Abstract

The design and development of high aspect ratio (HAR) microstructures for hydrophobic substrates are driven by heuristics and limited to the lithography technique at hand. Theoretical understanding of the dynamic wetting of HAR microstructures is lacking, primarily due to limitations in the resolution of experimental observations in dynamic scenarios. Therefore the role of flexural stiffness and morphology of the HAR microstructures on hydrophobicity and wetting reversibility is not fully understood.

The project aims at optimizing HAR microstructure (also known as micropillar) substrates, using three dimensional particle based meshless simulations. The goals of the optimization are increased hydrophobicity and reduced hysteresis with the pillar density, aspect ratio of pillars and flexural strength of the substrate material as the parameters. Incompressible single component fluid (with a free surface) interacting with deformable, complex shaped solid substrates will be simulated by meshless discretization of the continuum description. The capillary forces will be simulated by superimposing pairwise inter-particle forces on the continuum domain. The simulations will provide quantitative relationships between microstructure mechanical properties and the dynamic contact angles. Further, we aim to propose optimal HAR microstructure designs for different wetting regimes. As part of a priority program this project has the advantage of testing and validating the simulations against fabricated experimental surfaces. Also, the collaborations with experimental research groups would serve as a guide to keep the simulations as realistic as possible. The project aims at three groups of deliverables. The first is a set of validations of two and three dimensional drops on rigid HAR microstructures against theory and experiments. This group of studies would also differentiate between the effect of viscosity and inertia on the apparent contact angle. The second group of deliverables will introduce flexural stiffness as a parameter to identify different wetting regimes. The third group of deliverables will investigate micropillar aggregation during drop motion as well as drop evaporation.

Zusammenfassung

Die Gestaltung und Entwicklung von Mikrostrukturen mit hohem Aspektverhltnis (HAR) fr hydrophobe Substrate wird bislang durch Heuristiken vorangetrieben und durch die vorliegende Lithographietechnik limitiert. Theoretisches Verstndnis fr das dynamische Benetzungsverhalten von HAR-Mikrostrukturen fehlt jedoch. Ein entscheidender Grund dafr ist die begrenzte optische Auflsung bei der experimentellen Beobachtungen von dynamischen Vorgngen. Daher ist der Einfluss von Biegesteifigkeit und Morphologie der HAR-Mikrostrukturen auf die Hydrophobizitt sowie auf die Reversibilitt des Benetzungsvorgangs nicht systematisch verstanden.

Ziel des Projekts ist die Optimierung von HAR-Mikrostruktursubstraten (auch bekannt als Mikrosulen) unter Verwendung von dreidimensionalen gitterfreien Partikelsimulationen. Optimierungsziel ist eine erhhte Hydrophobizitt sowie die Verringerung der Hysterese. Als Designvariablen werden Dichte, Aspektverhltnis und Biegesteifigkeit der Sulen herangezogen. Die Interaktion zwischen der inkompressiblen Flssigkeit (mit einer freien Oberflche) und dem komplex geformten, festen Substrat wird durch eine

gitterfreie Diskretisierung des Kontinuums simuliert. Die Kapillarkrfte werden simuliert, indem das Kontinuum mit paarweise interpartikulren Krften berlagert wird. Mit diesen Simulationen knnen quantitative Beziehungen zwischen den mechanischen Eigenschaften der Mikrostruktur und den dynamischen Kontaktwinkeln hergestellt werden. Darber hinaus beabsichtigen wir optimale HAR-Mikrostrukturdesigns fr verschiedene Benetzungsregime vorzuschlagen. Als Teil eines Schwerpunktprogramms hat dieses Projekt den Vorteil, dass die Simulationen gegen experimentell hergestellte Oberflchen getestet und validiert werden knnen. Darber hinaus untersttzt die Kollaboration mit Experimentatoren bei der Bercksichtigung von Fertigungseinschrnkungen, so dass die, in der Simulation untersuchten Systeme, so realistisch wie mglich gehalten werden knnen.

