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# Project Description – Project Proposals

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Switchable substrates: From micro to macro models

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# Project Description

# 1 State of the art and preliminary work

## 1.1 State of the art

When it comes to designing microfluidic hardware, it is in general not possible to scale down conventional devices to the micro-scale. In order to control droplets on this scale, influencing the wettability of the substrate is important. This dynamic process of liquids wetting or dewetting various substrates is an important part in many technological applications. Here, the wetting process depends predominantly on the properties of the liquid-substrate and liquid-air interfaces. One way to influence the wetting process is altering the properties of the liquid-substrate interface by applying thin coatings on the substrate which change the liquid-substrate interfacial energy. Depending on its components, the coating my exhibit internal structures which can be changed by external electric or magnetic fields. This gives rise to switchable substrates. However, the origins of the wettability variation are still not sufficiently understood, although several mechanisms have already been proposed in literature [21].

From the mathematical point of view, the description of wetting or dewetting processes on such switchable coatings contains several challenges. The strong coupling between (de)wetting hydrodynamics and processes in the coating typically introduces additional time and length scales that do not exist in the (de)wetting of inert and rigid substrates. Strong couplings may also impact the mechanisms of energy dissipation and thereby alter the dynamics on a global scale. The numerical treatment of micro-scale models describing these effects precisely is in general very expensive. On the other hand, macroscopic models describing the setting in less detail are often derived as an approximation of the microscopic models under the assumption of a quasi-stationary state. Therefore, the reliability of these models is questionable when the system is far from equilibrium.
The aim of this project is to bridge the gap between precise, microscopic descriptions and approximate coarse scale descriptions.

### 1.1.1 Two-phase flow

For the description of two-phase flow, there are different modeling approaches at hand. The interface between the two fluids can either be described by a sharp defined interface or by a smooth transition area between the fluids. We start by recalling the governing equations for the two-phase incompressible fluid flow in a classical sharp interface model. Away from the interface the flow is governed by

$$\operatorname{div} \boldsymbol{v} = 0 \,, \tag{1.1}$$

$$\partial_t(\rho \boldsymbol{v}) + \operatorname{div}\{\rho \boldsymbol{v} \otimes \boldsymbol{v}\} = \operatorname{div} \boldsymbol{S} \,, \tag{1.2}$$

were $\boldsymbol{v}$ is the fluid velocity, $\rho$ is the mass density and

$$\boldsymbol{S} = -p\mathbb{1} + \eta(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) \tag{1.3}$$

is the symmetric stress tensor with the fluid viscosity $\eta$. Across the fluidic interface $\Gamma$, the jump conditions

$$[\boldsymbol{v}] = 0\,, \qquad [-\boldsymbol{S}]\boldsymbol{n}_\Gamma = \hat{\sigma}\kappa\boldsymbol{n}_\Gamma \tag{1.4}$$

hold true. Here, the jump across the interface is denoted by $[.]$ and $\boldsymbol{n}_\Gamma$ is the unit normal on the interface. $\hat{\sigma}$ is the surface energy density and $\kappa$ denotes the mean curvature. When both fluids touch a solid wall, a three phase contact line occurs and the corresponding contact angle $\Theta$ is given by

$$\hat{\sigma}\cos\left(\Theta\right) = -\Delta\sigma_{fs}\,, \tag{1.5}$$

where $\Delta\sigma_{fs}$ denotes the difference between the fluid-solid interfacial energies of the wetting fluids. If this difference becomes too large, i.e. $|\Delta\sigma_{fs}| > \sigma > 0$, complete wetting or dewetting occurs and one fluid detaches from the solid wall.

As topological changes, like droplet break-up, droplet coalescence, or detachment from a wall, are hard to capture with a sharp interface model, approaches based diffuse interface methods became popular in the last decades ( [1,22,42,43,56]). In [3], a diffuse interface for incompressible two-phase flows with different mass densities was derived. This model combines the advantage of a solenoidal velocity field with a thermodynamically consistent and frame indifferent description of the two-phase flow. The bulk equations in the spatial domain $\Omega$ read

$$\rho(\phi)\partial_t\boldsymbol{v} + ((\rho(\phi)\boldsymbol{v} - \partial_\phi\rho(\phi)m(\phi)\nabla\mu)\cdot\nabla)\,\boldsymbol{v} - \mathrm{div}\left\{\eta(\phi)\left(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T\right)\right\} + \nabla p = \mu\nabla\phi\,, \tag{1.6a}$$

$$\mathrm{div}\,\boldsymbol{v} = 0\,, \tag{1.6b}$$

$$\partial_t\phi + \boldsymbol{v}\cdot\nabla\phi + \mathrm{div}\left\{m(\phi)\nabla\mu\right\} = 0\,, \tag{1.6c}$$

$$\mu = -\sigma\delta\Delta\phi + \sigma\delta^{-1}W'(\phi)\,, \tag{1.6d}$$

and are accompanied by the boundary conditions

$$\boldsymbol{v} = 0\,, \tag{1.6e}$$

$$m(\phi)\nabla\mu\cdot\boldsymbol{n} = 0\,, \tag{1.6f}$$

$$\sigma\delta\nabla\phi\cdot\boldsymbol{n} = \gamma'(\phi)\,. \tag{1.6g}$$

on $\partial\Omega$. Here, $\rho(\phi)$ is a linear interpolation between the mass densities of the two fluids, $\eta$ is an interpolation of the viscosity, $m$ is the mobility, $\delta$ is a parameter connected to the width of the transition region, and $\sigma$ relates to the surface energy density via $\hat{\sigma} = c_W\sigma$, where $c_W$ is a constant depending on the choice of double-well potential $W$. The function $\gamma$ interpolates between the fluid-solid interfacial energy densities. Therefore, the boundary condition (1.6g) is a diffuse interface formulation of Young's formula for the contact angle (1.5) (cf. [65]). The existence of weak solutions was established in [2] and in [33]and [P6], where convergent finite element schemes were presented. This model was later extended by Campillo-Funolet et. al. in [16] to include dissolved ions which interact with external electric fields. The numerical treatment of the arising model was investigated by the applicant in [P7] and [P2] (see also Section 1.1.4 below).

