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Ensembles of sitting and sliding drops on elastic media - experiment, simulation and theory

Abstract

Droplets on soft elastic substrates are a paradigmatic example of adaptive wetting, where capillarity-induced elastic deformations dramatically affect the wetting properties. Recent work has shown that substrates made from cross-linked polymer networks offer versatile routes to manipulate contact angles of droplets, as well as their spreading, directed motion, condensation and splashing. However, the full richness of these phenomena is only beginning to be explored and at present there is even no fully quantitative understanding of the behaviour of single drops – let alone ensembles of drops. Key challenges lie in the intricate effects of solid surface tension, and how this affects the force balance near the contact line, while dynamics involves viscoelasticity of the substrate and elastocapillary interactions between droplets.

This project aims at developing and utilising experimental setups, detailed direct numerical simulations, effective long-wave models and a Smoluchowski-type statistical description to investigate the behaviour of drops of simple nonvolatile and volatile liquids on flexible substrates. The first part of the project focusses on single drops. We wish to go beyond the current approaches that are almost exclusively based on linear elasticity, and develop detailed simulations that reveal the large-deformation mechanics near the contact line. The goal is a first-principles fully quantitive description of the wetting behaviour of single drops. This will form the basis for the second part of the project, where we will investigate the collective behaviour of ensembles of drops on soft substrates. Experiments on droplet ensembles, driven by external forcing or evaporation-condensation, will be complemented by a multi-scale modelling approach where we resolve the dynamics on different levels of detail. We develop effective long-wave models that are calibrated from the experimental and full simulation results for single drops, which opens the way for simulations of a large number of droplets, and ultimately for statistical modelling of drop ensembles.

The consistent combination of experiment, simulation and theory offers a multi-scale framework that provides qualitative and quantitative insights into the wetting of flexible substrates. It will reveal the interplay of drop and substrate dynamics, and the emergent laws of sliding, stick-slip motion and coalescence of individual drops and their collective ensemble behaviour. At all stages, the project will be pursued in close cooperation between theory (Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, WWU), experiment and simulation (Physics of Fluids, University of Twente, UT) and is embedded into further collaborations within SPP2171.

1 State of the art and preliminary work

1.1 State of the art.

The laws of wetting are well-known for drops on rigid surfaces, but these change dramatically when the substrate is no longer rigid, but soft and deformable. The free energy associated to substrate deformation profoundly changes the wetting equilibrium (i.e. Young's law is no longer valid), while the dynamical behaviour of droplets can be completely dominated by the viscoelastic rheology of the substrate. Given the potential for application in the context of adaptive wetting, this has lead to a major effort in recent years, with the central goal to generalise the laws of wetting to (visco)elastic substrates. This continues to be a great challenge, both theoretically and experimentally, owing to the multi-scale nature of the problem, where macroscopic fluid & solid mechanics are coupled to the molecular-scale physical chemistry of soft interfaces.

Statics and open issues: An important breakthrough for the statics of wetting was the realisation that the surface tension of the solid plays an active role in the force balance at the contact line [1, 2, 3, 4, 5, 6, 7]. Namely, for materials with elastic moduli below $E \sim 1$ MPa, the elastic stresses cannot compete with the highly localised capillary forces at the contact line. Instead, the substrate strongly deforms and takes on the form of a "Neumann-balance", where the surface tensions of the *substrate* balance the force induced by the liquid-vapour surface tension. This scenario has been confirmed by various experimental techniques (Fig. 1, left) [4, 8] and molecular simulations [9, 10], and has allowed for the development of theoretical models based on linear elasticity [5, 6, 7].

Despite the progress, however, the capillarity of soft solids brings along a major complication as compared to liquid interfaces. Namely, in general one expects the surface free energy to depend on the surface-strain, an effect that is known as the Shuttleworth effect [A1][11, 12, 13, 14]. Therefore one needs to distinguish the (scalar) surface energy from the (tensorial) surface tension, neither of which can be treated as a universal material constant [15]. The influence of strain-dependent surface tension was recently explored experimentally by measuring wetting angles on strained substrates [16, 17], but the conclusions were contradictory. On the theoretical side, the Shuttleworth effect is only beginning to be explored for soft amorphous materials [A1, A2], but so far concrete predictions are limited to linear elasticity. It is clear that the critical next step for understanding the wetting of soft surfaces calls for calculations that account for large elastic deformations near the contact line (i.e. beyond linear elasticity) and with a self-consistent inclusion of a strain-dependent surface energy.

Dynamics and open issues: The situation is similar for the dynamics of wetting drops. Pioneering work by Shanahan & Carré [18, 19, 20] already showed that the motion of single drops slows down due to viscoelastic dissipation in the substrate, known as viscoelastic braking, complemented on the theoretical side by rheology-based calculations [21, 22]. The past 5 years, however, have revealed a variety of surprising dynamical phenomena of soft wetting, such as directed motion by gradients of stiffness [23] and gradients of dissipation [24], and stick-slip motion (Fig. 1, middle) [A4][25, 26, 27]. Another remarkable observation, which will play a central role in our project, is the Inverted Cheerios effect shown in the right panel of Fig. 1: liquid drops can attract or repel by the elastic deformation of the substrate [A3]. Some of these phenomena closely resemble the behaviour of biological cells, so even though in the planned project no biophysical systems will studied, the obtained results will be of importance in a biophysical context for the spreading behaviour of cell aggregates [28, 29] and biofilms [30]. Once again, theoretical progress

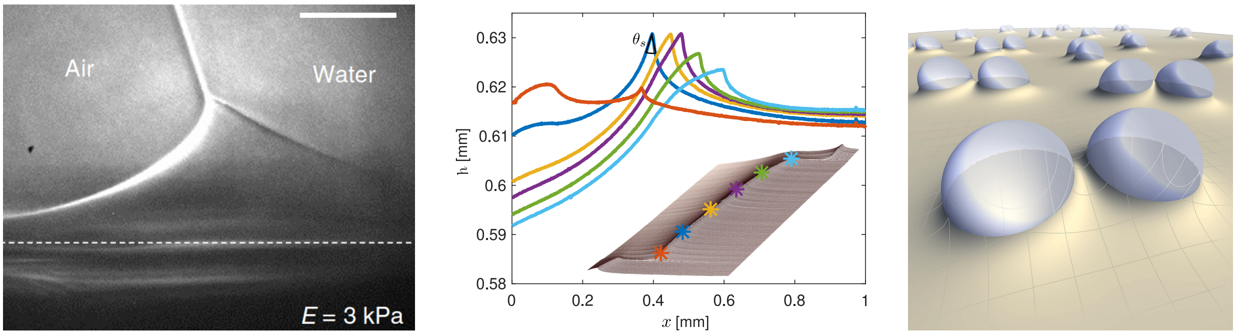


Figure 1: *Static and dynamics wetting on soft surfaces. (left) Xray microscopy image of a static wetting ridge of a water drop on a soft gel (scale bar 5 microns). The three surface tensions equilibrate according to a Neumann balance. Taken from [8]. (middle) Dynamical evolution of the wetting ridge during a stick-slip cycle. The inset shows a space-time diagram (cycle duration* ~ 0.5 *s). Unpublished experimental result (van Gorcum, Andreotti,* ***Snoeijer*** *& Karpitschka, available as arXiv:1807.07740). (right) The inverted Cheerios effect: liquid drops on soft solid substrates may attract or repel each through elastocapillary interactions. Created after [A3].*

for droplet motion was made by introducing solid surface tension, but with the same restrictions of small (visco)elastic deformations and without accounting for strain-dependent surface tension [A4, A3][24]. As a consequence, there is no fully predictive quantitive theoretical model that describes the motion of drops on soft surfaces, and the local dynamics near the contact line remains subject of debate [31, 32].