Das Projekt beinhaltet drei Bearbeitungsschwerpunkte. Der erste Schwerpunkt umfasst eine Reihe von Validierungsfllen, bei denen zwei- und dreidimensionale Tropfen auf starren HAR-Mikrostrukturen mit Theorie und Experiment verglichen werden. In diese Studien wird auch die Auswirkung von Viskositt und Trgheit auf den scheinbaren Kontaktwinkel differenziert betrachtet. Im zweiten Schwerpunkt wird die Biegesteifigkeit als Parameter zur Identifizierung unterschiedlicher Benetzungsregime eingefhrt. Der dritte Schwerpunkt wird zudem die Aggregation der Mikrosulen whrend der Tropfenbewegung sowie die Tropfenverdampfung untersuchen.

Project Description

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Optimization of micropillar carpets for reversible wetting using meshless simulations

1 State of the art and preliminary work

State of the art

a) High aspect ratio (HAR) microstructure

Two decades have passed since the discovery of the self cleaning mechanism of the leaves of a variety of plants [35]. The self cleaning happens essentially due to small area fraction of the substrate coming in contact with the liquid which also results in increased hydrophobicity and reduced resistance to the motion of the droplet, so that the droplet can pick up dust particles easily as it moves. Since then, biomimetic interests and nano fabrication advancements have resulted in innovative superhydrophobic substrates [7], specifically HAR microstructures also called micropillar carpets [18]. Several experiments have shown that the dynamic contact angle and reduced hysteresis are complex functions of the geometry of pillars, the chemical heterogeneity of their surfaces and the mechanical strength of the material [7, 15, 18]. However, all these studies have been heuristic studies based on the lithography technique available at their disposal. There has been no theoretical study to identify optimal combination of topology and material strength of micropillar substrates.

After seven decades since it was introduced, Cassie's [38] expression for the contact angle θ_C of a drop resting at equilibrium on a chemically heterogeneous substrate with species i of area fraction ϕ_i and corresponding contact angle θ_i remains the most general theory:

$$\cos\theta_C = \sigma_i \phi_i \cos\theta_i \tag{1}$$

For a liquid drop in Cassie state (where the roughness features of the substrate are not immersed in the drop) on a rough solid substrate, this equation takes the form [27]:

$$\cos\theta_R = r\phi\cos\theta_Y + \phi - 1 \tag{2}$$

where θ_R is the contact angle with the rough surface, r refers to the degree of roughness of the solid surface and θ_Y is the Young's equilibrium contact angle assuming a smooth plane surface. When droplet dynamics are considered, Eq. 2 fails to predict the difference between the contact angles at the advancing and receding edges of the droplet. This phenomenon, also known as contact angle hysteresis, is the source of resistance to the drop's motion on the surface. For self cleaning and other droplet based microfluidics applications it is desired to have a high contact angle with reduced hysteresis. Modified CB models exist in literature [20, 21, 36] which predict the receding angle, as the receding contact angle has larger room for variation as opposed to the advancing contact angle [9]. Most of these models match their own experimental results often considering only the features of the roughness at a cross section, neglecting the three dimensional distribution of roughness (or gratings) on the substrate. A theory that directly compares to experimental observations is therefore highly sought after [9]. Due to the complexities in describing microstructure morphology, chemical heterogeneity and the dynamics and flow regime of the drop, it seems sensible that different theoretical studies be performed for different regimes categorized by the solid area fraction.

b) High aspect ratio (HAR) microstructure

High aspect ratio (HAR) microstructures represent a subset where the surface area ratio of the liquid–solid contact is very small. Their properties, such as large mechanical compliance, large surface area, and topography that separates the underlying substrate have allowed the design and exploration of biomimetic reversible dry adhesives [25], dynamically tuned superhydrophobic wetting surfaces [30, 32] , mechanical sensors, efficient heat transfer [23] and substrates for cell mechanics [18, 33]. The elasticity and high aspect ratio of the fibers allow deformation under capillary forces. The flexibility of the fibre and its resistance to bending are crucial parameters that contribute to dynamic wetting. Moreover flexible HAR microstructure would enter complex regimes such as self-assembly regimes where the fibers crowd together (a visual analogy would be wet fur of dogs), further affecting the wetting characteristics. Attempts to understand these systems have mostly focused on wetting of rigid fibres [16, 19, 37] or on elasto-capillary effects in planar geometries [28]. Very few studies couple these two aspects in their models. For example, an analytical model was introduced to predict the critical volume of a drop for its spreading on a flexible fibrous substrates [15]. Another study [7] shows a remarkable reduction in hysteresis when the fibres are in a buckled state. Figure 1 shows the variation of the contact angle and the maximum drop volume that remains pinned to the substrate during its tilting as a function of the aspect ratio of the fibers. These graphs suggests that micromechanics behind wetting of flexible HAR fibers is extremely complex with several wetting regimes.