### 1.1.2   Micro-macro models

For the description of the thin coating, there are different approaches at hand which differ in accuracy, complexity, and the underlying assumptions (cf. [25]). In the most accurate description, the so called Doi or Doi–Hess model [13,23,39,44], liquid-crystalline systems are described as an ensemble of rods which evolve due to thermal motion and pairwise interactions. In these models the state of the liquid-crystalline system is given by a function $f(\boldsymbol{x}, \boldsymbol{d}, t)$ describing the

probability that a molecule at point $\boldsymbol{x}$ and a time $t$ is aligned in direction $\boldsymbol{d}$ which is an element of the unit sphere $\mathbb{S}^2$, i.e. $|\boldsymbol{d}| = 1$. In the case of head-to-tail symmetric, nonpolar, rodlike molecules, one cannot distinguish between the orientations $\boldsymbol{d}$ and $-\boldsymbol{d}$. This gives rise to the additional symmetry assumption $f(\boldsymbol{x}, \boldsymbol{d}, t) = f(\boldsymbol{x}, -\boldsymbol{d}, t)$ for all spatial points $\boldsymbol{x}$ in the given spatial domain $\Omega$, all times $t$, and all orientations $\boldsymbol{d} \in \mathbb{S}^2$. In absence of a velocity field, the evolution of the probability density $f$ is governed by

$$\frac{\partial f}{\partial t} = \frac{1}{\mathrm{De}} \mathcal{R} \cdot \left( f \mathcal{R} \left( \frac{\delta F}{\delta f}[f] \right) \right) , \tag{1.7}$$

where $\mathcal{R} := \boldsymbol{d} \times \frac{\partial}{\partial \boldsymbol{d}}$ denotes the gradient with respect to $\boldsymbol{d}$ restricted to the sphere and $\frac{\delta F}{\delta f}$ denotes the variational derivative of the free energy $F$ with respect to $f$. In other words, the evolution of $f$ is described by the gradient flow of the free energy functional $F$ which acts as a Lyapunov-type function. This property is the cornerstone for the mathematical analysis of the arising equations. The free energy consists of an entropic term $f \log f - f$, the contribution of the mean-field interactions of the molecules $F_{MI}$, and interactions with possible external fields $F_{ext}$. The mean field interactions are described by

$$F_{MI}(\boldsymbol{x}, \boldsymbol{d}, t) := f(\boldsymbol{x}, \boldsymbol{d}, t) \int_{\Omega} \int_{\mathbb{S}^2} \alpha(\boldsymbol{x} - \hat{\boldsymbol{x}}) \beta(\boldsymbol{d}, \hat{\boldsymbol{d}}) f(\hat{\boldsymbol{x}}, \hat{\boldsymbol{d}}, t) \mathrm{d}\hat{\boldsymbol{d}} \mathrm{d}\hat{\boldsymbol{x}} . \tag{1.8}$$

Here, $\alpha$ denotes a suitable localization term modeling the range of the interactions and the integral kernel $\beta$ describes how the molecules interact with each other. In the case of unpolar, rod-like molecules, typical choices for $\beta$ are Onsager's potential [61]

$$\beta(\boldsymbol{d}, \hat{\boldsymbol{d}}) = c|\boldsymbol{d} \times \hat{\boldsymbol{d}}| \tag{1.9}$$

with the constant $c > 0$ representing the coupling strength [20, 45], and the Maier–Saupe potential [57]

$$\beta(\boldsymbol{d}, \hat{\boldsymbol{d}}) \sim -(\boldsymbol{d} \cdot \hat{\boldsymbol{d}})^2 , \tag{1.10}$$

which is considered as an approximation (for small angles) of the cross product in (1.9). For the description of the interactions of "dipole-like" crystals, i.e. rods without head-to-tail symmetry, one may also use

$$\beta(\boldsymbol{d}, \hat{\boldsymbol{d}}) \sim -\boldsymbol{d} \cdot \hat{\boldsymbol{d}} . \tag{1.11}$$

In presence of an external magnetic field $\boldsymbol{H}$, $F_{ext}$ can be written as

$$F_{ext}(\boldsymbol{x}, \boldsymbol{d}, t) = -(\chi_{\|} - \chi_{\perp})(\boldsymbol{d} \cdot \boldsymbol{H})^2 f(\boldsymbol{x}, \boldsymbol{d}, t) \tag{1.12}$$

with susceptibilities $\chi_{\|}$ and $\chi_{\perp}$ parallel and perpendicular to the direction $\boldsymbol{d}$.

In the absence of external forces, the mathematical theorie is well established. Constantin et. al. proved the existence of solutions to (1.7) in [17], while the structure of stationary solutions was investigated in [55]. The inhomogeneous case which occurs, e.g., as a result of an externally imposed flow field with an $\boldsymbol{x}$-dependend velocity gradient is also well-understood: In [64], Otto and Tazavaras proved the existence of strong solutions to the Doi–Hess model coupled to a Stokes type equations. In [5,6], Bae and Trivisa proved global existence of weak solutions and extended this result to compressible fluid flow.

   We want to highlight that the structure of the Doi model is very similar to the micro-macro models used for the description of dilute polymeric solutions, where the mean-field interactions $F_{MI}$ are neglected and the constraint $|\boldsymbol{d}| \equiv 1$ is replaced by a relative entropy penalizing deviations of $f$ from a certain preferred distribution. These models are also well-understood, see e.g. [8,10] for analytical results and [9,11] for the discussion of discrete schemes. These results

were extended to the case of two-phase flow by Grün and Metzger in [P5]. Using Onsager's variational principle [59,60], they derived a thermodynamically consistent multiscale model. In this model $f$ was not interpreted as a probability density with a marginal equal to one. Instead, Grün and Metzger interpreted $f$ as a number density for the polymer chains and therefore the marginal provides the time-dependent number of polymers at a spatial point $\boldsymbol{x}$. The existence of weak solutions to the aforementioned model was also established in [P5] and an energy stable, convergent finite element scheme was proposed in [P1] together with simulations in two and three spatial dimensions (cf. Section 1.1.4 and Fig 2).