Collective behaviour: In practical applications such as condensation or printing, one is often interested in the *collective behaviour of large ensembles of drops.* This problem has attracted much interest, but apart from the two-drop interaction shown in Fig. 1 [A3] and a pioneering study on condensation [33], this was restricted to rigid surfaces. There, the interactions between individual drops and the resulting mass transfer processes determine the ensemble behaviour. In general, the long-time merging within such drop ensembles is a particular soft matter example of a coarsening process similar to the Ostwald-ripening of crystalline nanoparticles [34], quantum dots [35] or emulsion droplets [36] where the mean drop/cluster/dot size and their mean distance continuously increase following power laws.

For simple nonvolatile liquids on horizontal rigid substrates coarsening is well studied experimentally [37, 38, 39] and theoretically through simulations and asymptotic considerations based on thin-film equations [40, 41, 42]. Additionally including condensation, the process is also studied employing particle-based statistical models and Smoluchowski-type (cf. [43]) evolution equations for distribution functions of drop sizes [44]. With lateral driving forces, the dynamics of drop ensembles is dramatically different as the sliding speed strongly depends on drop size. The resulting relative motion of differently sized drops makes overall coarsening much faster than on horizontal substrates. However, instabilities may counteract coalescence and at large times the ensemble dynamics may converge to an almost stationary drop size distribution [A5] (see Fig. 2). Examples are drops that slide under an air flow or on an incline and spinodal decomposition under flow [45]. Condensing, coalescing drops with instantaneous sliding avalanches have also been described with particle-based statistical models and Smoluchowski-type equations [46].

As we above mentioned when discussing the Inverted Cheerios effect, the deformations induced by the softness of the substrate provide a new mechanism for interaction between neighbouring drops [A3]. As the drop-drop interactions on soft substrates can be attractive or repulsive, the interaction mechanisms is qualitatively different from any known for hard substrates. This implies that the behaviour of drop ensembles on soft substrates will exhibit unprecedented, intricate new features that remain to be explored. One of the key objectives of our project is to reveal these behaviours experimentally and theoretically.

Relevant thin-film modelling: As the long-time dynamical behaviour of drop ensembles is out of reach for present simulation techniques, a key step will be to derive and employ effective approximative approaches. In the description of wetting and dewetting dynamics one often uses the asymptotic approach of thin-film (or long-wave, or lubrication) models [47, 48]. They are only strictly valid when all interface slopes are small, but nevertheless show often quite good agreement with experiments/simulations at moderate contact angles. Within a gradient dynamics approach, the agreement can sometimes be strongly improved by employing better approximations for the energy functional (e.g., 'full curvature trick') while keeping the mobilities of the asymptotic model (see, e.g., [49] and discussion in [A6]).

Although a wide range of works exist for the dynamics of films and drops of simple liquids on solid or liquid substrates [47, 50, 48, 51][A6], the application of thin-film modelling to elastic and viscoelastic media is much less developed. Works on viscoelastic thin films on solid substrates study linear stability and linear relaxation modes [52, 53], asymptotic decay of dewetting fronts [54], and pattern formation in a soft thin film interacting with a rigid contactor [55]. A thin-film equation for viscoelastic liquids of Jeffreys type (special case of the generalized Maxwell model) is analysed in [56]. Two-layer films that combine viscose and linearly viscoelastic media are considered in [57] with a focus on surface instability and film rupture.

To our knowledge no thin-film studies exist that consider the viscoelastic braking of a sliding drop, the interaction between drops or the stick-slip motion of a receding contact line on elastic or viscoelastic substrates. One central aim of the project is to develop a simple thin-film model that captures these phenomena.

1.2 Preliminary work

The group of Prof. Snoeijer at UT is ideally placed to carry out the proposed research. An extensive line of research on "Soft Wetting" has been setup in the context of Snoeijer's ERC Consolidator Grant (expiring in April 2019). It is within this program that we discovered the attractive/repulsive interactions between two neighbouring drops – the Inverted Cheerios effect [A3] (Fig. 1, right) – that plays a central role for the proposed research on collective behaviour of drop ensembles. A second important work is on how the sliding dynamics is affected by the viscoelastic rheology of the substrate and how this leads to stick-slip motion [A4] . An experimental image of the dynamical depinning during stick-slip was already shown in the middle panel of Fig. 1, where we were able to track the ridge dynamics with unprecedented spatio-temporal resolution (unpublished). Thirdly, we pioneered the theoretical description of wetting in the presence of the Shuttleworth effect [A1], combining macroscopic experiments and theory [A2] with Molecular Dynamics simulations [13]. The group's international position is underlined by an invitation to write a review article on soft wetting, for the 2020 issue of Annual Review of Fluid Mechanics.

From a theoretical perspective, progress in the field was almost exclusively based on linear (visco)elasticity, accurate only for small deformations. The next step towards a fully quantitative description, however, must account for the large deformations in the vicinity of the contact line. To achieve this we initiated a collaboration with Prof. Harald van Brummelen (Eindhoven University of Technology), who recently developed numerical tools for simulating drops on elastic surfaces [58, 59] without the restriction of small deformation (Fig. 4). In this collaboration with Prof. van Brummelen we have performed preliminary FEM simulations where we include the Shuttleworth effect, using both diffuse and sharp interface descriptions for the liquid, providing a proof of principle for the proposed research.