c) Experimental and numerical approaches

Experiments are limited by resolution on the one hand. For example, the measurement of contact angle from a sessile drop much smaller than the capillary length scale ($\sqrt{\gamma/(\rho g)}$, where γ is the surface tension, ρ is the density of the liquid and g is the acceleration due to gravity) is difficult due to the fact that a drop touches the substrate of finite area due to the influence of gravity [24]. On the other hand, fabrication of different microstructures through a large parameter space in terms of fibre number density, flexural modulus and aspect ratio is expensive, time consuming, and in some cases, impossible. However optimal parameter combinations are important to motivate economically viable fabrications.

Numerical simulations could be extremely important to simulate wetting phenomena at the microscale to understand the interplay of flow regime, capillarity and the flexibil-

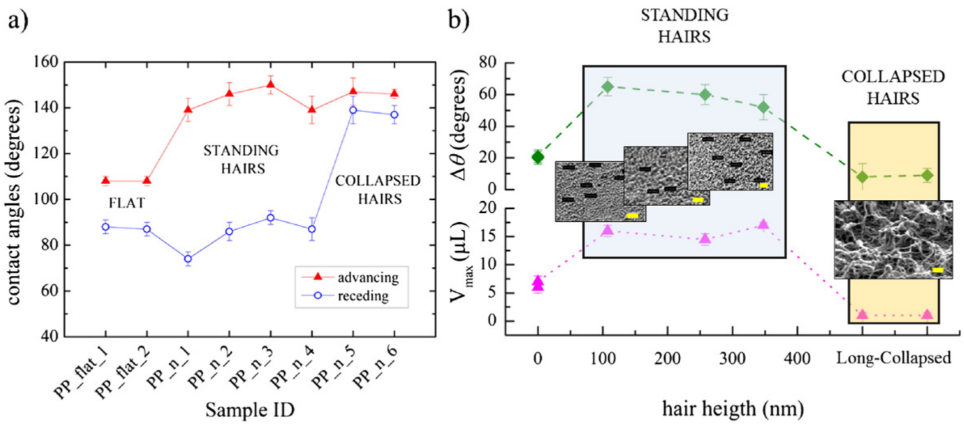


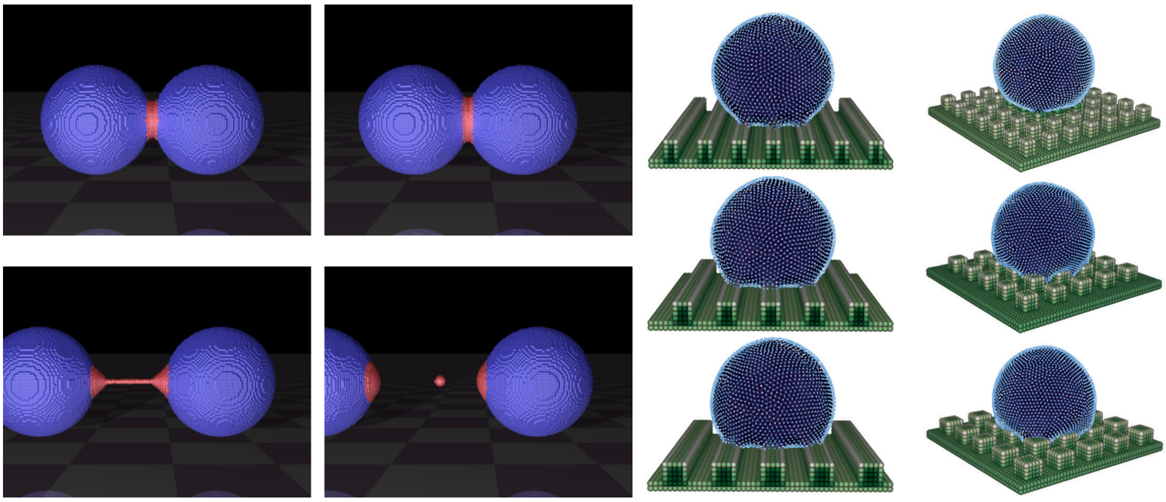
Figure 1: Variation of wetting parameters with aspect ratio (AR) of pillars in a micropillar substrate of two different materials, polypropylene and h-PDMS studied by [7]. Plot on the left shows increased hydrophobicity and reduced hysteresis as the AR increases. Even better hydrophobicity is observed when the pillars collapse due to buckling. The image on the right shows the decrease of hysteresis and the decrease in the minimum volume of the droplet required for it to roll during tilting [7].

