Project Description
within DFG priority program SPP-2171

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Efficient simulations of dynamic wetting of flexible substrates

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1 State of the art and preliminary work

Soft wetting. Wetting of flexible substrates (i.e. soft wetting) plays a major role in a broad variety of phenomena. Technical applications include the patterning of cells[1] or droplets[2] onto soft surfaces, the optimization of condensation processes[3] or the deposition of droplets in ink-jet printing or additive manufacturing. Also in biology, capillary interactions with flexible materials play a major role in self-organization of cell tissues[4], cell motility[5] and cancer cell migration [6]. Still, our understanding of the dynamics of such soft wetting processes lags by far behind of what is known about rigid surfaces[7]. Despite significant progress in computational modeling of (de)wetting of rigid substrates and the interaction of single fluids with elastic solids separately, the continuum modeling and simulation of wetting of elastic substrates has remained essentially unexplored [8].

One reason for this discrepancy is certainly the challenging nature of the problem which is inherently multi-scale in space (processes at the micro-scale determine dynamics on the macro-scale) and time (different time scales ranging from microseconds to seconds). Additionally, the strong coupling of hydrodynamics and substrate dynamics near the contact line requires special attention from a numerical point of view. Another reason for the lack of computational results in this field lies in the diversity of the required numerical techniques: the simulation of wetting typically employs interface capturing techniques (like the phase-field method), while the interaction of a fluid with an elastic structure is typically modeled by interface tracking techniques, in particular the ALE method. As most computational groups traditionally focus only on one of these methods, first simulations of wetting of elastic substrates appeared only very recently [8, 9, 10, 11]. We are fortunately experienced in both fields (phase-field modeling and fluid-structure interaction) and plan to combine these two branches to develop improved phase-field models of dynamic wetting of flexible substrates within this priority program (SPP).

Phase-field modeling. The phase-field model (also diffuse-interface model) is probably the most popular continuum model to describe wetting phenomena with moving contact lines. The idea is based on an order parameter, the phase-field function ϕ, which is used to indicate the fluid phases. To be consistent with the phase field variable, we label the fluids with the numbers 0 and 1, i.e. we define $\phi = 0$ in fluid 0, $\phi = 1$ in fluid 1. The phase-field function varies smoothly across the interface leading to a (thin) diffuse interface which is also physically motivated by the composition of real fluid-fluid interfaces [12]. This diffusive nature of the interface regularizes the stress singularity at the contact line, making it a very natural approach for moving contact lines. The rigorous thermodynamic substructure of the model allows for energy stable discrete formulations [A4] and robust time discretizations [A5] and makes phase-field models physically more sound than sharp interface models, like level-set or ALE, which typically need to introduce experimental fitting parameters[7].

Consistent boundary conditions for the phase-field modeling of wetting have been derived in [13, 14]. In [15] an improved phase-field model was derived from variational arguments and showed

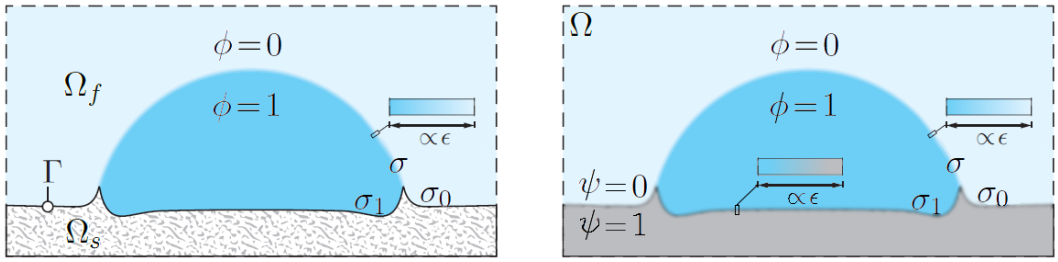


Figure 1: Illustration of the considered three-phase system. **Left:** In the typical phase-field-ALE framework, the fluid-fluid domain Ω_f and the solid domain Ω_s are separated by an interface Γ while the fluids are distinguished by a phase-field ϕ. **Right:** In a ternary phase-field model, an additional phase-field ψ is used to represent the solid domain.

impressive quantitative agreement to molecular dynamics simulations. In [A4] we have proposed a linear energy-stable discretization scheme for this model which enables the efficient solution, also in 3D.

Before we formulate the equations for the fluid-fluid-elastic three phase system, we begin by specifying the domains, see Fig. 1(left) for an illustration. The fluid-fluid system is contained in the time-dependent domain $\Omega_f \subset \mathbb{R}^d$, the time-dependent solid domain is denoted by $\Omega_s \subset \mathbb{R}^d$, for $d = 2, 3$. Both domains together form the computational domain $\Omega = \text{interior}(\bar{\Omega}_f \cup \bar{\Omega}_s)$. Both domains are separated by the time-dependent solid-fluid interface $\Gamma = \bar{\Omega}_f \cap \bar{\Omega}_s$. The behavior of the two-phase fluid in Ω_f can be described by the Navier-Stokes-Cahn-Hilliard equations [9, A8]:

$$\left.\begin{aligned} \partial_t^\bullet(\rho_f(\phi)\mathbf{v}) - \nabla\cdot\mathbf{S}_f &= \mathbf{F} \\ \nabla\cdot\mathbf{v} &= 0 \\ \partial_t^\bullet\phi &= \nabla\cdot(m\nabla\mu) \\ \mu &= \sigma\epsilon^{-1}W'(\phi) - \sigma\epsilon\Delta\phi \end{aligned}\right\} \text{ in } \Omega_f \tag{1}$$

where $\partial_t^\bullet = \partial_t + \mathbf{v}\cdot\nabla$ is the material derivative, $\rho_f(\phi)$ is the phase-dependent fluid density, $\mathbf{v}$ the volume-averaged velocity, $\mathbf{F}$ a body force, μ the chemical potential, ϵ controls the thickness of the diffuse interface and $m > 0$ is the mobility parameter. The double-well potential $W(\phi) = 18\phi^2(1-\phi)^2$ is here chosen to describe the phases by $\phi \approx 0, 1$ and to get rid of the scaling factor for the surface tension. Hence, σ is the physical fluid-fluid surface tension. Note, that we interprete ϕ here as volume fraction and consider a volume-averaged velocity formulation which ensures incompressibility of the mixture [16]. The stress of the complex fluid is given by

$$\mathbf{S}_f = \eta(\phi)(\nabla\mathbf{v} + \nabla\mathbf{v}^T) - p\mathbf{I} - \sigma\epsilon\nabla\phi\otimes\nabla\phi \tag{2}$$

where $\eta(\phi)$ is the phase-dependent viscosity, p the pressure and the last term represents the capillary stress. An additional term $M\rho'\mathbf{v}\otimes\nabla\mu$ can be added to the stress to ensure thermodynamic consistency of the model [16], but this will have only minor influence on simulation results, since ϵ is typically much larger than the physical interface thickness whereupon we aim to approach the sharp interface flow behavior, in which the term vanishes, see also our notable benchmark paper [A8]. In [8] an additional isotropic term has been included in the stress tensor, which essentially leads to a redefinition of the pressure.

Coupling Conditions. The set of equations (1) is supplemented by the following set of boundary conditions at the fluid-solid interface Γ

$$\left.\begin{aligned} \mathbf{S}_f \cdot \mathbf{n} &= \mathbf{S}_s \cdot \mathbf{n} + \sigma_s(\phi)\kappa\mathbf{n} + \nabla_\Gamma \sigma_s(\phi) \\ \partial_t^\bullet \phi &= -\nu \left(\sigma\epsilon \mathbf{n} \cdot \nabla\phi + \sigma_s'(\phi)\right) \\ \mathbf{n} \cdot \nabla\mu &= 0 \end{aligned}\right\} \text{ on } \Gamma \tag{3}$$

where $\mathbf{n}$ is the outer normal to Ω_f, $\mathbf{S}_s$ is the stress from the solid material, κ is the total curvature of the fluid-solid interface Γ and ∇_Γ is the surface gradient. The fluid-solid surface tension $\sigma_s(\phi) = (\sigma_1 - \sigma_0)(2\phi^3 - 3\phi^2) + \sigma_1$ is designed such that $\sigma_s(1) = \sigma_1$ and $\sigma_s(0) = \sigma_0$, where σ_1 and σ_0 are tensions between the solid and fluid 1 and fluid 0, respectively. In case of a flat rigid substrate, an equilibrium contact angle θ is related to these surface tensions by Young's relation $\sigma_1 - \sigma_0 = \sigma\cos(\theta)$.