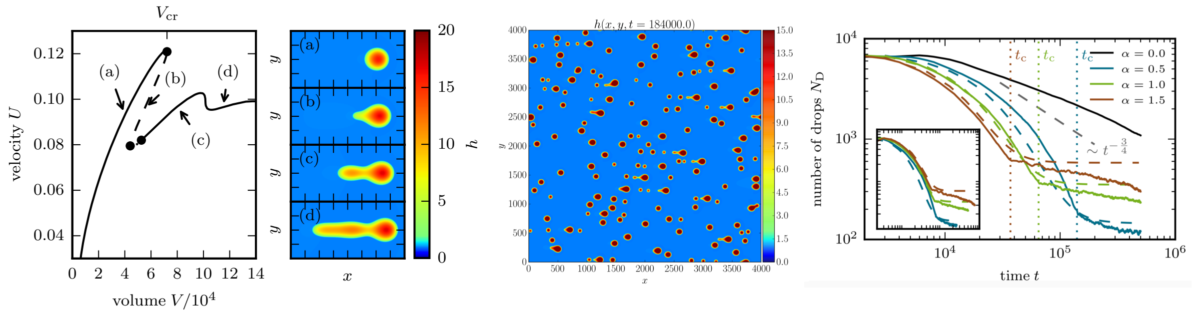


Figure 2: *(left) Bifurcation diagram for individual sliding drops giving velocity over volume at fixed lateral driving force. Stable [unstable] states are indicated by solid [dashed] lines. Selected height profiles at corresponding labels (a) to (d) are given to the right. The centre shows a snapshot from a large-scale direct numerical simulation (DNS), while the plot at the right compares the time evolution of drop size statistics for different inclinations α as obtained from DNS and a Smoluchowski-type statistical model. Reproduced from [A5][60].*

The group of Prof. Thiele's group at WWU provides complementary expertise, necessary for the understanding of collective behaviour for ensembles of drops. An important part of their activities focuses on investigations of self-organised structure and pattern formation in out-of-equilibrium soft matter and fluidic systems employing analytical and numerical methods of theoretical and computational physics and applied mathematics. Recently, the group gained an understanding of the collective dynamics of ensembles of interacting sliding drops of nonvolatile liquid on a smooth rigid substrate employing a novel multiscale approach that connects single-drop bifurcation analysis, large scale direct numerical simulations (DNS) employing a thin-film equation and a Smoluchowski-type statistical model [A5] (Fig. 2). Under lateral forcing, sliding speed strongly depends on drop size. The resulting relative motion of differently sized drops facilitates their coalescence making overall coarsening much faster than on horizontal substrates (cf. curves for $\alpha = 0$ and $\alpha \neq 0$ in Fig. 2 right). However, a pearling instability [61] counteracts coalescence by breaking large drops into smaller ones [60]. In consequence, at large times the ensemble dynamics reflects a balance of drop merging and splitting events and converges to an almost stationary drop size distribution [A5]. Its main features can be related to the bifurcation diagram and stability properties of individual sliding drops [60] obtained by numerical path continuation techniques [62, 63] (Fig. 2 left). Finally, the obtained single-drop information was employed to develop a Smoluchowski-type statistical model for the dynamics of the drop size distribution that well compares to the direct simulations [A5].

In a further preliminary step we have incorporated the deposition of liquid by condensation and heterogeneous wettability into our approach, i.e., we now closely approach realistic experimental settings. In this case, individual drops continuously condense onto the hydrophilic substrate defects and depin at a critical size under the influence of the lateral driving force. After depinning, drops slide, coalesce and split similar to Ref. [A5]. However, DNS shows that now a double-peaked drop-size distribution emerges. Its main features can be related to depinning and pearling thresholds, as obtained from single-drop bifurcation diagrams. We will adapt the developed methodology to thin-film models for drop ensembles on (visco)elastic substrates.

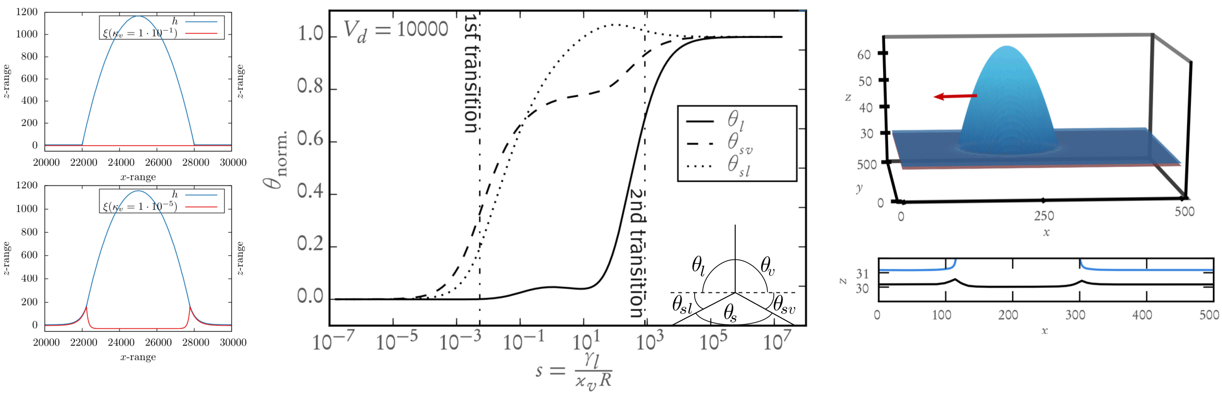


Figure 3: *(left) Profiles of drops sitting on a thin elastic substrate of low (top) and high (bottom) softness. Obtained via path continuation with a simple long-wave model. (centre) Shown are the interfacial angles (as defined in the inset) as a function of substrate softness s. One clearly discerns the two transitions described in the text. (right) Single liquid drop sliding on a viscoelastic substrate obtained via time-simulation of an amended two-layer thin-film model).*

In a second line of preliminary work, the applicants Thiele & Snoeijer have together developed first mesoscopic long-wave models for drops on soft substrates - based on their extended experience with gradient dynamics formulations of two-field models [A6][64], e.g., for two-layer liquid films [50] and surfactant-covered films [A7, A8]. In particular, a model for a drop of viscous liquid sitting on an elastic substrate is based on an energy functional in long-wave approximation that incorporates interfacial energies and higher order terms that account to lowest order for effects of substrate elasticity. Typical drop and substrate profiles are shown in Fig. 3(left) while the centre panel gives the Neumann angles at the contact line as a function of substrate softness s. With increasing s one observes two distinct transitions closely resembling results we obtained with a macroscopic model [5]: First, the cusp-like wetting ring rises ($\theta_{sl} + \theta_{sv}$ strongly increases) while the macroscopic contact angle θ remains nearly constant. Second, at larger softness, the cusp rotates, i.e., $\theta_{sl} + \theta_{sv}$ remains nearly constant while θ strongly increases. The developed simple approximation of the elastic energy has further been incorporated into a two-field gradient dynamics description. Numerical simulations have allowed us to obtain sliding drops on viscoelastic substrates (Fig. 3(right).

We believe that the presented overview well indicates how our project will bring together significant complementary experimental and modelling expertise and converging lines of preliminary work.

1.3 List of project-related publications

[A1] B. Andreotti and J. **Snoeijer**. Soft wetting and the Shuttleworth effect, at the crossroads between thermodynamics and mechanics. *Europhys. Lett.*, 113:66001, 2016.