ity of the microstructure. However, traditional computational fluid dynamics (CFD) tools such as the finite volume method (FVM) and finite difference method (FDM) suffer from severe difficulties to simulate such systems. The two major class of methods for simulating multiphase flows with capillary forces, namely, sharp interface [34] and diffuse interface [5] methods have their set of difficulties each. The former requires the contact angle to be an input parameter [22]. This does not distinguish between apparent and actual contact angles and uses ad hoc fixes to rectify the singularity that arises due to the non-slip wall boundary condition at the three phase contact line (TCL). Moreover simulating high density ratio similar to that of air-water systems require additional treatments [17]. The diffused interface methods which typically solves an equation for chemical potential (for example, the Cahn-Hilliard equation) [29] can handle heterogeneity of the substrates. But these methods are limited by the low density ratios that are achievable.

d) Smoothed particle hydrodynamics

Meshless methods such as smoothed particle hydrodynamics (SPH) method have the advantage of implicit mass conservation and interface tracking as a separate equation does not need to be solved for the position of the interface [31]. Though SPH is a discretization of continuum equations, it can be easily shown that the same equations of SPH can be obtained by a coarse-graining process from the molecular system. Hence SPH allows for seamless coupling between a coarse grained model and a continuum model. In fact, smoothed dissipative particle dynamics (SDPD) is one such method which is used for multiscale simulations [13].

The molecular interactions between particles can also be introduced in SPH in the context of capillary forces [6], owing to the molecular origin of surface tension [12]. In a recent publication we have shown how such molecular-like pairwise forces could be used in a way that does not interfere with the continuum viscosity formulation [2].



(a) (b)

Figure 2: Simulation of capillary phenomena using smoothed particle hydrodynamics (SPH). The image on the right taken from [4] shows the different apparent contact angles observed for different kinds of rectangular gratings on the substrate. Image on the left is result of our simulations showing formation and rupture of liquid bridge between two solid spheres that collide and depart [2].

This work presents several dynamic capillary phenomena where liquid interacts with complex shaped rigid bodies, where the contact angle manifests due to the balance of inter-particle forces between the different phases. In a recent study [4], the motion and pinning of droplets on inclined micrograted surfaces was extensively studied. This study does not involve explicitly imposed contact angles and the desired contact angle is achieved through energy balance at the phase interfaces. Figure 2 shows our SPH simulation of dynamic capillary phenomena and those of [4] for the wetting of micrograted surfaces using SPH.

In addition to the capillary forces, SPH has several other advantages. A single fluid formulation can be achieved where a one of the (lighter) phase's dynamics can be neglected and such free surface simulation [8] can be argued to be closer to air-water systems than simulations with low density ratios. An incompressible version of SPH which ensures strict incompressibility [7] yields accurate results comparable with mesh based approaches [26]. Complex shaped boundaries can be easily handled with SPH [14]. Interfacing fluids with different compressibility treatments is successfully demonstrated using SPH [4]. Other physical phenomena involving phase change and heat transfer such as evaporation and condensation can also be simulated using SPH accurately, thanks to the Lagrangian nature of the method [3].