Eq. (3_1) defines a balance of fluid traction, capillary stress and solid traction. The right hand side term $\nabla_\Gamma \sigma_s(\phi)$ is an additional contribution due to non-constant surface tension at the fluid-solid interface, also referred to as Marangoni force, see e.g. our works on interfaces with surfactants [A3]. In the sharp interface limit this force becomes singular at the three-phase contact-line and represents a line tension associated with changes in the contact line position.

Eq. (3_2) realizes a dynamic contact angle condition with an (inverse) relaxation time ν and has been derived in a variational model for moving contact lines [15] where it showed very good agreement with molecular dynamics simulations. Note, that when ν tends to infinity, Eq. (3_2) reduces to $\sigma\epsilon\mathbf{n} \cdot \nabla\phi = \sigma_s'(\phi)$ which realizes the static contact angle condition. Finally, Eq. (3_3) represents mass conservation (no penetration) at the fluid-solid interface.

The model (1-3) has been used in the previous work on wetting of flexible substrates [8, 9] in the static contact angle regime. In [10, 11] a similar model has been used based on the Navier-Stokes-Korteweg equations with neglected tension of the fluid-solid interface in Eq. (3_1).

Elastic structure. To close the system of equations it remains to specify the governing equations and stresses for the elastic structure. The defining property of soft condensed matter is a shear modulus, G, being much smaller than the bulk modulus [17]. As a consequence, all condensed soft matter is practically incompressible. This also holds for all materials that are soft enough to be significantly deformed by capillary forces of contacting droplets (unless they are extremely thin), and therefore for all materials discussed in this priority program (hydrogels, PDMS, etc.). Hence, it is effective and efficient to focus only on incompressible solid materials in the following, which provides many advantages, as we will see later.

One common way to specify the elastic stress is the neo-Hookean hyperelastic model which is based on the statistical thermodynamics of cross-linked polymer chains. The neo-Hookean model predicts the nonlinear stress-strain behavior of materials undergoing large deformations and is often the first choice for rubber-like materials and biological tissues[A2]. In previous work on wetting of flexible substrates [9, 10, 11], the simpler Saint Venant-Kirchhoff model was used which is based on a phenomenological description of the material behavior. This model agrees with the neo-Hookean model for small strains but might be less accurate and is less amenable to rigorous analysis since it is not based on a polyconvex energy function.
The stress of an incompressible visco-elastic neo-Hookean solid is given by

$$\mathbf{S}_s = G(\mathbf{B} - \mathbf{I}) - p\mathbf{I} + \eta_s(\nabla\mathbf{v} + \nabla\mathbf{v}^T) \tag{4}$$

where G is the material's shear modulus, $\mathbf{B} = \mathbf{F}\mathbf{F}^T$ is the left Cauchy-Green strain tensor and η_s is the additional viscosity when assuming Kelvin-Voigt visco-elasticity. Still in an Eulerian description

in the deformed configuration, the balance of mass and momentum takes the same form as in the fluid

$$\left.\begin{aligned} \partial_t^\bullet(\rho_s \mathbf{v}) - \nabla \cdot \mathbf{S}_s &= \mathbf{F} \\ \nabla \cdot \mathbf{v} &= 0 \end{aligned}\right\} \text{in } \Omega_s \tag{5}$$

ALE discretization. The standard method for discretization of fluid-structure interaction is the ALE method (Arbitrary Lagrangian-Eulerian) where the two domains Ω_s and Ω_f are discretized on two separate but connected, moving numerical grids. Grid points of the elastic structure and its surface move with the material velocity, i.e. they are material points. This also allows for easy calculation of $\mathbf{B}$ by memorizing the initial position X of each grid point by $\mathbf{B} = (\nabla X)^{-1}((\nabla X)^{-1})^T$, where gradients are understood with respect to the current configuration throughout this work. The grid points within the fluid structure are displaced in an arbitrarily prescribed way to obtain a mesh of proper shape, typically constructed by a harmonic map or pseudosolid movement. For example, if a harmonic map is used, the grid velocity $\mathbf{w}$ is the solution of

$$\left.\begin{aligned} \Delta \mathbf{w} &= 0 && \text{in } \Omega_f \\ \mathbf{w} &= \mathbf{v} && \text{in } \Gamma \\ \mathbf{w} &= 0 && \text{on } \partial\Omega_f \backslash \Gamma \end{aligned}\right\} \text{in } \Omega_s \tag{6}$$

and $\mathbf{w} = \mathbf{v}$ in Ω_s. The obtained grid velocity is then subtracted in the convective term of the equations, i.e., the material derivative $\partial_t^\bullet$ is replaced by

$$\partial_{t|\hat{x}} + (\mathbf{v} - \mathbf{w}) \cdot \nabla \tag{7}$$

where $\partial_{t|\hat{x}}$ defines the time derivative of a quantity on a moving grid point.

In the current literature on wetting of flexible substrates [8, 9, 10, 11], the governing equations in the solid domain are then discretized in the reference (undeformed) configuration of the grid, whereas the fluid equations are solved in the current spatial domain occupied by the fluid. Thereby, transformation functions are used to map from reference configuration to actual configuration. The fluid and solid subsystems are coupled in a partitioned scheme, i.e., both systems are solved alternatingly until convergence up to a prescribed tolerance is reached. This subiteration is typically done in every time step and can be enhanced by means of under-relaxation or modified-mass methods [18].

However, it has been found that for realistic applications of partitioned ALE methods for the soft wetting problem, there is a strong coupling between fluid and solid equations. Accordingly, in [8, 9] a severe under-relaxation was necessary to attain convergence in the subiteration process, leading to hundreds of subiterations in each time step. Additionally, small time steps have to be chosen, as several time scales are typically involved in the physical problem (kink formation in μs, ridge formation in ms, drop indentation in $\sim$ 100ms), making 3D simulations extremely challenging or even impossible.

One objective of this proposal is to relax this stiffness, which is not attributed to an added-mass effect [8] but to the interfacial coupling between binary fluid and elastic solid. To this end, we will formulate a monolithic coupling between both subsystems to enable stable large scale simulations of wetting of elastic substrates (see Sec. 2.3).

Phase-field modeling of fluid-structure interaction. While the ALE method provides a sound mathematical description and leads to a very accurate domain representation, it also comes with limitations on the evolution of the solid structure, which breaks down for large deformations or large translational and rotational movements. This has led to the development of alternative modeling approaches in recent years, in particular fully Eulerian formulations and interface capturing methods. In the recent decade numerical schemes have been developed to describe fluid–structure interactions in level-set methods [19, 20, 21] and volume-of-fluid methods [22].

We have very recently developed the first phase-field model for incompressible fluid-structure interaction [A1]. Thereby the governing equations in the fluid and solid domain are *not* defined by different sets of grid points, but a phase-field ψ is used the distinguish between the fluid region ($\psi = 0$) and the solid region ($\psi = 1$) in the full computational domain Ω. Hence, the equations for a *single* fluid and an elastic solid structure can be formulated similar to the fluid-fluid equations given in (1):

$$\left.\begin{aligned} \partial_t^\bullet(\rho(\psi)\mathbf{v}) - \nabla\cdot\mathbf{S}(\psi) &= -\sigma_s\epsilon\nabla\cdot(\nabla\psi\otimes\nabla\psi) \\ \nabla\cdot\mathbf{v} &= 0 \\ \partial_t^\bullet\psi &= \nabla\cdot(m\nabla\mu) \\ \mu &= \sigma_s\epsilon^{-1}W'(\psi) - \sigma_s\epsilon\Delta\psi \end{aligned}\right\} \text{ in } \Omega \tag{8}$$

for a constant fluid-solid surface tension σ_s. Thereby, the unified phase-dependent stress is given by

$$\mathbf{S}(\psi) = \eta(\psi)(\nabla\mathbf{v} + \nabla\mathbf{v}^T) - p\mathbf{I} + G\psi(\mathbf{B} - \mathbf{I}) \tag{9}$$

where the last term contributes the elastic stress. For example, choosing $\eta(\psi) = \eta_0(1-\psi)$ results in a classical fluid-structure interaction with viscosity η_0 in the fluid phase and elastic modulus G in the solid phase. The crucial part is the calculation of the left Cauchy-Green stress tensor $\mathbf{B}$. As no reference coordinates are available, $\mathbf{B}$ cannot be calculated directly from coordinate or displacement fields, but instead can be computed from the following evolution equation

$$\lambda(\psi)\left(\partial_t^\bullet\mathbf{B} - \nabla\mathbf{v}^T\cdot\mathbf{B} - \mathbf{B}\cdot\nabla\mathbf{v}\right) = -\alpha(\psi)(\mathbf{B}-\mathbf{I}) \qquad \text{in } \Omega \tag{10}$$

This is an Oldroyd-B like equation modeling the viscoelastic dissipation of the strain. By choosing the phase-dependent parameters $\alpha(\psi)$ and $\lambda(\psi)$ any combination of two phases, be it viscous ($\lambda = 0$), elastic ($\alpha = 0$) or viscoelastic ($0 < \lambda/\alpha < \infty$), can be modeled, for instance to simulate the interaction of a fluid with a viscoelastic Kelvin-Voigt or Maxwell-type material, see [A1(table 1)].