[A2] J. **Snoeijer**, R. Rolley, and B. Andreotti. Paradox of contact angle selection on stretched soft solids. *Phys. Rev. Lett.*, 121:068003, 2018.

[A3] S. Karpitschka, A. Pandey, L. Lubbers, J. Weijs, L. Botto, S. Das, B. Andreotti, and J. **Snoeijer**. Liquid drops attract or repel by the inverted cheerios effect. *Proc. Natl. Acad. Sci. USA*, 113:7403–7407, 2016.

[A4] S. Karpitschka, S. Das, M. van Gorcum, H. Perrin, B. Andreotti, and J. **Snoeijer**. Droplets move over viscoelastic substrates by surfing a ridge. *Nat. Commun.*, 6:7891, 2015.

[A5] M. Wilczek, W. Tewes, S. Engelnkemper, S. V. Gurevich, and U. **Thiele**. Sliding drops - ensemble statistics from single drop bifurcations. *Phys. Rev. Lett.*, 119:204501, 2017.

[A6] U. **Thiele**. Recent advances in and future challenges for mesoscopic hydrodynamic modelling of complex wetting. *Colloids Surf. A*, 553:487–495, 2018.

[A7] U. **Thiele**, A. Archer, and L. Pismen. Gradient dynamics models for liquid films with soluble surfactant. *Phys. Rev. Fluids*, 1:083903, 2016.

[A8] U. **Thiele**, J. **Snoeijer**, S. Trinschek, and K. John. Equilibrium contact angle and adsorption layer properties with surfactants. *Langmuir*, 35:7210–7221, 2018.

[A9] A. Marchand, S. Das, J. **Snoeijer**, and B. Andreotti. Capillary pressure and contact line force on a soft solid. *Phys. Rev. Lett.*, 108:094301, 2012.

[A10] J. **Snoeijer** and B. Andreotti. Moving contact lines: Scales, regimes, and dynamical transitions. *Annu. Rev. Fluid Mech.*, 45:269–292, 2013.

2 Objectives and work programme

2.1 Anticipated total duration of the project

36 Months.

2.2 Objectives

In this project we will reveal the behaviour of drops and drop ensembles of simple nonvolatile and volatile liquids on flexible (elastic and viscoelastic) substrates. To achieve this we will exploit the complementary expertises available at WWU & UT, and develop and utilise a combination of experimental setups, theoretical descriptions and numerical algorithms. Our objective is to consistently connect experiment and a multi-scale modelling framework, the latter consisting of detailed direct numerical simulations of macroscopic models, mesoscopic thin-film models and Smoluchowski-type statistical descriptions. Overall, this will lead to qualitative and quantitative insights into the intricate interplay of drop and substrate dynamics.

The research is organised along several work packages that will be outlined in detail below. Of core interest are the statics and dynamics of individual drops (WP1, WP2), the modes of interaction between two drops (WP3), and the resulting coarsening behaviour of drop ensembles on substrates without and with external driving (WP4, WP5). These work packages are organised in a way to optimise the interaction between the groups at WWU & UT, aiming at a synthesis between results obtained from the various methods. To ensure the dissemination of the resulting modelling toolbox, within the SPP and beyond, we dedicate a specific task to this purpose (WP 6).

Within the SPP these objectives are complementary to other projects where soft substrates play an important role allowing for a fruitful interaction. Collaborations are planned with projects on spreading drops (Harth), liquid-liquid decomposition on (Karpitschka), wetting rim dynamics for (Vollmer/Schmid), and drop impact on (Harth, Lecrivain) elastic substrates. We envision further interactions with projects involving liquid-infused (Hirtz), viscoelastic (Wagner/Seemann), elastic structured (Brinkmann) and switchable elastic structured (Ionov) substrates.

2.3 Work programme including proposed research methods

Work Package 1. Single static drops: calibration of experiment, simulation and thin-film model.

WP 1.1. Simulations beyond linear elasticity and including the Shuttleworth effect. A variety of experimental studies (performed amongst others at UT) have recently provided detailed information on how the contact angles depend on the stiffness of the substrate, and on the amount of stretching of the substrate. The effect of stretching is of particular interest to investigate the Shuttleworth effect, i.e. the strain-dependence of solid surface tension. Here we will use numerical modelling using FEM (Fig. 4): it allows to systematically account for both the Shuttleworth effect and the large deformation near the contact line (i.e. beyond the usual assumption of linear elasticity). With this we can settle some of the debates in the literature, and aim for a fully quantitative description of experiments. Further experimental data from microscopy will arise within the SPP in the project by Karpitschka, with whom we foresee close collaboration. From the theoretical perspective, we will focus on the limit of shallow angles and provide input for the mesoscopic modelling approach (cf. Fig. 3).

WP 1.2. Mesoscopic thin-film model. Here we employ our static thin-film model based on an energy functional containing interface, wetting and simplified elastic energies to investigate the double transition that occurs when increasing the substrate softness [5]. We further will incorporate the Shuttleworth effect into this description and determine bifurcation diagrams using substrate softness, drop volume and wetting characteristics as control parameters. We expect the transition between drop and flat film state to be of super- or subcritical character, hence, we will clarify under which conditions droplets need to have an overcritical size to be stable.

WP 1.3. Calibration. In an iterative comparative study, parameters of experiment, macroscopic and mesoscopic model are mapped onto each other in a parameter region where all should agree (small and moderate contact angle). Thereby, for the mesoscopic model long-wave and full curvature formulations are employed and compared to different orders of a gradient expansion of the full interface and elastic energies. Consistency conditions for macroscopic and mesoscopic approaches are determined (similar to the approach pursued for surfactant-laden drops in [A8], collaboration planned with K. John, Grenoble). The resulting consistent modelling toolbox shall be shared with other SPP projects.

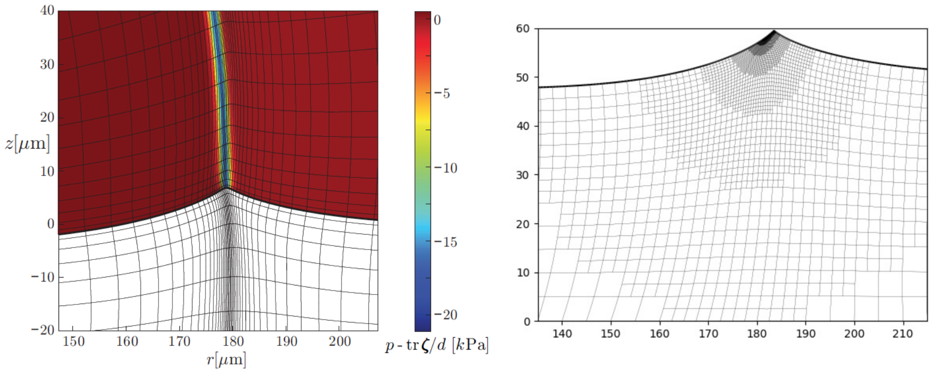


Figure 4: *FEM simulations of drops on an elastic solid, accounting for large deformation elasticity. (left) A liquid drop is modeled as a two-fluid model using a diffuse interface description (Cahn-Hilliard). Color indicates the local pressure. Taken from [58, 59]. (right) Adaptive grid-refinement near the contact line, for a sharp-interface model (preliminary result, proof of principle). These simulations will provide unprecedented insight in the structure of the contact line, including the Shuttleworth effect, large deformations, and viscoelastic dynamics.*

Work Package 2. Individual drop spreading and sliding.