Instead of considering the dynamics of the probability density $f$, which depends on the high-dimensional product space $\Omega \times \mathbb{S}^2$, one can simplify the model by considering only the evolution of the lowest-order moment of $f$ [20]. For nonpolar particles the first moment $\int_{\mathbb{S}^2} \boldsymbol{d} f(\boldsymbol{x}, \boldsymbol{d}, t) \mathrm{d}\boldsymbol{d}$ vanishes for all spatial points $\boldsymbol{x}$ at all times $t$. Therefore, it suffices to consider the evolution of the second moment $Q(\boldsymbol{x}, t) := \int_{\mathbb{S}^2} \left(\boldsymbol{d} \otimes \boldsymbol{d} - \frac{1}{3}\mathbb{1}\right) f(\boldsymbol{x}, \boldsymbol{d}, t) \mathrm{d}\boldsymbol{d}$ which gives rise to the so called $Q$-tensor theory [7, 20, 40]. At this point, we want to highlight that a stress tensor with a similar structure can be obtained by coarse graining density based descriptions of dilute polymeric solutions (cf. [P5], [P3]).

Under the assumption of uniaxial nematic states, which typically holds only for liquid crystals at low molecular weights (cf. [13]), the structural orientation in the liquid-crystalline systems can be fully described by the normalized eigenvector $\boldsymbol{d}$ to the eigenvalue with the largest absolute value This eigenvector is unique up to a multiplication with $-1$. This approach dates back to the results of Ericksen [26, 27], Leslie [46–48], Oseen [63], and Franck [29]. Similar to the probability distribution $f$ in the Doi-Hess description, the evolution of the nematic director $\boldsymbol{d}$ is governed by a free energy. Leslie [47] suggested to use the free energy density

$$F(\boldsymbol{d}, \nabla \boldsymbol{d}) := k_1(\nabla \cdot \boldsymbol{d})^2 + k_2(\boldsymbol{d} \cdot \nabla \times \boldsymbol{d})^2 + k_3|\boldsymbol{d} \times \nabla \times \boldsymbol{d}|^2 + (k_2 + k_4)(\operatorname{tr}(\nabla \boldsymbol{d})^2 - (\nabla \cdot \boldsymbol{d})^2),$$
(1.13)

an expression introduced by Oseen and Franck with the splay, twist, and bend elastic constants $k_1$, $k_2$, and $k_3$, and $(k_2 + k_4)$ describing the so called saddle-splay. To include an external magnetic field, one may follow the approach by de Gennes [20] and expand (1.13) by adding

$$F_{ext}(\boldsymbol{d}) = -\chi_\perp |\boldsymbol{H}|^2 - (\chi_\parallel - \chi_\perp)(\boldsymbol{d} \cdot \boldsymbol{H})^2$$
(1.14)

with an externally controlled magnetic field $\boldsymbol{H}$ and susceptibilities $\chi_\parallel$ and $\chi_\perp$ parallel and perpendicular to the director $\boldsymbol{d}$. A frequently used simplification of the Oseen-Franck free energy (1.13) is the so called "one-constant-approximation" with $k_1 = k_2 = k_3 = \frac{\gamma}{2}$ and $k_4 = 0$. In this case, the free energy density simplifies to

$$F(\boldsymbol{d}, \nabla \boldsymbol{d}) = \frac{1}{2}|\nabla \boldsymbol{d}|^2$$
(1.15)

(cf. [20,66]). A further simplification was introduced by Lin and Liu in [49], where they removed the algebraic restriction $|\boldsymbol{d}| = 1$ and rather added a Ginzburg–Landau penalty functional to the free energy density. In this case the free energy functional reads

$$F_\varepsilon(\boldsymbol{d}, \nabla \boldsymbol{d}) = \frac{1}{2}|\nabla \boldsymbol{d}|^2 + \frac{1}{4\varepsilon^2}\left(|\boldsymbol{d}|^2 - 1\right)^2.$$
(1.16)

Coupled with Navier–Stokes equations describing the evolution of the momentum, the arising model reads

$$\frac{\partial \boldsymbol{d}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{d} - \boldsymbol{d} \cdot \nabla \boldsymbol{v} = \Delta \boldsymbol{d} - \frac{1}{\varepsilon^2}\left(|\boldsymbol{d}|^2 - 1\right)\boldsymbol{d},$$
(1.17a)

$$\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} + \nabla p - \eta \Delta \boldsymbol{v} = -\nabla \cdot \left(\nabla \boldsymbol{d}^T \nabla \boldsymbol{d}\right),$$
(1.17b)

$$\nabla \cdot \boldsymbol{v} = 0 \,, \tag{1.17c}$$

where $\eta$ denotes the viscosity of the ambient fluid. Existence of strong solution to a simplified model was first established in [49] and later extended to a more general case in [50].

While the Doi–Hess model arises from molecular kinetic theory, the $Q$-tensor theory and the Ericksen–Leslie theory are phenomenological [38] and rely on phenomenological parameters which are often hard to determine from experimental results. Therefore, the connection of the later theories to the Doi–Hess model was intensely studied in the recent years [24, 38, 45, 67], as it allows to derive the unknown parameters from molecular quantities. However, the derivation of the $Q$-tensor theory and the Ericksen–Leslie theory from the Doi–Hess description relies on appropriate closure conditions and requires the system to be close to equilibrium [38, 67]. Consequently, it is not clear how the dynamics of these models relate in a state far from equilibrium.

### 1.1.3 Lubrication approximation of thin films

Dimension reduced models offer a pathway to reduce the numerical costs of computer simulations while still capturing significant features of wetting processes. In recent decades, various classes of thin-film type equaions have been derived by lubrication approximation under the general assumption that the ratio between typical vertical and horizontal length scales is small and that the liquid viscosity is sufficiently high (see [35, 62] and the references therein).