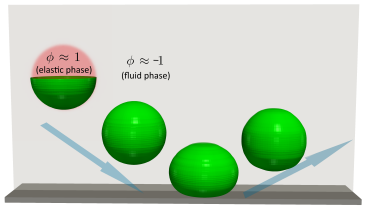
We have shown that Eqs. (8)-(10) approach the correct sharp interface equations of fluid-structure interaction as ϵ tends to zero. Also, the correct interface condition is recovered, namely that the jump between fluid and solid stress equals the interfacial surface tension force (here $\sigma_s\kappa\mathbf{n}$). A validation study showed excellent agreement to reference solutions from ALE simulations [A1].

The model is still brand-new and offers exciting new possibilities for modeling and simulation of fluid-structure interaction. For example topological transitions of elastic structures in flow (e.g. fluidization, melting) can be simulated or adhesive contact of elastic structures surrounded by a fluid [A1]. In the scope of this SPP, we believe that such a phase-field formulation of fluid-structure interaction is a natural choice to simulate wetting phenomena on flexible substrates, by introducing two phase-fields ϕ, ψ to represent the fluid-fluid and fluid-elastic interfaces. We will further elaborate on this in Sec. 2.3.

1.1 Project-related publications

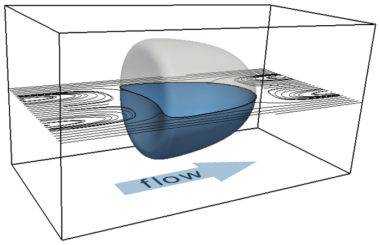
1.1.1 Articles published by outlets with scientific quality assurance, book publications, and works accepted for publication but not yet published

[A1] ***D. Mokbel***, *H. Abels,* ***S. Aland****. A phase-field model for fluid–structure interaction. J. Comp. Phys. 372 (2018)*



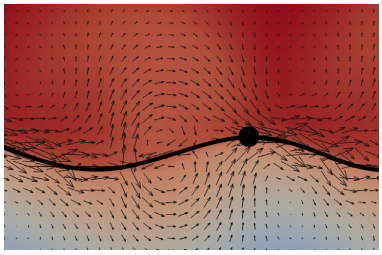
Summary: We present a first model for fluid-structure interaction where the elastic and fluid domain are described by a phase-field. The model can handle very large deformations, contact and adhesion of the solid to a wall. The method is carefully analyzed by matched asymptotic expansions and successfully benchmarked against reference solutions obtained by an ALE method. We highlight some distinct advantages of the new model, like the avoidance of re-triangulations and the stable inclusion of surface tension and illustrate that the model is capable to simulate any combination of viscous fluids, visco-elastic fluids and elastic solids.

[A2] ***M. Mokbel***, ***D. Mokbel***, *A. Mietke, N. Träber, G. Salvatore, O. Otto, J. Guck,* ***S. Aland****. Numerical Simulation of Real-Time Deformability Cytometry To Extract Cell Mechanical Properties. ACS Biomaterials, 3 (2017)*



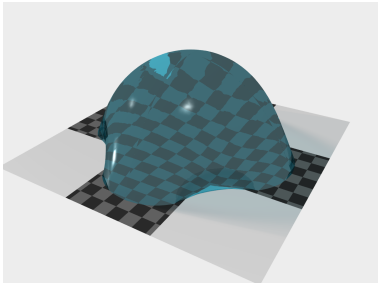
Summary: We study the fluid-structure interaction of an elastic biological cell traversing a flow channel and illustrate how the scenario can be used to extract cell mechanical parameters from matching simulations and experiments. We employ an ALE-model with elasticity formulated in the Eulerian framework. Energy variation is used to derive a very efficient, axisymmetric formulation for the elasticity of the cell surface as a thin linearly elastic shell.

[A3] ***M. Mokbel***, *S. Schwarzenberger, K. Eckert,* ***S. Aland****. The influence of interface curvature on solutal Marangoni convection in the Hele-Shaw cell. Int. J. Heat Mass Transfer. 115 (2017)*



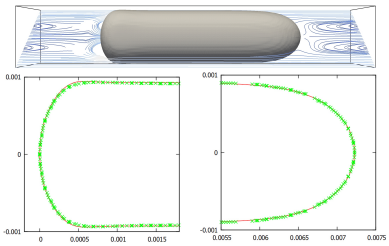
Summary: We study the impact of interfacial curvature on the Marangoni convection in a two-layer system of immiscible liquids with mass transfer of a surfactant. Interfacial curvature imposes concentration gradients along the interface as soon as the mass transfer starts. This leads to strong interfacial convection which initially enhances mass transfer but drastically reduces it at a later stage due to locking effects.

[A4] ***S. Aland***, *F. Chen. An efficient and energy stable scheme for a phase-field model for the moving contact line problem. Int. J. Numer. Meth. Fluids. 81 (2015)*



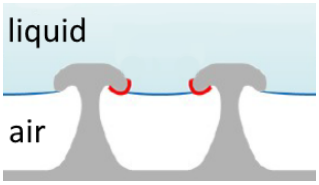
Summary: We propose for the first time a linearly coupled, energy stable scheme for the Navier–Stokes–Cahn–Hilliard system with generalized Navier slip boundary condition. We rigorously prove unconditional energy stability for the fully discrete finite element scheme. Using numerical tests, we verify the accuracy and demonstrate the effectiveness of our method through numerical simulations. The picture left shows equilibrium drop shape on a heterogeneous substrate.

[A5] ***S. Aland****. Time integration for diffuse interface models for two-phase flow. J. Comp. Phys. 262 (2014)*



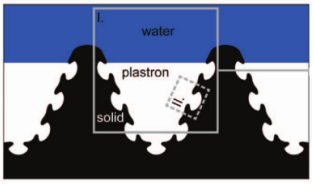
Summary: We propose a variant of the θ scheme for diffuse interface models for two-phase flow, together with linearization techniques that lower the stiffness arising from explicit coupling of interface and flow equations. We find that a monolithic coupling of these equations can even remove the time step restrictions completely. This coupling decreases the computation time of a Taylor flow scenario by several orders of magnitude, making diffuse-interface models faster than other interface capturing methods.

[A6] *R. Hensel, R. Helbig,* ***S. Aland****, H.G. Braun, A. Voigt, C. Neinhuis, C. Werner. Wetting resistance at its topographical limit. Langmuir, 29/4 (2013)*



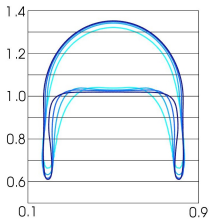
Summary: We study liquid wetting of microstructured surfaces as biologically found on the skin of springtails (Collembola). Using theory and numerical simulations we discover biological design principles that lead to hydrophobic and oleophobic surface properties. Our results pave the way for omniphobic surfaces with a high-pressure resistance irrespective of solid surface chemistry.