WP 2.1. Development of macroscopic dynamic model. The FEM modelling (Fig. 4) will be adapted to account for dissipation inside the solid. The relaxation dynamics will first be described phenomenologically, adding Kelvin-Voigt-like dissipation, but later more systematically using rheological input obtained from experiment. The simulations will extend the dynamical models that so far have been restricted to small deformations and constant surface tension, revealing the mechanics near the contact line in dynamical situations.

WP 2.2. Development of gradient dynamic mesoscopic model. We will incorporate the energy functionals developed in WP 1.2 into a gradient dynamics for two coupled fields, namely the height profiles of the elastic substrate and liquid film/drop. The corresponding mobilities shall be derived on the one hand on the basis of Onsager's variational principle employing a (visco-)elastic dissipation functional. One the other hand the systematic long-wave and gradient expansion employed in WP 1.3 is adapted to the dynamical case. We will then investigate how existing thin-film equations for the dynamics of a viscoelastic films ([56, 57] and our preliminary work in Fig. 3) relate to limiting cases of the developed models and perform a bifurcation study for individual sliding drop.

WP 2.2.M Incorporation of condensation/evaporation (Master project). The models developed in WPs 1.2 and WP 2.2 are supplemented by nonconserved terms that represent fluxes from and to the ambient vapour to the liquid film/drop. In an independent Master thesis, the resulting model shall be used to investigate modi of single-drop condensation and evaporation dynamics.

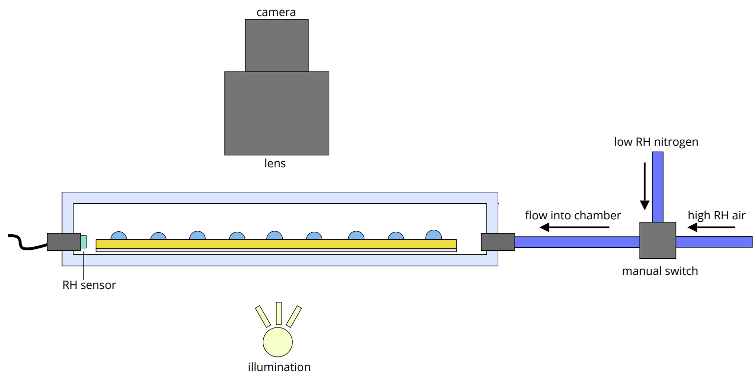
WP 2.3. Experiment and simulation. In an iterative comparative study of spreading and sliding drops, experiment, macroscopic and mesoscopic model are applied and adjusted in the parameter region of small and moderate contact angles. The focus is on the dynamic quantities, the static ones were already adjusted in WP 1.3. In a comparative study we analyse the properties of the asymmetric wetting ridge for a sliding drop and extract relevant power law dependencies (velocity on driving, critical parameter values on parameters) that are needed in WP 5 when developing the statistical model.

Work Package 3. Coarsening modes for two drops

WP 3.1. Bifurcation study with mesoscopic model. The coarsening of a pair of drops can occur via two modes: a mass transfer mode where liquid is transfered via the ambient air or the adsorption layer at the substrate between the drops that themselves remain at rest and a translation mode where the entire drops move towards each other. The relative importance of the two modes depends on drop size, distance etc. For rigid substrates, heterogeneities can stabilise these modes resulting in intricate bifurcation behaviour and state diagrams [65]. We expect that the softness of the here considered elastic substrates takes the role of heterogeneity strength for rigid substrate. We will employ the thin film model of WPs 1.2 and 2.2 to determine the corresponding bifurcation diagrams on horizontal soft substrates with substrate softness, drop volume and wettability as control parameters. Here continuation techniques shall be used for a 1d case and the gradient dynamics model of WP 1.2 will be supplemented by evaporation/condensation fluxes.

WP 3.2. From sitting to sliding drops. The study of WP 3.1 is extended to two dimensional substrates and the additional influence of a small lateral force is considered to investigate via continuation and time stepping how such a driving influences the coarsening behaviour in dependence of substrate softness. We expect that this will allow us to understand the transition between the attractive and repulsive mode of the Inverted Cheerios effect [A3] for sliding drops as a bifurcation that is the nonequilibrium equivalent of the coarsening transition of WP 3.1.

WP 3.3. Experiment. We will provide the experimental counterpart of the modelling on two-drop interactions of WPs 3.1 and 3.2. The experiments on drop-drop interaction in [A3] were limited to nonvolatile drops on an incline. Here we wish to perform the equivalent study on a horizontal substrate, and, importantly, consider volatile liquids. We will work with PDMS substrates of varying stiffness, with which we have ample experience with various liquids (volatile and nonvolatile) [A4, A3, A2]. The experiments including condensation and evaporation will be performed in a chamber of controlled relative humidity, by which we can manipulate the mass transfer. Note that within the SPP, we plan to compare our results to studies of the behaviour of pairs of impacting drops that interact through the elastic substrate (Lecrivain) and drop pairs on switchable elastic substrates (Ionov) and between elastic lamellae (Brinkmann).



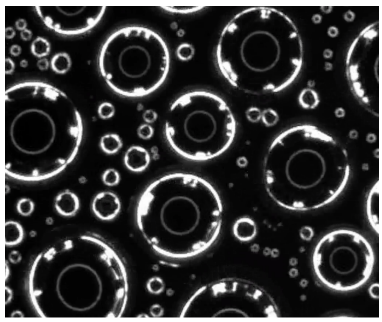


Figure 5: *(left) Schematic of the experimental setup to study droplet ensembles in the presence of condensation. The experiment is performed in a closed environment, with controlled temperature and relative humidity of the air, and controlled temperature of the substrate. (right) Typical condensation pattern taken from [38]. How will the statistical distribution change for soft substrates?*

Work Package 4. Drop ensemble experiments

WP 4.1. Sitting and sliding drops. We experimentally consider the dynamical evolution of large ensemble of drops. Our prime interest will be to gather statistical data from a large number of drops. Similar to [38], we will measure drops with radii ranging from several microns up to 500μm over a large field of view (typically mm). Parameters that can be varied are the substrate stiffness, contact angles, and the inclination to include the gravitational forcing. Besides global statistics, we will also zoom in and assess the (collective) behaviour on the drop-scale, showing to what extend the modes of motion and coarsening studied in WP 3 can be observed in large ensembles. We first focus on experiments with drops of nonvolatile liquids on a horizontal substrate, and then we systematically investigate how the forcing due to gravity alter the results.