In many cases, they come along with a gradient structure

$$\frac{\partial h}{\partial t} = \nabla \left[ Q(h) \nabla \left( \frac{\delta F}{\delta h} \right) \right] \,, \tag{1.18}$$

where $h$ is to describe the height of the liquid film above a substrate. $Q(.)$ is a usually degenerate mobility function – depending on the flow condition at the liquid–substrate interface, for instance $Q(h) \sim h^3$ in case of a no-slip condition. The underlying physics are captured by the energy

$$F(h) = \int_\Omega \frac{\gamma}{2} |\nabla h|^2 + f(h) \,. \tag{1.19}$$

Here, the Dirichlet integral models the energy of the liquid-gas interface and $f$ my be used to include further effects – for instance long-range van der Waals-interactions with a – possibly heterogeneous substrate. During the last 25 years, these fourth-order degenerate parabolic equations have been studied or are still under investigation. Concerning rigorous mathematical analysis, global existence of solutions has been studied ( [14, 15, 18, 32]) as well as the evolution of free-boundaries ( [19, 31]) or the regularity of free boundaries ( [30]). Convergent numerical schemes ( [36, 37]) have been used to validate thin-film models ( [12, 58]) and to predict new dewetting scenarios.

Thin films models have successfully been applied to the structure formation in thin liquid-liquid films. In that case, systems of degenerate fourth-oder parabolic equations are considered – and similarly as in the single-layer case, integral estimates become crucial both for analysis and numerics (for an overview, see [41] and the references therein).

In the recent years also a few results concerning liquid-crystalline films were obtained (see [51, 52] and the references therein). However, these results differ concerning a possible stabilizing or destabilizing effect of the elastic energy on the film. Those differences were recently traced back by Lin et. al. [51] to incompatible stress balance conditions at the free interface, which neglected the elastic stresses. By deriving a lubrication approximation for a thin film of nematic liquid crystal with strong anchoring conditions in two spatial dimension, Lin et. al. established the stabilizing effect for the case of compatible interface conditions. In [52], Lin et. al. derived a

Figure 1: Ionic droplet in an electric field (published in [P2]): Droplet shape (left) and cross section with dissolved ions (right).

lubrication approximation for a thin liquid-crystalline film and investigated the influence of the anchoring direction on the substrate on the spreading of the film. However, the instantaneous adjustment of the directors to their unique steady state was used as a key assumption in order to avoid dealing with multiple time scales. It is not clear whether this assumption is also appropriate for more intricate scenarios which include interactions with am additional wetting fluid and external fields.

### 1.1.4 Preliminary work on the numerical treatment of micro-macro models and electric effects

The importance of stable and efficient schemes for the simulation of complex flow problems is undeniable. First, the different involved length scales lead to high-dimensional systems which can not be treated monolithically. Secondly, the interactions between different physical components (like coating and wetting fluids) induce a strong coupling in the arising partial differential equations. To reduce these couplings, specific discretization techniques are necessary. In [P6] a special time approximation of the transport velocity was used to drive a convergent numerical scheme for two-phase flow which decouples the Cahn–Hilliard and Navier–Stokes equations and thereby reduces the computation time drastically. This approach was refined in [P7] and [P2] for a Cahn–Hilliard–Poisson–Nernst–Planck–Navier–Stokes system. The resulting finite element scheme then allows for a sequential treatment of the different blocks of the model and thereby omits the employment of a fixed point method. To show the practicality of the schemes, simulations of ion induced topology changes were performed. Due to the electric field induced by the electrodes depicted as red and blue lines on right-hand side of Fig. 1, the uncharged molecules (green) decompose to charged ions (red and blue) which move towards the electrodes. Thereby, the droplet gets stretched and finally breaks.

Special attention has also to be paid to artificial diffusion induced by the numerical scheme. As shown in [P2], a reduction of artificial diffusion allows for larger time increments without loss of accuracy. Based on these techniques, the applicant derived a convergent finite element scheme for a Cahn–Hilliard–Fokker–Planck–Navier–Stokes system describing two-phase flow of dilute polymeric solutions. To investigate the influence of the dissolved polymer chains on the oscillatory behavior of a droplet, simulations in two and three spatial dimensions were made. The resulting pictures, which show the oscillating droplet and the additional stresses induced by the deformation of the polymer chains, are depicted in Fig. 2.
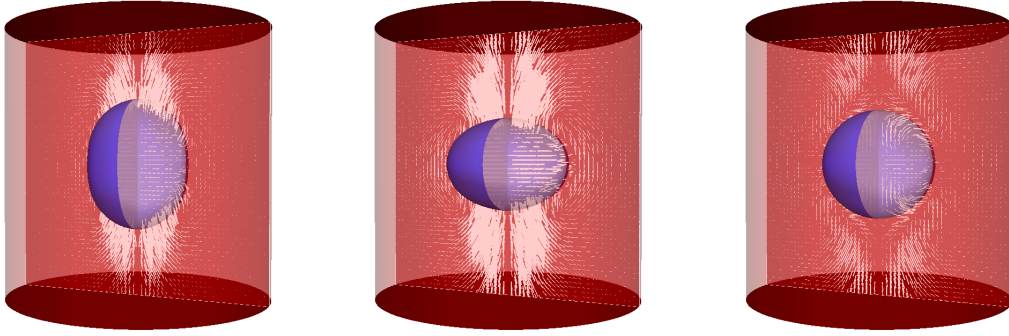
Figure 2: Simulation of two-phase flow of dilute polymeric solutions (published in [P1]).

## 1.2 Project-related publications

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

[**P1**] S. Metzger, *On convergent schemes for two-phase flow of dilute polymeric solutions*, ESAIM: Mathematical Modelling and Numerical Analysis, Forthcoming article, accepted 2018, 52 pages.

[**P2**] S. Metzger, *On stable, dissipation reducing splitting schemes for two-phase flow of electrolyte solutions*, Numerical Algorithms, Forthcoming article, accepted 2018, 32 pages.

[**P3**] G. Grün, S. Metzger, *Micro-Macro-Models for Two-Phase Flow of Dilute Polymeric Solutions: Macroscopic Limit, Analysis, and Numerics*, Chapter in Transport Processes at Fluidic Interfaces, Springer International Publishing, 2017, 291–304.

