavtsev (Univ. Oxford), I will also work on extension of this framework to cell-motility, e.g. cf. [44]. This task is the practical application of WP2-1, so that there is the possibility to interchange the (timely) order of tasks in WP2 and WP3.

#### **Task WP3-4:** *Modeling of elastic/deformable substrates with moving contact lines (4 months).*

**Description WP3-4:** Based on the theoretical work on the dissipation modeling for suspension two-phase flows [23], this workpackage uses a similar flow-map based approach for a dissipative fluid-solid coupling. We will model the quasi-static evolution with a dissipation in the fluid  $\Omega$  and



**Figure 9:** Simulation of gravitational fingering instability of a suspension flow as in Eq. (15) on inclines with angles increasing from left to right and density indicated by the shading. Numerical method is based on gradient flow.

the solid  $\bar{\Omega}$

$$\mathcal{D}(\mathbf{u}_\ell, \dot{\mathbf{u}}_s) = \int_{\bar{\Omega}} R_{\text{visc}}(\mathbb{D}\dot{\mathbf{u}}_s) \, dx + \int_{\Gamma} R_\Gamma(\dot{\mathbf{u}}_s - \mathbf{u}_\ell) \, ds + \int_{\Omega} \boldsymbol{\tau}(\mathbf{u}) : \nabla \mathbf{u} \, dx,$$

where  $\mathbf{u}$  is the fluid velocity and  $\mathbf{u}_s$  is the solid deformation velocity. The most natural interface condition would emerge from  $R_\Gamma(w) = \mu_\Gamma |w|^2$  and gives rise to a Navier-slip condition and  $R_{\text{visc}}$  gives rise to viscoelastic material behavior. In the presence of a moving contact line the dissipation  $R_{\text{visc}}$  leads to a localization of the dissipation at the contact line [70] and thereby should create an effective law for a dynamic contact line. The elastic energy will, as usual, be given in Lagrangian coordinates as  $\mathcal{E}_{\text{elast}}(\mathbf{u}_s) = \int_{\bar{\Omega}_{\text{ref}}} W_{\text{elast}}(F) \, dx_{\text{ref}}$  with the deformation gradient  $F = \nabla_{\text{ref}} \mathbf{u}_s$ . This modeling approach will be used to work with Barbara Wagner and Ralf Seemann on dissipative effects in coupling flow with soft elastic substrates. This will allow us to systematically study the effect of viscoelastic dissipation, e.g., cf. [71], in particular studying its impact on the effective contact line dynamics and thereby its impact on the overall dewetting process. Martin Brinkmann studies the effective dynamics and pattern formation of droplet arrays between arrays of elastic lammelas. We will cooperate on aspects of the consistent coupling and on the emergence of hysteretic behavior by dissipation modeling due to contact line dynamics.

## 2.4 Data handling

Research data at WIAS is subject to frequent backups and kept for at least 10 years. Software developed in all work packages will be documented and published, e.g., as in the repository <https://github.com/dpeschka/thinfilm-freeboundary> from [P8]. Publishing data is supported by WIAS by providing DOIs and storage capacity, e.g., see the work [21] featuring research data published at [www.wias-berlin.de/resdata/3/](http://www.wias-berlin.de/resdata/3/).

## 2.5 Other information

none.

## 2.6 Descriptions of proposed investigations involving experiments on humans, human materials or animals as well as dual use research of concern

none.

## 2.7 Information on scientific & financial involvement of international cooperation partners

none.

## 2.8 Information on scientific cooperation within Priority Programme

To foster the exchange between theoretical groups working with continuum-theoretical approaches within the SPP, we have initiated an informal network, which at the moment includes **M. Brinkmann**, **S. Gurevich**, **D. Peschka**, **J. Snoeijer**, **H. Stark**, **U. Thiele**, **A. Voigt** and **B. Wagner** and which is open to others. There, we will coordinate aspects of the training of the involved young researchers within the SPP, and meet sporadically to discuss details of our approaches and ongoing work. Several groups in the SPP are working on numerical algorithms for flows on rigid (**A. Voigt**, **A. Reusken**, **S. Aland**, **H. Stark**) and agreed to define numerical benchmark problems, where also dynamic contact angles will be considered. With **B. Rapp & D. Helmer** we plan to compare experiments and simulations for chemically structured substrates. With **U. Thiele** I will investigate the coupling of long-wave multiphase transport and nontrivial contact angle dynamics. With **B. Wagner** and **R. Seemann** we will discuss dissipative substrate-flow coupling for soft substrates. With **M. Brinkmann** I will work on hysteresis for soft and porous substrates.

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## 4 Requested modules/funds

### 4.1 Basic Module

#### 4.1.1 Funding for Staff

1 full time position E13 TVöD for three years (Eigene Stelle).