2 Preliminary work

For the proposed project we plan to employ an SPH code that has been in continuous development since 2012 [2], by the applicant of this proposal. The applicant is a post

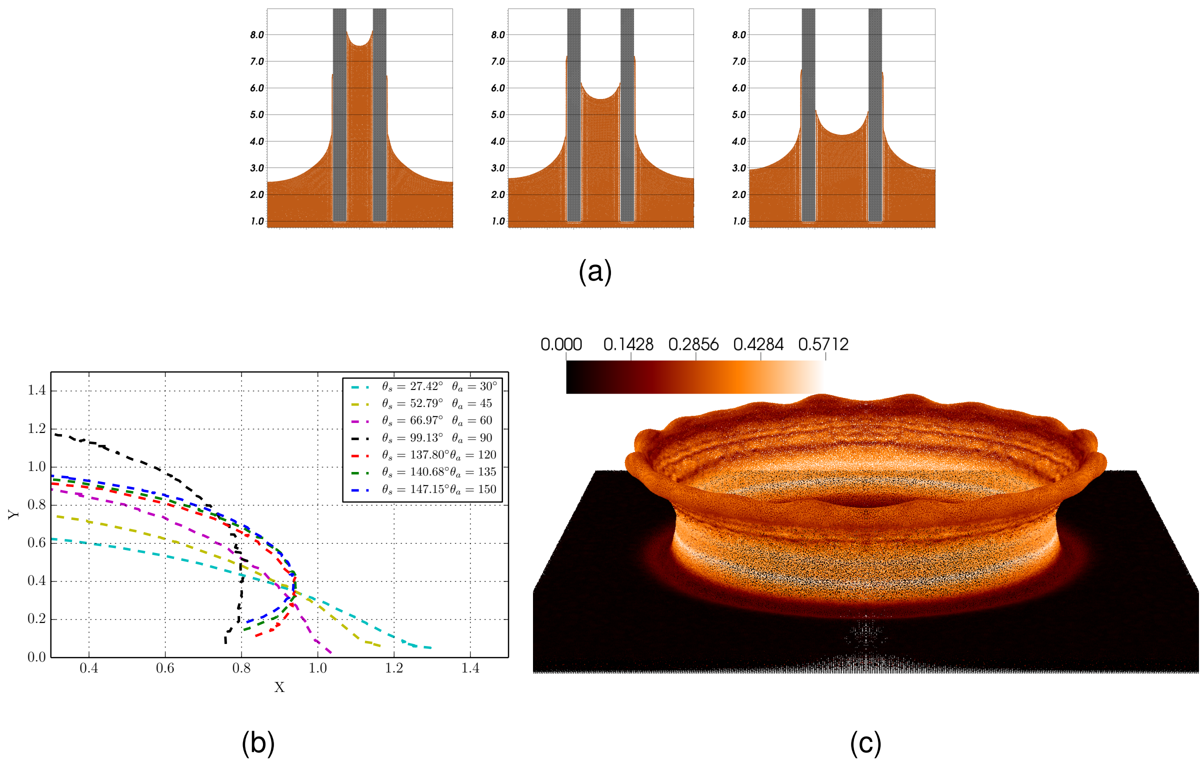


Figure 3: SPH simulations using the pairwise force model for dynamic capillarity: (a) Simulation of 2D capillary rise for different pore diameters (b) Simulated contact interface with different apparent contact angles. (c) 3D simulation of splash crown following impact of drop on a film of liquid, the simulation captures the crown's radial spread accurately and the splash wavelength realistically [2].

doctoral fellow at the Institute for Multiscale Simulation, Friedrich-Alexander University of Erlangen-Nürnberg since 2016. The expertise of the institute in particle based methods and multiscale modelling has been now incorporated into the SPH method [2]. The improved code was successfully applied to a variety of problems, including notoriously difficult systems such as additive manufacturing applications [1].

The SPH program uses a variant of SPH namely incompressible SPH (ISPH) which solves for the condition of isochoricity for incompressibility [7] and can accurately simulate free surface flows [8]. The program has been applied to study fluid-solid interaction problems encountered in water entry of solids of different shapes and density [5] in two and three dimensions. Recently we introduced a dynamic capillary model based on the molecular theory of surface tension to simulate wetting scenarios where capillary, inertial and viscous forces are of comparable time scales [2]. The algorithm was also applied to study liquid bridge formation and rupture [6].

As a preparation for this proposal, we have implemented the following features in this multiphysics SPH program with extensive validation:

– Surface tension using a pairwise force model that recovers the macroscopic surface tension coefficient and contact angle [2].