[**P4**] H. Abels, H. Garcke, G. Grün, and S. Metzger, *Diffuse interface models for incompressible two-phase flows with different densities*, Chapter in Transport Processes at Fluidic Interfaces, Springer International Publishing, 2017, 203–229.

[**P5**] G. Grün, S. Metzger, *On micro-macro-models for two-phase flow with dilute polymeric solutions – modeling and analysis*, Mathematical Models and Methods in Applied Sciences **26** (2016), no. 05, 823–866.

[**P6**] G. Grün, F. Guillén-González, and S. Metzger, *On fully decoupled, convergent schemes for diffuse interface models for two-phase flow with general mass densities*, Communications in Computational Physics **19**, (2016), no. 5, 1473–1502.

[**P7**] S. Metzger, *On numerical schemes for phase-field models for electrowetting with electrolyte solutions*, Proceedings in Applied Mathematics and Mechanics **15** (2015), no. 1, 715–718.

### 1.2.2 Other publications

Not applicable.

## 1.3 Patents

Not applicable.

# 2 Objectives and work programme

## 2.1 Anticipated total duration of the project

The project's intended duration is 6 years. The application period is 36 month.
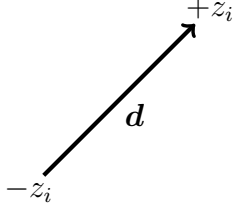
Figure 3: Sketch of a dipole.

## 2.2 Objectives

This project aims for a better understanding of wetting phenomena on flexible and switchable substrates. The properties of theses substrates are often dominated by thin coatings covering their surface. As the size of the structures in these coatings is significantly smaller than the lateral extension of the wetting droplet, different length scales are inherent to the problem. This makes monolithic numerical simulations very expensive, as the size of the computational domain is prescribed by a macroscopic length scale (e.g. the diameter of the wetting droplet), while the resolution is prescribed by a microscopic length scale (e.g. size of the structures in the coating) which is magnitudes smaller. In addition, changes on the microscopic length scale may happen very fast in comparison to the macroscopic evolution of the droplet. Therefore, resolving these changes leads to severe restrictions on the size of the time increment. As a consequence, identifying and separating the involved spatial and temporal scales is of great importance.

The aim of our project is threefold:

- We wish to provide a better understanding of the microscopic interactions at the fluid-solid contact line and – in particular – at the three phase contact line. For this reason, we will derive thermodynamically consistent microscopic models which are able to capture the interactions between the structures of the coating and the ambient fluid. Here, we will adapt liquid crystal models (cf. Section 1.1.2) to describe the coating, as these models include the orientation of structures as well as their interactions.

- Secondly, we shall derive effective macroscopic models which still include the main dynamics from the micro scale but allow for a more efficient treatment.

- Finally, we will derive stable and efficient numerical schemes for the aforementioned models and aim for a comparison of numerical and experimental results.

### 2.2.1 Micro-macro models for fluid-substrate interactions

As a first part of the project, we will derive thermodynamically consistent models describing the interactions between the wetting fluid and the underlying switchable substrate. Thereby, we will concentrate on the setting depicted in Fig. 4: A solid substrate $\Omega_s$ is coated by a thin nematic layer $\Omega_c$ of height $l$. On top of this layer, two immiscible fluids are placed. At the three phase contact line, the fluids form the contact angle $\theta$, which depends on the surface tension between the fluids and the phase-dependent interfacial energy density on the fluid-coating interface $\Gamma_{c,f}$. The peculiarity of this approach is that the interfacial energy density on $\Gamma_{c,f}$ depends not only on the fluid phases but also on the orientation of microstructures in the nematic coating. To influence the orientation of liquid-crystalline structures, we will employ an external electric field. In a first step, we shall adapt the approaches by Campillo et. al. [16], Fontelos et. al. [28] and by Grün and Metzger [P5] to derive a Doi-type model. In addition to the spatial domain which is denoted by $\Omega \subset \mathbb{R}^3$, we consider a larger domain $\Omega^* \supset \Omega$ for the electric field in order to reduce the bias introduced to the electric field by the finite size of the domain. The orientation

of a rod-like liquid crystal molecule is described by the probability density function $f$ which depends on the spatial coordinate $\boldsymbol{x} \in \Omega$, the time $t$ and the orientation vector $\boldsymbol{d} \in \mathbb{S}^2$ with $\mathbb{S}^2$ denoting the unit sphere. These molecules are assumed to have electric dipole properties, i.e. positive and negative bound charges occur which, for simplicity, are assumed to be at the endpoints of the rod. Therefore, we may describe the polarization of a molecule by $z\boldsymbol{d}$, where $z \geq 0$ denotes the magnitude of the occurring charges in one molecule (cf. Fig. 3). The derivation of the model starts from balance equations for the probability density and the momentum, and Gauss's and Ampère's laws describing the electric field. Assuming that the fluid is incompressible and that magnetic fields can be neglected, we have the balance equation

$$\partial_t f + \operatorname{div}_{\boldsymbol{x}} \left\{ \boldsymbol{v} \nabla_{\boldsymbol{x}} f \right\} + \operatorname{div}_{\mathcal{R}} \left\{ \boldsymbol{d} \times \nabla_{\boldsymbol{x}} \boldsymbol{v} \boldsymbol{d} \psi \right\} + \operatorname{div}_{\boldsymbol{x}} \left\{ \boldsymbol{J}_{f,\boldsymbol{x}} \right\} + \operatorname{div}_{\mathcal{R}} \left\{ \boldsymbol{J}_{f,\boldsymbol{d}} \right\} = 0 \qquad (2.1\text{a})$$

for the density $f$ on $\Omega \times \mathbb{S}^2$ with the rotational differential operator $\mathcal{R} := \boldsymbol{d} \times \frac{\partial}{\partial \boldsymbol{d}}$ and the correspondingly defined divergence operator $\operatorname{div}_{\mathcal{R}}$. The momentum balance with incompressibility condition is given as