WP 4.2. Condensation and evaporation. In a further series of experiments we will look at the effects of condensation and evaporation. We will investigate the same questions as in WP 4.1, but as in WP 3.3 the experiments will be carried out in a closed box of controlled relative humidity (see Fig. 5). Ensembles of growing drops at elastic substrates may also be created by liquid-liquid phase separation (Karpitschka) and between stacks of elastic lamellae (Brinkmann) - comparison to these approaches will allow us to find out if the influence of the elastic substrate on coarsening has universal features across different systems.

Work Package 5. Statistical model for drop ensembles.

WP 5.1. Large-scale time simulation with long-wave model. The thin-film model developed in WP 2.2 is employed in large-scale direct numerical simulations (DNS) of ensembles of sitting and sliding drops on elastic substrates. In this way, benchmark data for the statistical model are extracted, in particular, the necessary time constants, the length scale for the 'laning effect' (expected to be of larger importance than in [A5] because of the inverted Cheerios effect). We plan to investigate the dependencies on overall volume, driving force, substrate softness and wetting properties.

WP 5.2. Development and simulation of statistical model The data extracted from the DNS in WP 5.1 and the bifurcation properties and scaling laws obtained for individual drops in WPs 2.2 and for pairs of drops in 3.2 are employed to derive a coarse-grained macroscopic statistical model of Smoluchowski type that describes the time-evolution of the drop size distribution. The model is simulated at parameters comparable to the DNS in WP 5.1 and experiments in WP 4. Comparison of the three approaches shall allow us to adapt model details and parameters across all levels of modelling. The question is pursued whether it is possible to utilise the statistical properties of ensembles of driven droplets to determine aspects of mesoscale wetting energies, elasticity and dissipation in the elastic substrate.

Work Package 6. Creation of hands-on Tutorials. Hands-on tutorials are created for the mesoscopic models that detail how the numerical results are obtained allowing even bachelor and master students to easily reproduce them. The tutorials are shared with the wider community enabling groups working experimentally or with other model/simulation types to nearly instantaneously master the pursued gradient dynamics modelling approach und to implement their own versions of thin-film models for flexible substrates. For this WP a dedicated Student Research Assistant (wissenschaftliche Hilfskraft) shall be employed (see Sec. 4.1).

Time line of the project. Figure 6 represents the tentative time line of the project and the dependencies between the work packages.

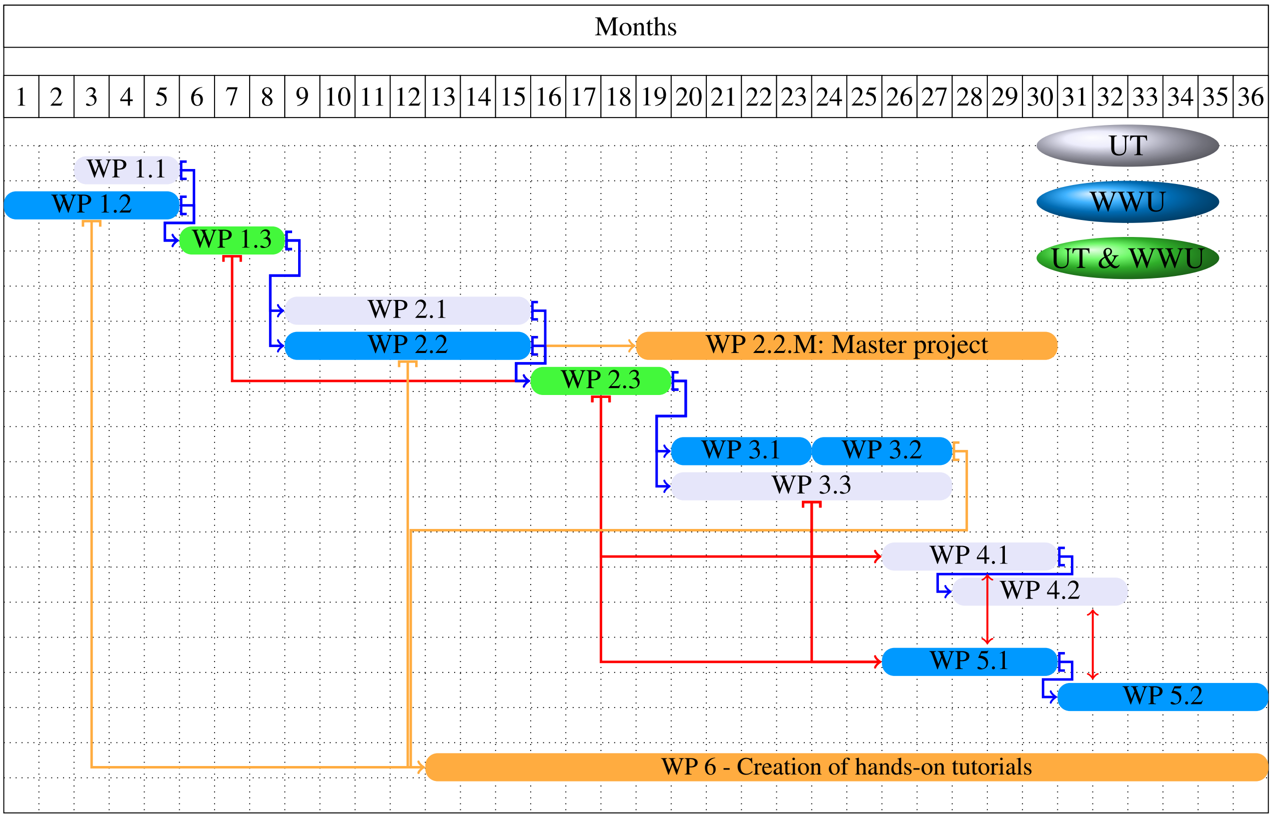


Figure 6: *Time line and main data flow in the project. For clarity we only include main connections between WPs. Exchange between experiment, simulation and theory is continuously ongoing.*

2.4 Data handling

The gained research data will be handled according to the guidelines of UT and WWU. All scientific results will be published in international peer-reviewed journals and be presented at international conferences. Following our past best practice, parallel to journal submission all manuscripts will be uploaded to the preprint server *arXiv* guaranteeing full open access to our results. The data behind all publications and theses related to the project will be archived in a structured way. Furthermore, we plan to bring essential parts of the developed numerical algorithms for the mesoscale models into tutorial form and make them available to the wider international community (see WP 6). Short project descriptions and regularly updated main results will be provided on the web pages of the SPP, WWU and UT.

2.5 Other information

Not applicable.