[A7] *R. Hensel, R. Helbig,* ***S. Aland****, A. Voigt, C. Neinhuis, C. Werner. Tunable nano-replication to explore the omniphobic characteristics of springtail skin. Nature Asia Materials, 5 (2013)*



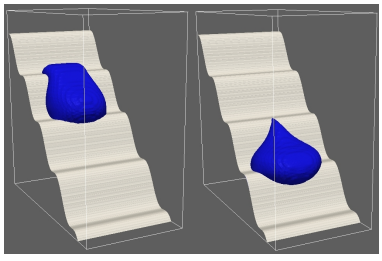
Summary: We explore the Cassie–Wenzel transition of springtail skin by in situ experiments and phase-field simulations. The results obtained unravel the decisive role of nanoscopic surface structures for the protection of springtails against wetting, and explain how the evolved nanotopography enables the production of omniphobic surfaces even from intrinsically hydrophilic polymer materials.

[A8] ***S. Aland****, A. Voigt. Benchmark computations of diffuse interface models for two-dimensional bubble dynamics. Int. J. Numer. Meth. Fluids. 69 (2012)*



Summary: In this quite popular paper, we conduct the first quantitative benchmark of phase field models for two-phase flow and compare the results with other numerical methods. We find good agreement among the models and convergence as the diffuse interface thickness tends to zero. In a balanced regime of modeling error (due to finite interface thickness) and numerical error (due to finite grid size), phase-field methods are found to need a similar computational effort as other two-phase flow models.

[A9] ***S. Aland****, J. Lowengrub, A. Voigt. Two-phase flow in complex geometries: A diffuse domain approach. Comp. Model. Eng. Sci., 57 (2010)*



Summary: We present a method for simulating two-phase flows in complex geometries, where we combine the diffuse domain method for solving PDEs in complex geometries with the phase-field method for simulating multiphase flows. In this approach, the complex geometry is described implicitly by an additional phase-field variable, that can be directly calculated from imaging data of the complex geometrical structure. The fluid and component concentration equations are reformulated and solved in larger regular domain with the boundary conditions being implicitly modeled by source terms.

2 Objectives and work programme

2.1 Anticipated total duration of the project

36 months, starting October 1, 2019

2.2 Objectives

Working at the small scales of typical droplets (often at a length scale L$< 100\mu$m), surface tension forces become dominant as they are scaled with L^3. This makes the coupling between flow and interface motion extremely stiff, such that severe time step restrictions are introduced. Hence, the time step size is not controlled by the desired accuracy of the solution, but by the stability of the numerical algorithm, resulting oftentimes in admissible time step sizes being several orders of magnitude smaller than physically necessary [A5]. As a consequence, numerical simulations with real-world parameters are impossible, if no stabilization mechanism is included.

Along these lines, it has been reported that a severe underrelaxation was necessary to stabilize the coupling between a wetting fluid and an elastic substrate with partitioned ALE approaches [8, 9], slowing down the solution by a factor ~ 100. While parallelization nowadays enables the solution of large 3D systems, integration in time still has to be done step-by-step and is therefore the bottleneck for relevant simulations. In particular for the soft wetting problem, where typical experimental times (drop movement, coalescence, phase separation) are in the range of 1-100 seconds, time step sizes of microseconds (as used in the available literature on soft wetting [8, 9, 11]) may make the system unfeasible for simulations of the dynamics, even in 2D.

Accordingly, The goal of this project is to develop improved numerical methods for the coupling of two-phase flow to elastic bodies and substrates. We will derive efficient numerical algorithms using adaptive methods and efficient and robust time discretizations. A highly parallel discretization in space will enable 3D simulation results, which we will validate in collaboration with experimentalists and theoreticians within the SPP. Beyond the mathematical point of view, the methods will make it possible to get new insight on exciting phenomena that have been discovered in experiments.

Accordingly, the objectives are arranged into 6 work packages with the aim to

- Develop improved ALE formulations for wetting of elastic substrates (WP1)
- Develop a ternary phase-field model for two fluids and one elastic solid (WP2)
- Define a first benchmark problem for soft wetting dynamics (WP3)
- Understand single drop dynamics and stick-slip motion (WP4)
- Present first simulations of wetting of elastic structured surfaces (WP5)
- Explore the interaction of drops through a soft substrate (WP6)

Thereby, we hope to establish a deeper understanding of the fundamental physics behind the dynamic wetting of flexible substrates and to help developing foundations for future technologies that utilize such phenomena.

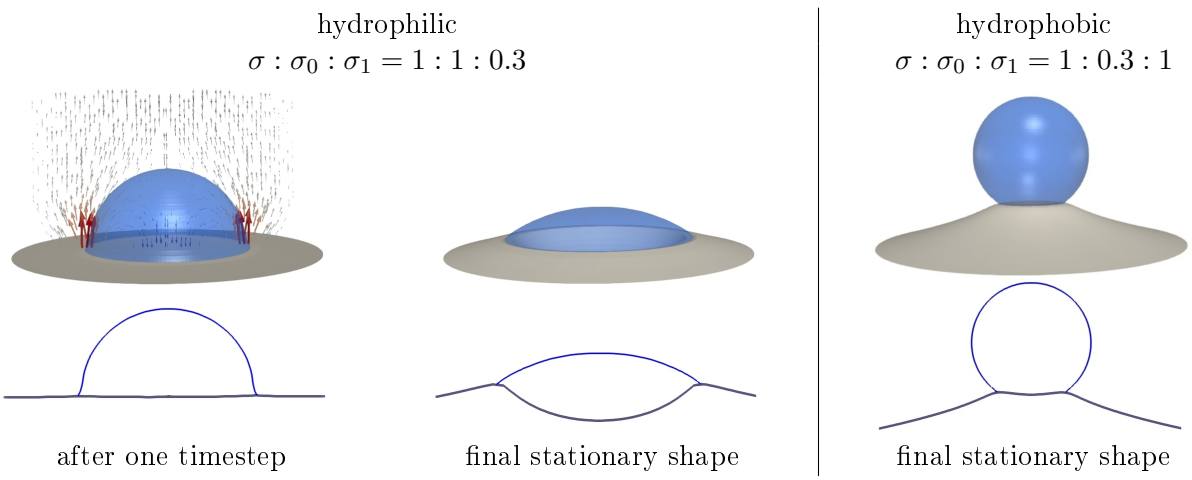


Figure 2: A first simulation of an initially half spherical fluid drop on a flexible surface for two different surface tension ratios. **Left:** Hydrophilic drop induces strong upward flow at the contact line at the start of the simulation. **Middle/Right:** Stationary shape of hydrophilic/hydrophobic drop.

2.3 Work programme incl. proposed research methods

WP1: Development of improved ALE formulations for wetting of elastic surfaces
As illustrated in the Sec. 2.2, a stable time integration is the most pressing issue in the numerical solution of wetting problems on elastic substrates. We will address this issue in the following. We will start with the absolute standard method for fluid-structure interaction problems, the ALE method. Thereby, we will solve Eqs. (1)-(5) combining our present ALE code for fluid-structure interaction [A2] and our phase-field code for moving contact lines [A4].

WP1.1: Code validation for a segregated model

In the first part, we plan to set up a segregated scheme where the fluid equations (1)-(2) and the solid equations (4)-(5) are solved alternating. Both equations are coupled through the boundary condition (3_1) including the Marangoni term and the continuity condition of the velocity field. As in [9] we will use an under-relaxation to stabilize this coupling.

Our available codes of fluid-structure interaction and two-phase flow are dimension-independent and can therefore switch between 2D, 3D and axisymmetric. Grid adaptivity is realized by a jump residual estimator. The implementation involves only the coupling of these two codes and should be straight-forward as we have many years of experience in phase-field modeling, wetting, fluid-structure interaction and Marangoni forces. For illustration, we have set up a simple ALE discretization to simulate the wetting of a single axisymmetric drop on a thin elastic surface. Thereby, the system (1)-(3) is solved, but the stress of the elastic surface is modeled as given in [A2,Sec.6]. Fig. 2 shows the initial and stationary states for two Parameter combinations.

In contrast to usual ALE schemes, the equations are here formulated in an Eulerian frame of reference, which eliminates an explicit evaluation transformations from the reference domain to the current domain. This may already have a positive influence on the stability of the system. Also, the direct enforcement of the incompressibility constraint makes the system more efficient and should also make it more stable than previous formulations [8, 9, 11], which used a huge first Lamé constant to make the material nearly-incompressible.

We will test the code for its performance and validate the numerical results in collaboration with H. van Brummelen (TU Eindhoven, Netherlands), who has presented a comparison of numerical

and experimental data of stationary wetting ridge shapes [8, 9]. As these results are given for an axisymmetric drop, they are amenable for very efficient axisymmetric simulations.