$$\partial_t \boldsymbol{v} + \operatorname{div}_{\boldsymbol{x}} \left\{ \boldsymbol{v} \otimes \boldsymbol{v} \right\} - \operatorname{div}_{\boldsymbol{x}} \boldsymbol{S} + \nabla_{\boldsymbol{x}} p - \boldsymbol{k} = 0 \,, \qquad (2.1\text{b})$$

$$\operatorname{div}_{\boldsymbol{x}} \boldsymbol{v} = 0 \qquad (2.1\text{c})$$

in $\Omega$, and the electric field is governed by Ampére's and Gauss's laws

$$\epsilon \partial_t \boldsymbol{E} + \chi_\Omega \int_{\mathbb{S}^2} z \boldsymbol{d} \partial_t f = 0 \,, \qquad (2.1\text{d})$$

$$\operatorname{div}_{\boldsymbol{x}} \left\{ \epsilon \boldsymbol{E} \right\} = - \operatorname{div}_{\boldsymbol{x}} \left\{ \chi_\Omega z \int_{\mathbb{S}^2} \boldsymbol{d} f \right\} \qquad (2.1\text{e})$$

in $\Omega^* \supset \Omega$. Here, $\chi_\Omega$ denotes the characteristic function of $\Omega$. A powerful tool for the determination of the unknown quantities in (2.1), which are the fluxes $\boldsymbol{J}_{f,\boldsymbol{x}}$ and $\boldsymbol{J}_{f,\boldsymbol{d}}$, the symmetric stress tensor $\boldsymbol{S}$, and the force term $\boldsymbol{k}$, is Onsager's variational principle [59, 60] – an approach which has already been applied successfully in [3, 16, 65] and [P5]. Separating the terms which only contribute to the work and do not produce entropy, provide an expression for $\boldsymbol{k}$. To determine the remaining, entropy producing terms, we apply Onsager's variational principle.

This principle states that the first variation $\delta$ with respect to $\boldsymbol{J}_{f,\boldsymbol{x}}$, $\boldsymbol{J}_{f,\boldsymbol{d}}$, and $\boldsymbol{S}$ of the sum of the rate of energy $\mathcal{E}$ and a dissipation functional $\Phi$ disappears. In particular, it states

$$\delta \left( \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} + \Phi \right) \overset{!}{=} 0 \,. \qquad (2.2)$$

Concerning the energy, we want to consider the following contributions: The kinetic energy $\frac{1}{2} \int_\Omega |\boldsymbol{v}|^2$, the (negative) entropy $\int_\Omega \int_{\mathbb{S}^2} f \log f - f$, the contribution of the electric field $\frac{1}{2} \int_{\Omega^*} \epsilon |\boldsymbol{E}|^2$, the orientation energy of the dipoles $\int_\Omega \int_{\mathbb{S}^2} \boldsymbol{E} \cdot \boldsymbol{d} z f$, and the interaction of potential of the molecules which has the form

$$\frac{1}{2} \int_\Omega \int_\Omega \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \alpha(\boldsymbol{x} - \hat{\boldsymbol{x}}) \beta(\boldsymbol{d}, \hat{\boldsymbol{d}}) f(\hat{\boldsymbol{x}}, \hat{\boldsymbol{d}}, t) f(\boldsymbol{x}, \boldsymbol{d}, t) \, \mathrm{d}\hat{\boldsymbol{d}} \, \mathrm{d}\boldsymbol{d} \, \mathrm{d}\hat{\boldsymbol{x}} \, \mathrm{d}\boldsymbol{x} \qquad (2.3)$$

with an appropriate localization term $\alpha$ and $\beta$ defined in (1.10) or (1.11), depending on whether the influence of the charges on the mean-field interactions is negligible or not. In combination with the the mass conserving boundary conditions

$$\boldsymbol{v} = 0 \,, \qquad (2.4)$$

$$\boldsymbol{J}_{f,\boldsymbol{x}} \cdot \boldsymbol{n}_{\boldsymbol{x}} = 0 \qquad (2.5)$$

9

on $\partial\Omega$ and the dissipation functional

$$\Phi\left(\boldsymbol{J}_{f,\boldsymbol{x}}, \boldsymbol{J}_{f,\boldsymbol{d}}, \boldsymbol{S}\right) := \int_\Omega \int_{\mathbb{S}^2} \frac{|\boldsymbol{J}_{f,\boldsymbol{x}}|^2}{2fD_{\boldsymbol{x}}} + \int_\Omega \int_{\mathbb{S}^2} \frac{|\boldsymbol{J}_{f,\boldsymbol{d}}|^2}{2fD_{\boldsymbol{d}}} + \int_\Omega \frac{|\boldsymbol{S}|^2}{4\eta}\,, \tag{2.6}$$

this approach gives rise to the following set of equations. The evolution of the density $f$ is governed by

$$\partial_t f + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \operatorname{div}_{\mathcal{R}}\left\{\boldsymbol{d} \times \nabla_{\boldsymbol{x}} \boldsymbol{v} \boldsymbol{d} f\right\} = \operatorname{div}_{\boldsymbol{x}}\left\{D_{\boldsymbol{x}} f \nabla_{\boldsymbol{x}} \mu_f\right\} + \operatorname{div}_{\mathcal{R}}\left\{D_{\boldsymbol{d}} f \mathcal{R} \mu_f\right\} \tag{2.7a}$$

on $\Omega \times \mathbb{S}^2$. The chemical potential $\mu_f$ is the first variation of the free energy with respect to $f$, i.e.