2.6 Explanations on the proposed investigations

No experiments on humans, human materials and animals are planned.

2.7 Information on scientific and financial involvement of international cooperation partners

Close collaboration with Prof. Harald van Brummelen from TU Eindhoven (TUE, NL) is planned on aspects of WPs 1.1 and 2.1 - centred around his coupled fluid-structure code that takes into account large deformation elasticity. Our project collaborates in the further development of the code towards the incorporation of further elasticity models beyond linear elasticity, of the Shuttleworth effect and (visco)elastic dynamics.

Prof. van Brummelen will closely collaborate in the supervision of the researcher based at UT and is involved in the discussions regarding the matching of macroscopic and mesoscopic approaches. We plan for bi-monthly meetings between the researchers from TUE, UT and WWU. Further, we plan for an exchange of the involved PhD candidate and postdoc, i.e., they shall spend up to 2-4 weeks per year at the partner group.

Further, we will discuss aspects of the mesoscopic modelling and development of numerical algorithms with our present common collaborator, Dr. Karin John (Grenoble). In particular, this relates to WP 1.3. where she will contribute to the derivation of consistency conditions for macroscopic and mesoscopic approaches and, in general, will be involved in the development of gradient expansion techniques for nonlinear elastic media. Visits of Dr. John at UT and WWU are financed through university funds. Further, we will discuss aspects of the project with further international collaborators, e.g., Prof. B. Andreotti (ENS Paris) and Prof. A. Hazel (Manchester).

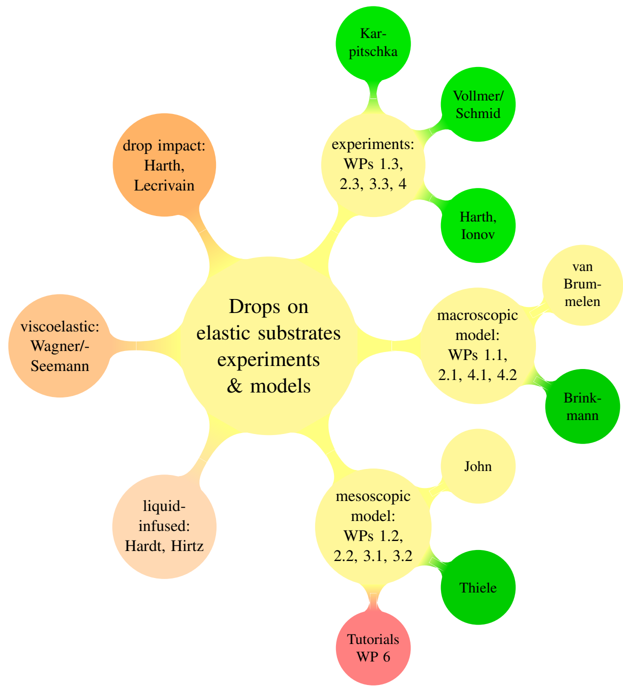


Figure 7: *Scheme that shows how our WPs relate to other SPP projects and external collaborations on (i) experiments, (ii) macroscopic approaches and (iii) mesoscopic models for similar systems.*

The postdoctoral researcher, PhD candidates and master students working on the project will be embedded into the SPP 2171 funded by the DFG. For the PhD candidate at WWU a cotutelle is planned between UT and WWU.

2.8 Information on scientific cooperation within SPP 2171

Beside the international collaboration with van Brummelen and John we envision a number of fruitful interactions with partners working within SPP 2171 on projects that are complementary to ours. This is briefly described in our objectives (see sec. 2.2 and visualised in Fig. 7). This includes connections to (i) experiments (WPs 1.3, 2.3, 3.3 and 4), (ii) macroscopic models for related systems (WP 1.1, 2.1, 4.1, 4.2), and (iii) mesoscopic approaches to similar systems (WPs 1.2, 2.2, 3.1, 3.2).

(i) In particular, results of our experimental WPs on drop behaviour will be shared with projects on drop impact and drop spreading on soft substrates (Harth), on liquid-liquid decomposition and the behaviour of liquid-liquid systems on soft substrates (Karpitschka), on wetting on polymer gels (Vollmer/Schmid), on switchable elastic substrates (Ionov) and drops between elastic lamellae (Brinkmann). They will provide us with complementary characterisations of relevant substrate materials, substrate-liquid couplings and the dynamics of the wetting rim. In turn we provide them with our data and explore adapting our models to their systems.

(ii) Our advances in the macroscopic approach will be shared with and compared to the FEM & phase field model approach to drop impact on soft substrates (Lecrivain), to dissipative particle dynamics results for wetting phenomena on polymer gels (Vollmer/Schmid) and to simulations of the behaviour of droplets between elastic lamella (Brinkmann).

(iii) We plan to match our mesoscopic models and results not only to our own macroscopic results but will also compare them with other projects that pursue mesoscopic models for the (de)wetting dynamics on viscous (liquid-infused) and viscoelastic substrates (Wagner/Seemann). We expect that, in particular, our gradient dynamics modelling approach [A6] will promote a number of extensions that allow for an easy adaptation to related experimental systems, e.g., liquid-infused (Hardt, Hirtz). The development of part of the numerical continuation techniques will be coordinated with a project on mesoscopic models for adaptive substrates (Thiele). The corresponding expanded numerical algorithms will be entered into a pool of tools available to all projects (see WP 6).

Further, to foster the exchange between theoretical groups working with continuum-theoretical approaches within the SPP, we have initiated an informal network, which includes the groups of Brinkmann, Gurevich, Peschka, Snoeijer, Stark, Thiele, Voigt and Wagner and is open to others. There, we will coordinate aspects of the training of the involved young researchers within the SPP, and meet sporadically to discuss details of our approaches and ongoing work.

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4 Requested modules/funds

4.1 Scientific personnel

1. Postdoctoral researcher at UT, who will realise the experimental and full simulation WPs: 30 months of 100% TVL (DFG flat rate E 13 level 3 to E 14 level 2)

Justification The postdoctoral researcher will be responsible for the usage and further development of the full simulation methods, as well as for the adaptation of the existing experimental setups to obtain results for drop ensembles. (S)he will also be responsible for documentation of the experiments and simulations, communication with the collaborators at WWU and Eindhoven, and publication of the results in journals and at international conferences. (S)he will organise the collaboration meetings in Enschede. Because of the large responsibility and broad spectrum of knowledge (direct simulation and experiment), a 100% TVL-13/14 (postdoc) position is necessary. This is equivalent to the usual rate for postdoctoral researchers at UT.[1]

[1]Note, that the postdoc at TU shall start about two months after the PhD candidate at WWU and finish about 4 months earlier. In this way the PhD candidate has additional time to enter the field and to finalise their thesis,

2. Doctoral Candidate at WWU, who will realise the theoretical WPs: 36 months, 75% TVL (DFG flat rate E 13 level 2 to E 14 level 1)

Justification The doctoral candidate will together with the PI at WWU develop the mesoscopic (asymptotic long-wave) models, implement the models into time stepping and path continuation algorithms, validate the numerical method and perform the numerical investigations possibly supported by a Master student (WP 2.2.M). The scientist will organise the exchange with the collaborators at UT and Grenoble and keep close contact with the collaborating theory groups within the SPP. (S)he will organise project collaboration meetings in Münster.