To validate the dynamics, we will collaborate with H. van Brummelen and S. Karpitschka (MPI Göttingen, within the SPP). S. Karpitschka can provide dynamic morphologies of the wetting ridge for moving droplets as well as measurements of droplet speeds for variously-sized droplets on inclined surfaces, see also WP4.

WP1.2: stable monolithic fluid-fluid-elastic ALE system

It is known that monolithic schemes give higher accuracy while enabling larger time steps (or significantly less subiterations) [23]. Accordingly we will formulate a monolithic scheme of the fluid-fluid-elastic ALE system in this work package. A complete description of the time discretization of the complete problem is beyond the range of this proposal. Rather, we focus on the presentation of the ideas to develop an linear and implicit time stepping scheme.

The Eulerian formulation of fluid and solid equations (1)-(5) enables a unified weak formulation and discretization. Let us consider the momentum equation for an illustration. By adding up the usual weak forms of Eqs. (1_1) and (5) and using the boundary condition (3_1), one obtains the single (weak) momentum equation for both phases:

$$\int_\Omega \partial_t^\bullet(\rho\mathbf{v})\cdot\alpha + \eta(\nabla\mathbf{v}+\nabla\mathbf{v}^T):\nabla\alpha + p\nabla\cdot\alpha\ dx + \int_{\Omega_f}\sigma\epsilon\nabla\phi\otimes\nabla\phi:\nabla\alpha\ dx + \int_{\Omega_s} G(\mathbf{B}-\mathbf{I}):\nabla\alpha\ dx = \int_\Gamma(\sigma_s(\phi)\kappa\mathbf{n}+\nabla_\Gamma\sigma_s(\phi))\cdot\alpha\ dx \tag{11}$$

for some test function α, e.g. $\alpha\in H^1(\Omega)^d$.

The most significant point is the intrinsic inclusion of the interfacial balance in this formulation, since the boundary condition (3_1) is naturally incorporated. From two-phase flow simulations it is known that such a treatment can completely stabilize the coupling of two different phases. The remaining boundary integral of the solid surface tension force can be made essentially implicit. For example, the interface curvature κ can be evaluated at the new time step by expressing it as the previously computed κ plus a correction involving the new velocity field. This approach, introduced by Dziuk [24], is standard in sharp interface methods for two-phase flows and is known to stabilize surface tension forces significantly. Also note, that the velocity is, in accordance with α, chosen from a Sobolev space defined on whole Ω which automatically ensures continuity of the velocity across the fluid-solid interface.

Hence, the above formulation of unified momentum equation is expected to have superior stability properties. In particular an implicit time-stepping can be formulated. In [A5] we have shown an unconditionally stable implicit coupling strategy for the capillary stress, which can be adapted to the current problem. The only remaining explicit term in Eq. (11) is the left Cauchy-Green strain tensor $\mathbf{B}$. If the explicit evaluation of this term poses problems for the stability of real-world applications, we can go to linear elasticity. In this case a displacement field $\mathbf{u}$ can be calculated by the evolution

$$\partial_t^\bullet\mathbf{u} = \mathbf{v} \qquad \text{in } \Omega_s \tag{12}$$

and the elastic stress $G(\mathbf{B}-\mathbf{I})$ is replaced by $G(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$.

To discretize the unified momentum equation (11) in time, the material derivative is replaced by the ALE derivative (7) and a backward Euler scheme is used. The unified momentum equation can

be discretized in space by finite-elements coupled to the incompressiblity condition and the Cahn-Hilliard equations. This coupling can be done monolithically as we have shown in [A5], i.e. the final linear system of equations for all degrees of freedom is assembled in *one* common matrix, taking into account all couplings. We have shown in [A5] that such a coupling can completely remove the stiffness of interfacial forces and result in a very efficient numerical scheme.

While the discontinuity of ρ and η across the sharp fluid-solid interface can be easily handled by using appropriate quadrature rules, special care has to be taken for the pressure finite-element space, which needs to be enriched to deal with discontinuity of p across Γ. But since Γ is placed on the nodes of grids, the resulting extended finite-element space only requires one additional degree of freedom for the pressure at each node on Γ, which is easy to implement in our FEM toolbox AMDiS[25].

Finally, we arrive at a stable monolithic ALE discretization which should produce robust and accurate results without subiterations and therefore be several magnitudes faster than present numerical models [8, 9]. It should also be possible to develop energy stable scheme similar to our work in [A4]. We will again collaborate with H. van Brummelen regarding exchange of knowledge and code comparison.

WP2: Ternary phase-field model for wetting of flexible substrates

Parallel to the improvements of existing ALE models, we will develop a very interesting alternative model to describe the interaction of two fluids with an elastic body or substrate. The idea is to combine the novel phase-field model for fluid-structure interaction [A1] with the phase-field model for moving contact lines. That is, we develop a three-phase model for the two fluids and one solid phase. The resulting system will offer exciting new possibilities, for example the motion of an elastic body through a two-phase fluid (without remeshing), topological transitions of the elastic structures (e.g. melting) or adhesive contact of elastic structures immersed in a two-phase fluid, see [A1].

To develop the model, we can build upon present models for three-phase flows developed by our long-standing collaborator J. Lowengrub [26], improved in [27] and analyzed in [28]. Using the same ideas here, we can represent the three distinct phases by the fields ψ ($=1$ in the solid phase), ϕ ($=1$ in fluid 1) and ξ ($=1$ in fluid 0). Of course, the concentrations of all phases sum up to 1, i.e., the admissible states are restricted by the condition $\psi+\phi+\xi=1$. This condition is enforced by an additional term in the chemical potential and reduces the unknown phase variables effectively to two fields, ϕ and ψ from which the third field can be computed, here $\xi=1-\phi-\psi$. See Fig. 1(right) for an illustration.

Following the approach in [26, 27], we obtain the system

$$\left.\begin{aligned} \partial_t^\bullet(\rho(\psi,\phi)\mathbf{v}) - \nabla\cdot\mathbf{S}(\psi,\phi) &= \mathbf{F} \\ \nabla\cdot\mathbf{v} &= 0 \\ \partial_t^\bullet A &= \nabla\cdot(m\nabla\mu_A) && \text{for } A=\phi,\psi \\ \mu_A &= \epsilon^{-1}W'(A) - \epsilon\Delta A - \epsilon^{-1}\phi\psi(1-\phi-\psi) && \text{for } A=\phi,\psi \end{aligned}\right\} \text{in } \Omega \quad (13)$$

where the stress $\mathbf{S}(\psi,\phi)$ now contains phase-dependent viscosity, pressure, elastic stress and the surface tension stress of the three contact lines:

$$\begin{aligned} \mathbf{S}(\psi,\phi) =& \eta(\psi,\phi)(\nabla\mathbf{v}+\nabla\mathbf{v}^T) - p\mathbf{I} + G\psi(\mathbf{B}-\mathbf{I}) \\ & - \epsilon\sigma\nabla\phi\otimes\nabla\phi - \epsilon\sigma_0\nabla\psi\otimes\nabla\psi - \epsilon\frac{\sigma+\sigma_0-\sigma_1}{2}\left(\nabla\psi\otimes\nabla\phi+\nabla\phi\otimes\nabla\psi\right). \end{aligned} \quad (14)$$

Additionally, Eqs. (13)-(14) are coupled to Eq. (10) for the evolution of the strain tensor $\mathbf{B}$. For illustration and to check the feasibility, we have performed a first three-phase flow simulation without elastic stress shown in Fig. (3).

We will analyze the resulting model in terms of sharp interface limit, numerical properties and benchmark against reference solution from ALE models [8, 9], in collaboration with J. Lowengrub. We see several advantages of this phase-field model as compared to ALE simulations: **(i)** the superior stability due to the consistent Eulerian description as a three-phase-fluid model, **(ii)** the easy monolithic coupling of interface advection and flow equations, similar to our work in [A5], lifting any stiffness-related time step restrictions, **(iii)** the possiblitity to simulate large translational and rotational movements of the elastic phase without grid remeshing, and **(iv)** the thermodynamic substructure of the system allowing for linear energy-stable schemes, similar to our work in [A4].