– Conduction heat transfer across a free surface.

– Phase change using a model that modifies the specific heat near the interface.

– Initial complex geometry input through a triangulated surface geometry file (for example, the STL format).

– High viscosity simulations using an implicit velocity solver, which makes the time step independent of the coefficient of viscosity.

– An improved free surface algorithm that semi-analytically applies Dirichlet boundary conditions at free surfaces and two phase interfaces where only one phase is solved for, enabling the breakup of domain and other intertial interfacial phenomena to be simulated more accurately and robustly [8]. This also allows for pressure gradients tangential to the free surface close to the free surface in contrast to other SPH codes available for academic use.

– Non-uniform interfacial tension by separate Marangoni force model.

– A volume conserving pressure equation is used, which ensures incompressibility is better satisfied, without compromising on efficiency [7, 9].

– The code can also handle rigid and primitively defined bodies [5] with 6 degrees of freedom.

– Species concentration equation and reaction diffusion equation can be added to the set of governing equations without major modifications.

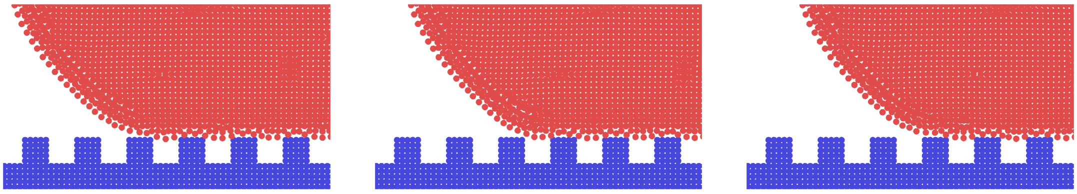
We have performed a number of validation cases to ensure the accuracy of the current code.

Figure 3 shows different simulation results from the implementation of a pairwise force model for surface tension for various interfacial flow phenomena. In Fig. 3a, the capillary rise is validated against theoretical results. The three phase contact angle, which is a macroscopic parameter is recovered with good accuracy from the pair-wise force model (see Fig. 3b). Contact angles are also relevant for the modeling of thin films as the approaching bubbles maintain a certain contact angle depending on the interaction between the air-liquid interfaces. A shared memory parallel simulation of a splash caused by the impact of a droplet on a thin liquid film is shown in Fig. 3c. This recent result shows accurate prediction of the instability that leads to a "crown" formation following the splash. The number of waves on the crown corresponds to experimental observations for the same film Weber number. The use of particle method also enables study of material migration and locally unsteady phenomena.

The liquid phase is modelled here using a one-fluid formulation, neglecting the presence of air and is governed by the incompressible Navier–Stokes equation given by:

$$\frac{d\vec{u}}{dt} = -\frac{1}{\rho}\nabla P + \nabla \cdot \left(\frac{\mu}{\rho}\nabla \vec{u}\right) + \vec{f}^{\text{int}} + \vec{f}^{\text{B}}. \tag{3}$$

Here P is the pressure, μ is the coefficient of viscosity, $\vec{f}^{\text{int}}$ is the interfacial force acting at the free surface and at the liquid–solid interface and $\vec{f}^{\text{B}}$ is the body force per unit mass acting on the system. The hydrodynamic pressure is $P = p + \tilde{p}$, where $\tilde{p}$ is a background or ambient constant pressure which does not contribute to the pressure gradient force due to incompressibility of the medium. The pressure p is not coupled