Because of the large field of responsibility and broad spectrum of knowledge including the mathematical modelling of complex fluids, advanced numerical time stepping and path continuation methods and analytic approaches of theoretical physics, a 75% position is necessary for the complete duration of the project.

3. Student Assistant at WWU, who will in month 12-36 create the hands-on tutorials (WP 5). (24 Months, 10hrs/week SHB, monthly 542€ , **in total 13.008€**)

Justification In current publications, results are often presented in a rather compact manner and dissemination of novel techniques etc. to students and young scientists entering into interdisciplinary field has high thresholds. The planned creation of detailed hands-on tutorials shall lower these threshold for entry into gradient dynamics modelling - a field where knowledge from several areas must be quickly acquired. The tutorials shall detail how the numerical results are obtained allowing even bachelor and master students to easily reproduce results. The SPP shall provide a platform for the creation and sharing of these tutorials allowing all groups within the SPP and the wider community (including groups working experimentally or with other model/simulation types) to nearly instantaneously master the gradient dynamics modelling approach und to easily implement their own multi-field thin-film models.

4.2 Scientific devices (requested by UT)

Device	WWU in €	UT in €
Microdrop dispenser to deposit drops in controlled fashion (WP 4.1)		1.400
Materials and workshop costs to build controlled chamber (WP 4.2)		1.000
Sum	**0**	**2.400**

4.3 Consumables (requested by UT)

	WWU in €	UT in €
Chemicals (liquids, gels, surface preparation) needed for experiments developed in WP 3.3 and used in subsequent experimental WPs		6.000
Sum	**0**	**6.000**

respectively.

4.4 Travel costs

Event	WWU in €	UT in €
SPP Advanced School 2019 (20 person days [pd])	1.200	1.200
SPP PhD candidate Workshop 2020 (8 pd)	520	520
SPP Workshop 2019 & 2020 (32 pd)	2.080	2.080
SPP International Conference 2021 (20 pd)	1.200	1.200
Cooperation within project & SPP	5.280	5.280
11th Liquid Matter Conf., Prague 2020 (15 pd)	2.400	1.200
35th Conf. ECIS, Crete 2021 (15 pd)	1.400	2.800
Sum for all three years	**13.980**	**14.180**

Justification

- The doctoral candidates at WWU & UT attend all SPP events, both PIs attend all SPP events except the PhD Workshop [in total 80 person days (a 80€) and 18 return travels (a 200€)]
- Visits of PhD candidates and PIs to collaborating groups (2 visits each year, PIs 2 days each, PhD candidates 4 days each), in total 72 days and 24 times return travel
- The *Liquid Matter Conf.* (tri-annual conference of the Liquid Physics Section of EPS) and *Conf. of European Colloid and Interface Society* (yearly) provide ideal interdisciplinary audiences to present our results to the liquid, soft matter and interface communities. One PI and both doctoral candidates shall respectively attend the two (each 5 days a 100€ , return travel a 200€ /400€ and conference fees of about 500€).

4.5 Publication costs

	WWU in €	UT in €
Publication costs	750 per year	750 per year
Sum	**2.250**	**2.250**

5 Project requirements

5.1 Employment status information

Prof. Snoeijer and Prof. Thiele are both full professors on permanent positions.

5.2 First-time proposal data

n.a.

5.3 Composition of the project group

1. **Prof. Uwe Thiele**, WWU, is responsible for mesoscopic modelling, exchange between experiment, simulation and theory and overall coordination (paid by WWU).

2. **T. Frohoff-Hülsmann**, WWU, PhD candidate, uses 10% of his time to supports the implementation of the numerical path continuation approach and bifurcation analysis (paid by the university).
3. **Prof. Jacco Snoeijer**, UT, is responsible for the experiments and full simulation, exchange between experiment, simulation and theory (paid by UT).

5.4 Cooperation with other researchers

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

International collaboration with Prof. H. van Brummelen (Eindhoven) and Dr. K. John (Grenoble) as laid out in sec. 2.7. Collaboration with partners within the SPP as summarised in Sec. 2.8.

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

U. Thiele: Prof. AJ Archer, Loughborough University (UK); Prof. T Betz, Univ. Münster; Prof. L Chi, Shuzhou Univ. (China); Prof. H Gomez, Univ. A Coruna (Spain); Dr. SV Gurevich, Univ. Münster; Prof. A Hazel, Univ. Manchester; Prof. A Heuer, Univ. Münster; Prof. E Knobloch, Univ. Berkeley (USA); Prof. T-S Lin, National Chiao Tung Univ. Hsinchu (Taiwan); Profs. O Manor & L Pismen, Technion Haifa (Israel); Dr. DN Sibley, Loughborough Univ. (UK); Prof. H Stark, TU Berlin; Dr. D Tseluiko, Loughborough Univ. (UK); Prof. H Uecker Univ. Oldenburg;

J. Snoeijer: Prof. B Andreotti, ENS Paris (France); Prof. P Brunet, Univ. Paris Diderot; Prof. H-J Butt, MPI Mainz; Prof. C Clanet, Polytechnique, Palaiseau (France); Prof. P Colinet, Univ. Libre de Bruxelles (Belgium); Prof. K Daniels, North Carolina State Univ. (USA); Prof. E Dufresne, ETH Zurich (Switzerland); Prof. J Eggers, Univ. Bristol (UK); Prof. H Gardeniers, Univ. Twente (Netherlands); Prof. J Harting, Erlangen-Nürnberg; Dr. S Karpitschka MPIDS Göttingen; Prof. R Lammertink, Univ. Twente; Prof. D Lohse, Univ. Twente; Prof. D van der Meer, Univ. Twente Prof. C-D Ohl, Nanyang Technological Univ. (Singapore); Prof. D Quéré, ESPCI Paris (France); Prof. J Vancso, Univ. Twente; Prof. C Venner, Univ. Twente; Prof. M Versluis, Univ. Twente; Prof. E Villermaux, Univ. Marseille (France); Prof. D Vollmer, MPI Mainz;

5.5 Scientific equipment available for the project

- Local Computing Cluster at ITP, WWU & PoF, UT
- High Performance Computing (Palma 2 at WWU, access to SURFsara Netherlands)
- All necessary licences for the needed software (UT & WWU)

5.6 Project-relevant interests in commercial enterprises

There are no connections between the project and an enterprise.

6 Additional information

This proposal has not been submitted to a third party.