Further by choosing the parameters accordingly, we can simulate any combination of two fluids being in contact with a liquid, elastic or viscoelastic third phase, which is essentially any combination interesting for this SPP. Parts of this work package will be done in agreement with A. Voigt (within the SPP) who develops a very similar model. In particular we will supply A. Voigt with the phase-field code for fluid-structure interaction from [A1] and share work efficiently whenever possible.

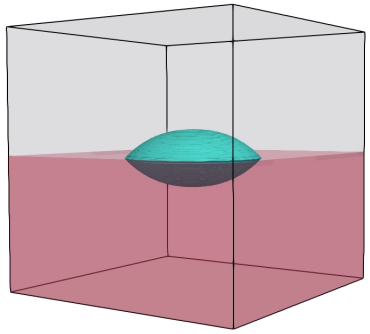


Figure 3: A first three-phase flow simulation: Stationary state of an initially circular liquid lens located at an interface between two other immiscible fluids.

WP3: A wetting benchmark

In the absence of exact, analytical reference solutions, numerical benchmarking (i.e. code-to-code comparison) is needed to assess the accuracy of numerical models. Good benchmarking is not only important for verification and validation of numerical codes, but can be extremely helpful for code development, in particular for new groups entering this computational field. Within this SPP we plan to define and conduct a first benchmark for wetting and soft wetting in collaboration with the groups of A. Voigt (TU Dresden) and A. Reusken (RWTH Aachen). We plan to simulate the relaxation of an initially half-spherical drop on a substrate with three different numerical methods: the ALE method (see WP1), the ternary phase-field method (see WP2) and a level-set formulation for three viscous phases. The total benchmark should consider four substrate rheologies: viscous, elastic, viscoelastic and rigid. The use of realistic physical parameters will ensure that the benchmark is also amenable to experiments, providing a tool to assess computational modeling errors as well as experimental measurement errors.

WP4: Single drop dynamics and stick-slip motion

The motion of drops on flexible surfaces is highly relevant for technical processes (printing, coating) as well as to understand biolgical systems governed by similar physical processes (e.g. cell motility, wound healing). However, our understanding of the dynamics of a single drop on an elastic substrate lags far behind of what is known about rigid surfaces[7]. Experiments have shown that the softness drastically slows down the wetting dynamics in comparison to rigid solids. The theoretical description of moving contact lines over soft solids is so far limited to global dissipation arguments, which, already for wetting of rigid solids, are known not to capture the entire physics behind the process[29].

Together with S. Karpitschka (within the SPP) we plan to reveal the physical mechanisms governing the dynamics of soft wetting. Thereby we plan to work in a close bilateral subsequent collaboration, where alternating experiments and simulations inspire, support and assist each other in a feedback loop, leading to a gradual increase of understanding of soft wetting. As detailed in his proposal, S. Karpitschka can provide data on droplet speed on inclined surfaces, time-resolved profiles of dynamic wetting ridges and dynamic strain fields during drop motion.

The few current numerical works address mostly the stationary state, where the morphologies of drop and substrate depend only on elastic and surface properties. By simulating the dynamics, also the visco-elasticity of the substrate has to be considered. Just recently an alternating stick and slip behavior, termed stick-slip motion was discovered on viscoelastic substrates, with its physical origin being still under debate[29]. It has been shown in the work of our collaborator, that realistic theoretical predictions can only be achieved when geometrical non-linearities and realistic rheologies are included [29]. Our phase field model developed in WP2 includes a neo-Hookean material law as well as three different visco-elastic models: Kelvin-Voigt, Maxwell and Jeffrey (see also [A1]) and is therefore ideally suited to tackle realistic simulations of droplet dynamics. Motion of the contact line can be triggered in the experiments by gravity (substrate inclination), by droplet inflation through a syringe pump, or by pumping fluid through a cylindrical cavity. The latter two cases are even amenable for axisymmetric simulations, which provides a way to extremely efficient and accurate simulation results. S. Karpitschka will use two liquids instead of a liquid/gas system, which reduces the density and viscosity ratios by several orders of magnitude for the benefit of the numerical simulations. The according experimental setup is designed to tune material parameters individually to disentangle nonlinearities arising from wetting ridge deformation and substrate rheology. Accordingly, we believe that this collaboration between the simulations, theory and experiments will provide a significant contribution towards understanding of the physics of soft wetting.

WP5: Elastic structured surfaces

The ALE method is ideally suited to describe elastic bodies of complex topography with fine surface structuring. Compared to phase-field models, only a small amount of degrees-of-freedom is necessary to resolve slender structures of the elastic body, due to the sharp and mesh-fitted surface representation. We will exploit this feature by presenting the first simulation results for wetting of elastic micro-structured surfaces.

The slenderness of microscopic surface structures leads to strong elastic deformations, and intensifies the complex interplay of droplet dynamics and substrate elasticity. Additional effects arising from the complex geometry (e.g., the Cassie-Wenzel transition, see [A7]) make such problems particularly interesting, especially in view of the massive scientific efforts to create robust omniphobic surfaces.

We have already considered wetting of complex (rigid) topographies in [A6,A7] in a joint experimental and theoretical work. For illustration we have also conducted a toy simulation of wetting of a hairy substrate in Fig. 4. Now, we aim to proceed to elastic substrates and plan a close collaboration with K. Harth (within the SPP) who will consider wetting of micro-structured subtrates. K. Harth will provide strain fields of the elastic deformation in the bulk and on the surface as well as high resolution imaging data of drop shapes. In the start of the collaboration, we will conduct a small validation study considering the impact of a single drop on a planar elastic substrate. Using the same materials, we will then move to structured surfaces with elastic pillars (10-100μm) and compare numerical and experimental data. We will consider a single drop moving by substrate inclination and investigate the influence of substrate elasticity on the drop velocity and at the pinning and detachment dynamics of single pillars. Particular interest will also be put on the influence of elasticity on the Cassie-Wenzel transition and the apparent contact angle which is strongly related to the creation of omniphobic surfaces. As wetting of structured elastic surfaces has not been simulated before, the problem is already interesting in reduced dimensions. Hence, we will start with 2D simulations to understand the influence of elasticity on contact line motion and then turn to 3D simulations within the experimental collaboration.

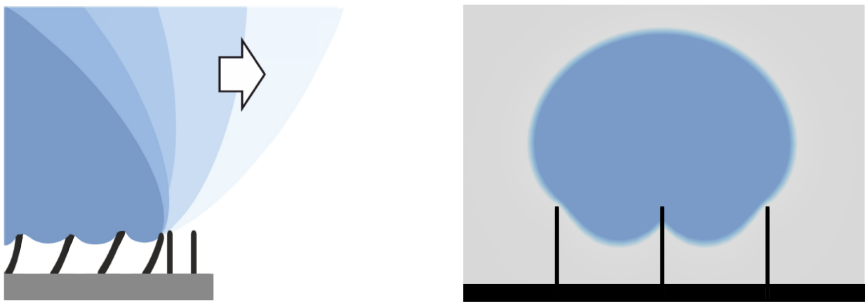


Figure 4: Wetting of elastic structured surfaces illustrated by a single drop on a hairy substrate. **Left:** Schematic image from the SPP coordinators. **Right:** A first 2D simulation of a single liquid drop on a hairy substrate *without* elasticity. Shown is the stationary state at contact angle $\theta = 135°$.

WP6: Durotaxis and substrate-mediated liquid interaction

In this work package we plan to go further to consider the interaction of liquid morphologies with an heterogeneous elastic substrate, which gives rise to many interesting effects. One of these is durotaxis, i.e. the motion of drops along gradients in substrate stiffness, which offers new technical applications, for example the patterning of liquid drops[2]. Computationally, durotaxis has only been addressed in a first paper [10].

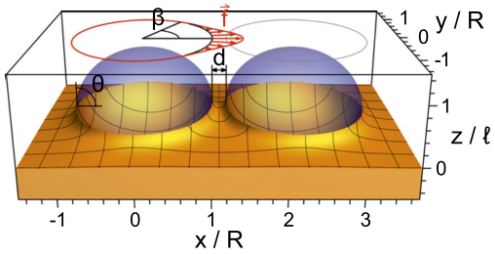


Figure 5: Illustration of the cheerios effect: The elastocapillary meniscus leads to long-range attraction of two drops. Image reproduced from [30].