#### 4.1.2 Direct Project Costs

5,250 EUR p.a. (see below)

##### 4.1.2.1 Equipment up to €10,000, Software and Consumables

none.

**4.1.2.2 Travel Expenses** Two annual visits of major international conferences (ICIAM, ECMI, APS DFD meeting, Free Boundary Problems Theory and Application) and additional networking activities (see Sec. 2.8) are planned, for which 3,000 EUR p.a. are requested.

**4.1.2.3 Visiting Researchers** External cooperation partners (G. Kitavtsev, L. Heltai) are invited for one week each p.a., for which 1,500 EUR p.a. are requested.

**4.1.2.4 Expenses for Laboratory Animals:** none.

**4.1.2.5 Other Costs:** none.

**4.1.2.6 Project-related publication expenses:** For support of open access publications 750 EUR p.a. are requested.

#### 4.1.3 Instrumentation

**4.1.3.1 Equipment exceeding €10,000:** none.

**4.1.3.2 Major Instrumentation exceeding €50,000:** none.

## 5 Project requirements

### 5.1 Employment status information

Dirk Peschka has a fixed term contract as research assistant until December 31, 2018 funded by Einstein Center for Mathematics Berlin in the MATHEON project *OT8 Modeling, analysis, and optimization of optoelectronic semiconductor devices driven by experimental data*.

### 5.2 First-time proposal data

Does not apply. The applicant was one of the proposers in the DFG SPP 1506 project *Mathematical modeling, analysis, numerical simulation of thin liquid bilayers and validation experiments*.

### 5.3 Composition of the project group

Does not apply.

## 5.4 Cooperation with other researchers

### 5.4.1 Researchers with whom you have agreed to cooperate on this project (external)

**K. Jacobs (Universität des Saarlandes, Saarbrücken)** develops experimental methods for dewetting flows from rigid coated substrates to be probed by AFM. We agreed to compare the developed models with existing experiments for dewetting patterns from coated substrates.

**L. Heltai (SISSA, Trieste)** is an expert in high performance computing with a focus on free boundary and fluid-structure interaction problems. We will jointly develop higher-order ALE methods using mapped finite-elements. We have preliminary results within the deal.ii finite-element library.

**A. Mielke (WIAS, Berlin)** develops analytical methods for evolutionary  $\Gamma$ -convergence based on energetic solution concepts. He showed the emergence of rate-independent dissipation in the homogenization of an evolution problem with microstructure (wiggly energy landscape). We will jointly work on transferring this concept to heterogeneous/rough surfaces.

With **T. Surowiec (Philipps Universität Marburg)** and **M. Hintermüller (WIAS, Berlin)** I will cooperate on nonsmooth variational problems and gradient structures for electrowetting. With **V. John** and **A. Linke (both WIAS, Berlin)** I will discuss the numerical analysis of flow problems. With **M. Thomas (WIAS, Berlin)** I will discuss modeling and analysis of rate-independent systems with elasticity and fracture mechanics and possible applications in geophysics. With **G. Kitavtsev (Univ. of Oxford)** I will work on gradient flow formulations for cell-motility problems.

### 5.4.2 Researchers with whom you collaborated scientifically within the past three years

Ralf Seemann<sup>a</sup>, Karin Jacobs<sup>a</sup> Thomas Surowiec<sup>b</sup>, Patricio Farrell<sup>c</sup> Michael Hintermüller<sup>d</sup>, Barbara Wagner<sup>d</sup>, Marita Thomas<sup>d</sup>, Nella Rotundo<sup>d</sup>, Thomas Koprucki<sup>d</sup>, Alexander Mielke<sup>d</sup>, Ansgret Glitzky<sup>d</sup> Andreas Münch<sup>e</sup>, Georgy Kitavtsev<sup>e</sup>, Andrea Bertozzi<sup>f</sup>, Luca Heltai<sup>g</sup>.

a) Universität des Saarlandes, b) Philipps-Universität Marburg, c) TU Hamburg, d) Weierstrass Institute,

e) University of Oxford, f) University of California Los Angeles, g) SISSA Trieste

## 5.5 Scientific equipment

Infrastructure, office space and all other preconditions for carrying out the proposed work will be granted by WIAS for the whole period of the project. A related declaration is attached to the accompanying letter.

**5.6 Project-relevant cooperation with commercial enterprises:** none.

**5.7 Project-relevant participation in commercial enterprises:** none.

## 6 Additional information

The proposer also submitted a DFG proposal **PE 1782/1-1** entirely devoted to the subject of extending methods known for Bingham flows to study contact line hysteresis, with a more mathematical focus. The goal of this proposal in the Priority Programme is the substrate-flow coupling with energy-dissipation structures, where the influence of hysteresis is also present but not the primary objective.