$$\begin{aligned}
\mu_f(\boldsymbol{x}, \boldsymbol{d}, t) =& 2\nabla_{\boldsymbol{x}} V(\boldsymbol{x}, t) \cdot \boldsymbol{d} z + \log f(\boldsymbol{x}, \boldsymbol{d}, t) + \tfrac{1}{\epsilon}\left(\int_{\mathbb{S}^2} z f(\boldsymbol{x}, \hat{\boldsymbol{d}}, t)\,\mathrm{d}\hat{\boldsymbol{d}}\right) \cdot \boldsymbol{d} z \\
&+ \int_\Omega \int_{\mathbb{S}^2} \alpha(\boldsymbol{x} - \hat{\boldsymbol{x}})\beta(\boldsymbol{d}, \hat{\boldsymbol{d}}) f(\hat{\boldsymbol{x}}, \hat{\boldsymbol{d}}, t)\,\mathrm{d}\hat{\boldsymbol{d}}\,\mathrm{d}\hat{\boldsymbol{x}}\,.
\end{aligned} \tag{2.7b}$$

For the momentum, we obtain the Navier–Stokes equations with an additonal stress tensor depending on the microstructures.

$$\begin{aligned}
\partial_t \boldsymbol{v} + \operatorname{div}_{\boldsymbol{x}}\left\{\boldsymbol{v} \otimes \boldsymbol{v}\right\} - \operatorname{div}_{\boldsymbol{x}}&\left\{\eta\left(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T\right)\right\} + \nabla_{\boldsymbol{x}} p \\
&= \int_{\mathbb{S}^2} \mu_f \nabla_{\boldsymbol{x}} \psi + \operatorname{div}_{\boldsymbol{x}}\left\{\int_{\mathbb{S}^2}(\boldsymbol{d} \times \mathcal{R}\mu_f) \otimes \boldsymbol{d} f\right\}\,,
\end{aligned} \tag{2.7c}$$

$$\operatorname{div}_{\boldsymbol{x}} \boldsymbol{v} = 0\,, \tag{2.7d}$$

in $\Omega$. Finally, the electrostatic potential $V$, which prescribes the electric field via $\boldsymbol{E} = -\nabla_{\boldsymbol{x}} V$, is given by

$$\operatorname{div}_{\boldsymbol{x}}\left\{\epsilon \nabla_{\boldsymbol{x}} V\right\} = \operatorname{div}_{\boldsymbol{x}}\left\{\chi_\Omega \int_{\mathbb{S}^2} z f \boldsymbol{d}\right\} \tag{2.7e}$$

in $\Omega^*$. In order to include anchoring conditions in (2.7), we will add

$$\int_\Omega \int_{\mathbb{R}^3 \setminus \Omega} \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \alpha(\boldsymbol{x} - \hat{\boldsymbol{x}})\beta(\boldsymbol{d}, \hat{\boldsymbol{d}})\psi(\hat{\boldsymbol{x}}, \hat{\boldsymbol{d}}, t) f(\boldsymbol{x}, \boldsymbol{d}, t)\,\mathrm{d}\hat{\boldsymbol{d}}\,\mathrm{d}\boldsymbol{d}\,\mathrm{d}\hat{\boldsymbol{x}}\,\mathrm{d}\boldsymbol{d} \tag{2.8}$$

where $\psi$ is the extension of the preferred orientation on $\partial\Omega$. The interplay between the wetting fluid and the internal structures of the liquid crystalline film can the be included by making the extension $\psi$ fluid dependent.

The numerical treatment of the Doi–Hess model derived above is expected to be rather expensive as the evolution is governed by a Fokker–Planck type equation on the high-dimensional product space $\Omega \times \mathbb{S}^2$ and includes the non-local contributions of the interaction potential (2.3). However, when deriving a simpler looking director field model, the standard approach [54] yields

$$\partial_t \boldsymbol{d} + (\boldsymbol{v} \cdot \nabla)\,\boldsymbol{d} - \boldsymbol{d} \cdot \nabla \boldsymbol{v} = -\frac{\delta F}{\delta \boldsymbol{d}}\,, \tag{2.9}$$

i.e. the director $\boldsymbol{d}$ is governed by an $L^2$-gradient flow of the free energy $F$. This approach captures the long-time behavior of the liquid-crystalline film, but not the current dynamic evolution. Therefore, we intend to derive a director model which includes the variation of the energy not only by an $L^2$-gradient flow, and therefore will capture the dynamic evolution of the system in addition to its long time behavior. We will also investigate the existence of weak solutions to the arising partial differential equations. The construction of weak solutions is usually based
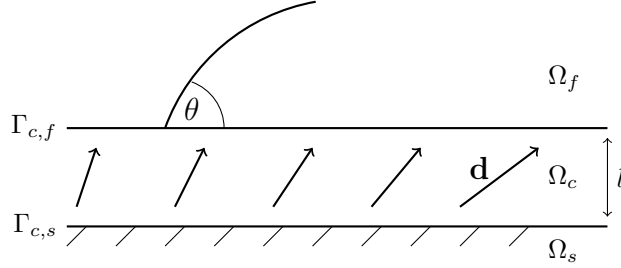
Figure 4: Sketch of a droplet on a switchable coating.

on global energy estimates and suitable (weak) compactness methods and therefore requires an understanding of the underlying structure of the model and the identification of important quantities that can be controlled by energy estimates. Consequently, establishing the existence of weak solutions will not only prove the well-posedness of the derived model, but will also indicate which properties of the model should be conserved in the subsequent coarse-graining process.

To validate the freshly derived microscopic model, we shall derive stable numerical schemes and compare our simulations of microscopic phenomena to experimental results which can be provided by the group of J. Hussong and E. Gurevich. Based on our experience (see Figure 2) with the numerical treatment high-dimensional, microscopic problems [P1], we intend to derive stable finite element schemes. As we expect the simulations to be very costly, it will be crucial to improve the splitting techniques successfully used in [P6], [P1], and [P2] to decouple as many parts of the model as possible without losing stability. In this part of the project, we intend to collaborate with the group of R. Stannarius and E. Eremin concerning the modeling of the interactions between the liquid-crystalline film and the wetting fluid, and with C. Liu concerning the derivation of improved Ericksen-Leslie type models.

### 2.2.2 From multi-scale to effective models

The second part of the project aims for a better understanding of the different involved spatial and temporal scales. By separating the different scales it is often possible to simplify the model by using macroscopic, averaged quantities without losing the information from the microscopic scale completely.