Alternatively, substrate heterogeneity may stem from local deformation of the elastic material, for example due to the presence of an other contact line. In this case our collaborator S. Karpitschka has found an *inverted cheerios effect*, which is defined as substrate-mediated attraction of nearby drops [30]. Similar interactions occur in drop condensation experiments, where the surface softness leads to increased attraction but decelerated fusion of drops [3]. A numerical investigation of the dynamics governing these effects remains open.

We will study the cheerios effect with two drops and extend this to multiple drops to investigate the coarsening dynamics on a soft substrate. The drops will be initially placed on the substrates in different distances and geometrical configurations. As the cheerios effect is an intrinsically slow process, relatively large time steps can be used to capture the physical evolution. The robust time discretizations developed in WP1 and WP2 make this possible, as they should lift time step restrictions from numerical stiffness. The results of the benchmark comparison (WP4) will determine whether we use the ternary phase-field or the phase-field-ALE model. In collaboration with A. Voigt we will look at connections to the coarsening dynamics of solid materials governed by surface diffusion or attachment/detachment processes.

Experimentally, we will collaborate with the SPP project Seemann/Wagner and again with S. Karpitschka who first reported the cheerios effect. The group of R. Seemann will conduct dewetting experiments where substrate-mediated droplet interaction should occur after complete dewetting at the late stage of the experiments. We will use the dewetted droplet pattern as a starting point for the simulation study and compare the long-time evolution of drops to experimental results.

S. Karpitschka will provide experimental data on the cheerios effect and investigate the phase separation of an initially homogeneous mixture on soft substrates. Such processes are particularly

exciting as they are tightly related to fog harvesting which becomes increasingly popular in regions of water shortage. The dynamics of phase separation are governed by the ratio of volume and surface area of emerging nuclei. As tiny drops tend reduce their surface area by sinking into soft substrates, the dynamics of phase separation is expected to be largely influenced by substrate stiffness. Computationally, nucleation on soft substrates is completely unexplored but can be included in the phase-field model by using a different double-well potential and an additional noise term satisfying the fluctuation-dissipation theorem [31]. However, due to time restrictions we may have to leave this advanced project part for the second funding period of the SPP.

Extension: Efficient parallelization
Whenever it is appropriate, we will use axisymmetric configurations, such that the simulations can be effectively reduced to 2D computations leading to a very efficient discretization in space. However for many physically relevant configurations this might not be possible and the space discretization will result in big systems of equations, which can only be solved by parallel computing. Our finite element toolbox AMDiS already contains an advanced parallelization based on domain decomposition, MPI communication and PETSc data structures and solvers. The current parallelization has been shown a good weak scaling efficiency for up to 1024 cores [25]. It is ready to work with any system of equations, such that we should be able to use it for the soft wetting problem without any effort. Together with the monolithic time discretization from WP1.2 or WP2, we expect that this will result in very efficient high performance simulations of soft wetting in 3D.

In the unlikely case that a much larger number of processors has to be employed in the course of the project, it might be necessary to improve the efficiency of the parallelization. In this case, we can adapt the FETI-DP method to the current problem. FETI-DP is a highly scalable parallelization [32] which has been shown to scale for up to 65,536 cores [33]. The method has already been used for Stokes problems and can easily be implemented in AMDiS. Access to the Saxonian high performance computer TAURUS (40,000 cores) in Dresden ensures that we can exploit the potential of FETI-DP for large scale 3D soft wetting problems.

Extension: Adaptive and Switchable surfaces
Adaptive and switchable surfaces are another branch of this SPP which we have not explicitly addressed in this proposal. However, the numerical methods that we develop here provide a general and flexible tool in which physical parameters can be freely functionalized. Accordingly, the effects of adaptive and switchable surfaces can be incorporated into the method with only minor modifications. For example, one could easily make the surface tension energies dependent on an external switch or local properties (flow rate, surface strain, etc.) to realize adaptivity and switchability. Though this goes beyond the scope of the first three years of this SPP, we are open to make use of these capabilities as new collaborations may arise in the course of the SPP funding period.

Work schedule
The targeted work schedule is depicted in Fig. 6

2.4 Data handling

All data will be handled and stored according to the "Suggestions of best practice" and "Guidelines on the Handling of Research Data" of DFG. The state of Saxony provides an open access document server (Qucosa) which will allow for long-term storage and sustainable usage of project results and raw data. Additionally, we are committed to publish in high quality journals listed in the Directory of Open Access Journals (DOAJ) and published by members of the Open Access Scholarly Publishers Association (OASPA).

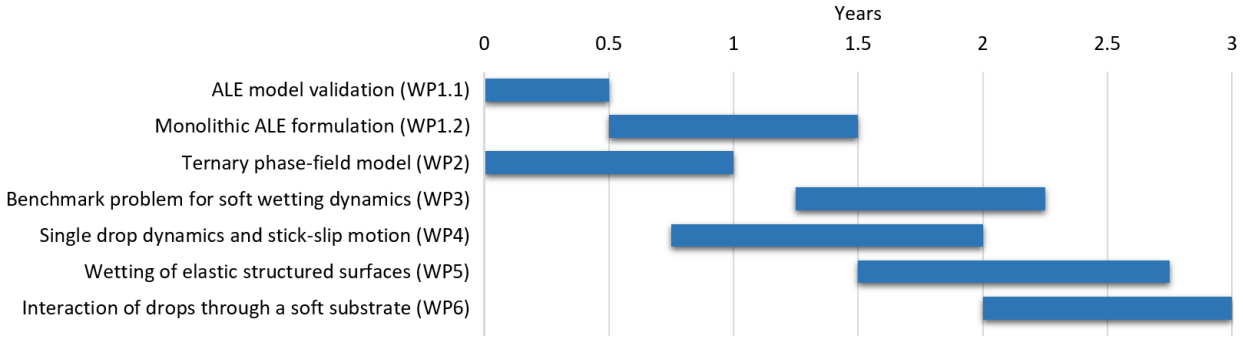


Figure 6: Planned work schedule.

2.5 Information on scientific cooperation within SPP 2171

Dr. Kirsten Harth (Uni Magdeburg)	Elastic micro-structured surfaces	WP5
Dr. Stefan Karpitschka (MPI Göttingen)	Single drop dynamics on viscoelastic substrates Cheerios effect and nucleation	WP4 WP6
Prof. Dr. Arnold Reusken (RWTH Aachen)	Soft wetting benchmark	WP3
Prof. Dr. Ralf Seemann (Uni Saarbrücken)	Substrate-mediated droplet interaction	WP6
Prof. Dr. Axel Voigt (TU Dresden)	Ternary phase-field model, soft wetting benchmark	WP2, WP3
Prof. Dr. Barbara Wagner (TU Berlin)	Substrate-mediated droplet interaction	WP6

Loosely concerted collaborations

Dr. Florian Kummer (TU Darmstadt)	Code comparison

3 Bibliography

[1] D. E. Discher, P. Janmey, and Y.-l. Wang. "Tissue cells feel and respond to the stiffness of their substrate". In: *Science* 310.5751 (2005), pp. 1139–1143.

[2] R. W. Style et al. "Patterning droplets with durotaxis". In: *Proceedings of the National Academy of Sciences* 110.31 (2013), pp. 12541–12544.

[3] M. Sokuler et al. "The softer the better: fast condensation on soft surfaces". In: *Langmuir* 26.3 (2009), pp. 1544–1547.

[4] M. L. Manning et al. "Coaction of intercellular adhesion and cortical tension specifies tissue surface tension". In: *Proceedings of the National Academy of Sciences* 107.28 (2010), pp. 12517–12522.

[5] C.-M. Lo et al. "Cell Movement Is Guided by the Rigidity of the Substrate". In: *Biophysical Journal* 79.1 (2000), pp. 144 –152.

[6] S. Douezan, J. Dumond, and F. Brochard-Wyart. "Wetting transitions of cellular aggregates induced by substrate rigidity". In: *Soft Matter* 8.17 (2012), pp. 4578–4583.

[7] D. Bonn et al. "Wetting and spreading". In: *Reviews of modern physics* 81.2 (2009), p. 739.

[8] E. Van Brummelen et al. "Binary-fluid–solid interaction based on the Navier–Stokes–Cahn–Hilliard Equations". In: *Fluid-Structure Interaction*. de Gruyter, 2017, pp. 283–328.