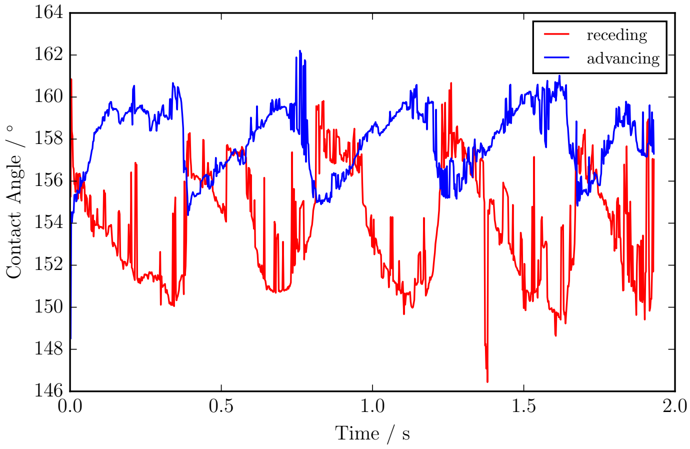


Figure 4: Simulation showing the stick shift behavior of apparent contact angles as a drop moves over a grated surface. The top row shows the instance of receding edge sliding from first to the second image and the jump from one grating to the other in the third image when the receding contact angle undergoes a sharp change. Bottom plot shows the variation of the contact angles over time.

to the density and serves to ensure an incompressibility constraint such as a zero divergence velocity field

$$\nabla \cdot \mathbf{u} = 0, \tag{4}$$

or equivalently, an isochoric deformation given by a unit determinant of deformation gradient tensor $\vec{F}$ [7]

$$\det(\vec{F}) = 1. \tag{5}$$

The free surface of the fluid and its intersection with a solid surface (called the contact line) are subject to capillary forces modelled as inter-particle forces.

Figure 4 shows the simulation of a 2D drop sliding over a micro grated surface. A bubble of about 1 mm width sliding over microgratings of width 100 micrometers is shown. The microgratings modify the average contact angle measurable using an experimental technique. Whereas the simulation shows the instantaneous configuration of the drop. In Fig. 4, we see that as the drop slides through a flat part of the grating, the apparent contact angle remains the same. However, as the drop moves further, the receding edge jumps from one grating to the other causing an abrupt change in its apparent contact angle. This stick-shift motion is shown in graph at the bottom of this figure. Simulations thus reveal the micromechanics with a greater resolution than experiments. A particle simulation like ours is free from heuristic input paramters and therefore captures the dynamics in way that resembles nature.

2.1 List of project-related publications

2.1.1 Articles which at the time of proposal submission have been published or officially accepted by publication outlets with scientific quality assurance, listed in standard format; and book publications

[1] M. Blank, P. Nair, and T. Pöschel. "Capillary viscous flow and melting dynamics: Coupled simulations for additive manufacturing applications". In: *International Journal of Heat and Mass Transfer* (2018), Accepted.

[2] P. Nair and T. Pöschel. "Dynamic capillary phenomena using Incompressible SPH". In: *Chemical Engineering Science* 176 (2018), pp. 192–204.

[3] N. Agrawal, P. Nair, T. Pöschel, and S. Roy. "Isotropy of sphere packings in a cylindrical confinement". In: *Chemical Engineering Journal* (2018).

[4] P. Nair and G. Tomar. "Simulations of gas-liquid compressible-incompressible systems using SPH". In: *Computers & Fluids* 179 (2018), pp. 301–308.

[5] P. Nair and G. Tomar. "A study of energy transfer during water entry of solids using incompressible SPH simulations". In: *Sādhanā* 42.4 (2017), pp. 517–531.

[6] P. Nair and T. Pöschel. "Structural changes in wet granular matter due to drainage". In: *EPJ Web of Conferences*. Vol. 140. EDP Sciences. 2017, p. 09005.

[7] P. Nair and G. Tomar. "Volume conservation issues in incompressible smoothed particle hydrodynamics". In: *J Comp. Phys.* 297 (2015), pp. 689–699.

[8] P. Nair and G. Tomar. "An improved free surface modeling for incompressible SPH". In: *Comput. & Fluids* 102 (2014), pp. 304–314.

2.1.2 Other publications

[1] M. U. Blank. "Dynamics of melting solids using SPH". Masters thesis. Friedrich-Alexander Universität Erlangen-Nürnberg, 2017.

[2] P. Nair. "Modeling Free Surface Flows and Fluid Structure Interactions using Smoothed Particle Hydrodynamics". PhD thesis. Bangalore: Department of Mechanical Engineering, Indian Institute of Science, 2015.

2.1.3 Patents

– not applicable

3 Objectives and deliverables

3.1 Anticipated total duration of the project

- 3 + 3 years. This proposal is for the first phase—3 years.