As we assume the liquid-crystalline film to be very thin in comparison to its lateral extension, there is an obvious difference in the occurring spatial length scales. We intend to make use of this difference in the length scales and employ a lubrication approximation. This is a standard approach for the description of thin films (cf. Section 1.1.3). However, we do not expect the approximation to be as straightforward as in e.g. [51] and [52], as the instantaneous adjustment of the directors to their steady state was a key assumption in these publications. Hence, considering only the time scale corresponding to the evolution of the film is sufficient and the faster time scale corresponding to the evolution of the director can be neglected. In our case, i.e. in presence of external forces and interactions with the additional Newtonian film, it is not clear whether the director field attains the global or a possible local energetic minimum, and therefore, whether the fast time scale can be completely neglected. To overcome this obstacle, we shall consider also a faster time scale reflecting the changes in the orientation of the director. Adapting an approach from homogenization, we assume local periodicity in lateral direction. This allows us to split the model into multiple decoupled fine scale problems describing evolution of the director on the fast time scale, and a coarse scale problem describing the evolution of the coating and the wetting Newtonian film on the larger time scale.

We intend to investigate the resulting equations numerically.

At this point we want to highlight that the focus of this project is not on the spreading of the

liquid-crystalline thin film or the occurrence of precursor layers, but on the interplay between the anchoring conditions on the solid substrate, the influence of external magnetic or electric fields, and the anchoring conditions on the fluid-coating interface which give rise to switchable boundary conditions for the overlying film of a simple liquid.

## 2.3 Work programme incl. proposed research methods

### 2.3.1 Microscopic models

To derive the microscopic models for liquid-crystalline films, we apply an energetic variational approach [53]. The evolution of the director is governed by the deformation induced by a flow field $\boldsymbol{v}$. In particular, the evolution equation for the deformation tensor $\boldsymbol{\mathcal{F}}$ in the observer's coordinates reads

$$\partial_t \boldsymbol{\mathcal{F}} + \boldsymbol{v} \cdot \nabla \boldsymbol{\mathcal{F}} = \nabla \boldsymbol{v} \boldsymbol{\mathcal{F}} . \tag{2.10}$$

As the director $\boldsymbol{d}$ depends on its initial data $\boldsymbol{d}_0$ via $\boldsymbol{d} = \boldsymbol{\mathcal{F}} \boldsymbol{d}_0$ the kinematic equation for the director reads

$$\partial_t \boldsymbol{d} + \boldsymbol{v} \cdot \nabla \boldsymbol{d} - \boldsymbol{d} \cdot \nabla \boldsymbol{v} = 0 \tag{2.11}$$

with an a priori unknown velocity field $\boldsymbol{v}$. Here, $\boldsymbol{v}$ Combining the least action principle with Onsager's maximum dissipation principle will allow us to determine the velocity field based on the total energy and the dissipation of the system (see e.g. [68]).

### 2.3.2 Lubrication approximations

In the second year of the funding period, we will derive a lubrication approximation of the aforementioned models. We will use an asymptotic expansion and approximate the problem by considering the leading order terms. This will be a collaboration with G. Grün.

### 2.3.3 Numerical simulations

We plan to start with the numerical study of the microscopic models derived in Section 2.2.1 at the beginning of the second year of the funding period. We will implement the finite element schemes in our inhouse package `EconDrop` [4, 34],[P1],[P2]. `EconDrop`, which was developed in the group of G. Grün, is a finite element framework written in `C++` and allows for adaptivity in space and time. In the past various schemes for different models including two-phase flow [4], [P6], [P2] and micro-macro models [P1] have been implemented successfully in `EconDrop`.
The investigation of the numerical treatment of the coarse grained models derived in Section 2.2.2 will start at the end of the second year of the first funding period. Again, we plan to use the framework of `EconDrop` for the implementation, as it was also already used successfully used for simulations based the (stochastic) thin film equation.

## 2.4 Data handling

Not applicable.

## 2.5 Other information

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

Not applicable.

## 2.7 Information on scientific and financial involvement of international co-operation partners

Not applicable.

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# 4 Requested modules/funds

## 4.1 Basic Module

### 4.1.1 Funding for Staff

To carry out the research programme, we apply for funding of the following positions.

| Official position | Number | Duration | Salary | Total Cost |
|---|---|---|---|---|
| Doctoral researcher | 0.75 | 36 months | TV-L E13 | 145.125 Euro |
| Student assistant (B. Sc.) | 1 | 36 months | | 19.269 Euro |

### 4.1.2 Funding for direct project costs

### 4.1.3 Module Project-Specific Workshop

For travelling to the SPP2171 related meetings, we apply for 19.600 Euro.
To present results on conferences and invite other scientist, we apply for an assistance of 3000 Euro.

# 5 Project requirements

## 5.1 Employment status information

Stefan Metzger
Research associate A13 (for at least three years starting on August 20, 2019), University of Erlangen-Nürnberg

## 5.2 First-time proposal data

Stefan Metzger

## 5.3 Composition of the project group

## 5.4 Cooperation with other researchers

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

J. Hussong and E. Gurevich for a comparison of numerical and experimental results.
R. Stannarius and E. Eremin for modeling of liquid crystal - fluid interactions. C. Liu for the derivation of Ericksen–Leslie type models. G. Grün for the derivation a lubrication approximation.

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

H. Abels and H. Garcke (Regensburg University), G. Grün (Friedrich–Alexander University of Erlangen–Nürnberg), F. Guillen-Gonzalez (University of Sevilla, Spain), P. Knabner (Friedrich–Alexander University of Erlangen–Nürnberg), I. Rybak (University of Stuttgart), E. Süli (Oxford University, UK).

## 5.5 Scientific equipment

For numerical simulations, the PI has direct access to the computer infrastructure of Chair of Applied Mathematics 1 at Erlangen University which includes two workstations (2×6 cores, 48 GB RAM, and 2×10 cores, 128 GB RAM, respectively) and a compute server (4×10 cores, 512 GB RAM).

## 5.6 Project-relevant cooperation with commerical enterprises

Not applicable.

# 6 Additional information

G. Grün will also assist in the supervision of Ph.D. candidates.