[9] E. Van Brummelen, M Shokrpour-Roudbari, and G. Van Zwieten. "Elasto-capillarity simulations based on the Navier–Stokes–Cahn–Hilliard equations". In: *Advances in Computational Fluid-Structure Interaction and Flow Simulation*. Springer, 2016, pp. 451–462.

[10] J. Bueno et al. "Wettability control of droplet durotaxis". In: *Soft matter* 14.8 (2018), pp. 1417–1426.

[11] J. Bueno et al. "Three-dimensional dynamic simulation of elastocapillarity". In: *Meccanica* 53.6 (2018), pp. 1221–1237.

[12] J. van der Waals. "The thermodynamic theory of capillarity flow under the hypothesis of a continuous variation of density. Verhandel Konink Akad Weten 1. Translation Published by Rowlinson JS". In: *J Stat Phys* 20 (1893). cited By 1, pp. 200–244.

[13] D Jacqmin. "Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling". In: *Journal of Computational Physics* 155.1 (1999), pp. 96–127.

[14] W. Ren and W. E. "Boundary conditions for the moving contact line problem". In: *Physics of Fluids* 19.2 (2007), p. 022101.

[15] T. Qian, X.-P. Wang, and P. Sheng. "A variational approach to moving contact line hydrodynamics". In: *Journal of Fluid Mechanics* 564 (2006), pp. 333–360.

[16] H. Abels, H. Garcke, and G. Grün. "Thermodynamically Consistent, Frame Indifferent Diffuse Interface Models for Incompressible Two-Phase Flows With Different Densities". In: *Math. Mod. Meth. Appl. Sci.* 22.03 (2012), pp. 1150013–1.

[17] D. Johannsmann. *The Quartz Crystal Microbalance in Soft Matter Research*. Springer, 2014.

[18] E. Van Brummelen. "Partitioned iterative solution methods for fluid–structure interaction". In: *International Journal for Numerical Methods in Fluids* 65.1-3 (2011), pp. 3–27.

[19] G. Cottet, E. Maitre, and T. Milcent. "Eulerian formulation and level set models for incompressible fluid-structure interaction". In: *ESAIM: M2AN* 42.3 (2008), pp. 471–492.

[20] A. Legay, J. Chessa, and T. Belytschko. "An Eulerian-Lagrangian method for fluid-structure interaction based on level sets". In: *Computer Methods in Applied Mechanics and Engineering* 195.17 (2006), pp. 2070–2087.

[21] P. He and R. Qiao. "A full-Eulerian solid level set method for simulation of fluid–structure interactions". In: *Microfluidics and Nanofluidics* 11.5 (2011), p. 557.

[22] K. Sugiyama et al. "A full Eulerian finite difference approach for solving fluid-structure coupling problems". In: *Journal of Computational Physics* 230.3 (2011), pp. 596–627.

[23] C. Michler et al. "A monolithic approach to fluid–structure interaction". In: *Computers & Fluids* 33.5 (2004). Applied Mathematics for Industrial Flow Problems, pp. 839 –848.

[24] G. Dzuik. "An algorithm for evolutionary surfaces". In: *Numer. Math.* 58.6 (1991), pp. 603–611.

[25] T. Witkowski et al. "Software concepts and numerical algorithms for a scalable adaptive parallel finite element method". In: *Advances in computational mathematics* 41.6 (2015), pp. 1145–1177.

[26] J. Kim and J. Lowengrub. "Phase field modeling and simulation of three-phase flows". In: *Interfaces and free boundaries* 7.4 (2005), pp. 435–466.

[27] J. Kim. "Phase field computations for ternary fluid flows". In: *Computer Methods in Applied Mechanics and Engineering* 196.45-48 (2007), pp. 4779–4788.

[28] F. Boyer and C. Lapuerta. "Study of a three component Cahn-Hilliard flow model". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 40.4 (2006), pp. 653–687.

[29] S. Karpitschka et al. "Droplets move over viscoelastic substrates by surfing a ridge". In: *Nature Communications* 6 (2015), pp. 1–7. arXiv: `1406.5547`.

[30] S. Karpitschka et al. "Liquid drops attract or repel by the inverted Cheerios effect". In: *Proceedings of the National Academy of Sciences* 113.27 (2016), pp. 7403–7407.

[31] L. Gránásy et al. "Phase field theory of heterogeneous crystal nucleation". In: *Physical review letters* 98.3 (2007), p. 035703.

[32] C. Farhat, M. Lesoinne, and K. Pierson. "A scalable dual-primal domain decomposition method". In: *Num. Lin. Alg. Appl.* 7 (2000), pp. 687–714.

[33] A. Klawonn and O. Rheinbach. "Highly scalable parallel domain decomposition methods with an application to biomechanics". In: *Z. Angew. Math. Mech.* 90.1 (2010), pp. 5–32.

4 Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

Funding is requested for one doctoral researcher (PhD student) according to standard tariff TV-L E13. The position is planned for my very bright student Julian Karwowski, who obtained a Master's degree in Mathematics by implementing a fluid-structure interaction problem.

We are convinced that excellent students should be involved in research early on in their career to gain hands-on experience and to be nudged to pursue a career in academia. Therefore we request additional money for a student assistant to conduct minor implementation tasks and parameter studies. This will be helpful for the PhD student in obtaining comprehensive datasets and additionally strengthen his profile through experience in supervision.

Category	Duration	Working hours (in 40h/week)	EUR/year
doctoral researcher	3 years	75%	48,375 EUR
student assistant	3 years	25%	6,000 EUR

4.1.2 Direct Project Costs

4.1.2.1 Travel Expenses

We request

- 1,500 EUR per year for SPP internal traveling (annual SPP meeting for PI and PhD candidate, annual workshop for PhD candidate)
- 2,500 EUR per year for traveling to one national and one international conference
- 1,500 EUR per year for exchange with our collaboration partner H. van Brummelen, to enable the PhD student to visit the lab in Eindhoven for 2 weeks per year or to invite H. van Brummelen to Dresden
- 0 EUR for long-term PhD student exchange (2-6 weeks) with our main collaborator S. Karpitschka as included in the central funding of the SPP

4.1.2.2 Project-related publication expenses

To disseminate our results in highly ranked open-access journals we apply for publication expenses of 750 EUR per year. Additional funding can be provided by the state of Saxony.

Total amount of Direct Project Costs: 6,250 EUR per year

5 Project requirements

5.1 Employment status information

Sebastian Aland: permanent faculty position as full-time professor at the Faculty of Informatics/Mathematics at HTW Dresden - University of Applied Sciences.

5.2 Composition of the project group

Currently, my group consists of the following people:

Name	Title	Status	Funding	Expertise
Marcel Mokbel	M.Sc.	PhD student	DFG	Marangoni flow and elastic surfaces
Lucas Wittwer	M.Sc. ETH	PhD student	SMWK	Phase-field models for multiphase flow
Dominic Mokbel	M.Sc.	PhD student	TU Dresden	Phase-field modeling of fluid-structure interaction

5.3 Cooperation with other researchers

5.3.1 Researchers with whom you have agreed to cooperate on this project

Researchers within the SPP (see Sec. 2.5 for details)
Dr. Kirsten Harth (Uni Magdeburg), Dr. Stefan Karpitschka (MPI Göttingen), Dr. Florian Kummer (TU Darmstadt), Prof. Dr. Arnold Reusken (RWTH Aachen) , Prof. Dr. Ralf Seemann (Uni Saarbrücken), Prof. Dr. Axel Voigt (TU Dresden), Prof. Dr. Barbara Wagner (TU Berlin)

Researchers outside of the SPP

Prof. John Lowengrub (UC Irvine)	Ternary phase field modeling and asymptotic analysis	WP 2
Prof. Harald van Brummelen (TU Einhoven)	ALE model validation and monolithic ALE solver	WP 1.1, 1.2

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

H. Abels (Uni Regensburg), J. Allard (UC Irvine), F. Chen (Baruch College New York), K. Eckert (TU Dresden), E. Fischer-Friedrich (MPI Dresden), J. Guck (MPI Erlangen), D. Iber (ETH Zürich), J. Lowengrub (UC Irvine), R. Nürnberg (Imperial College London), O. Otto (Uni Greifswald), A. Voigt (TU Dresden)

5.4 Scientific equipment

We have access to the high performance computer TAURUS (40,000 cores) in Dresden, currently at a quota of 240,000 CPU-hours per year, which can be extended, if needed.