3.2 Objectives

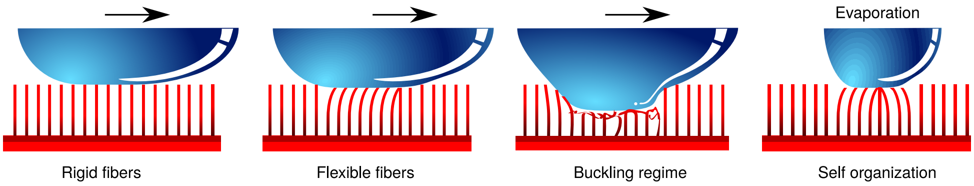


Figure 5: Schematic showing the different flow and fiber deformation regimes considered in this project. The arrow shows the direction of motion of the drop resulting in contact angle hysteresis.

The project aims at optimizing HAR microstructures (also known as micropillar substrates), in terms of pillar density, aspect ratio and bending strength, for increased hydrophobicity and reduced hysteresis, using three dimensional particle based meshless simulations.

Incompressible single component fluid (with a free surface) interacting with deformable, complex shaped solid substrates will be simulated by meshless discretization of the continuum description. The HAR microstructures will be modelled as a chain of particles, similar to the ropes modelled in ship mooring simulations in [8] with bending resistance as a mechanical parameter. The interface forces, both surface tension and wetting, will manifest as a result of inter particle forces between the particles representing the liquid as well as between particles representing the liquid and the solid. The usage of a single line of particles to model HAR would allow us to simulate a large number of pillars in 3D.

The simulations are aimed at providing quantitative relationships between microstructure mechanical properties and the dynamic contact angles. Further, we aim to propose optimal HAR microstructure designs for different wetting regimes. As part of a priority program this project has the advantage of testing and validating the simulations against fabricated experimental surfaces. Also, experimental projects in this direction would help us to reduce the parameter space to investigate.

In Fig. 5 we show the different droplet wetting regimes we expect for different assumed situations. We start with the study of wetting of rigid micropillar arrays, introduce bending of the pillars, consider the cases where the pillars are in a buckled state. Finally we focus on the aggregation and self organization of the pillars due to evaporation or translation of the droplet as is evidenced through experiments in literature. We organize the research plan for the first 3 years into work packages with their respective sets of deliverables.

3.3 Work programme including proposed research methods

Our plan for relating micropillar geometry and strength properties to dynamic wetting regimes can be broadly divided into three subsequent work packages and is described below.

a) Work package # 1 (WP1)
Rigid micropillar array
Duration: 0.5 years

Based on the confidence we have from our proof of concept simulations described in Sec. 2 and shown in Fig. 4, we readily propose to simulate motion of droplets of length scale below the capillary length scale given by

$$L_c = \sqrt{\gamma/(\rho g)}, \tag{6}$$

where γ, ρ and g are, respectively, the surface tension coefficient, density of liquid and acceleration due to gravity. For different aspect ratio and consequently different solid area fraction of wetting, we check for the equilibrium contact angle and the apparent advancing and receding contact angles. The drop's Reynolds number will be set to low values. Due to evidence in literature that the receding contact angle has a dependence on inertia in the system [11], we plan to not assume a strict Stoke's regime. Also, we have observed stick-shift motion of the drops with complex detachment and attachment dynamics of the receding contact line. In two dimensions a simulation typically takes one to two days, due to time step restrictions that arise from the capillary time scale, even though the velocity of the drop may be low. In 6 months we plan to complete a parameter study in two dimensions and also perform 3D simulations based on interesting regimes observed in 2D.

b) Work package # 2 (WP2)
Flexible micropillar array
Duration: 1.5 years

During the second work package we plan to extend the understanding we have on the wetting of micropillar arrays when rigid pillars were assumed. The pillars, modelled as a chain of particles which interact with the fluid through potential forces will be given a bending resistance. The chain forming each pillar preserves its length during the deformation. However, its curvature will be computed and resistance to the bending will be assigned according to elastic property of the material simulated.

We plan to replicate micropillars that are practically feasible to prepare. For example, we start with the strength properties of epoxy micropillars as used in [18]. The flexural modulus of epoxy resins is in the range of 10 GPa. We plan to use this value as a reference value and move down to the flexural modulus of hydrogels ($\approx$ 100 kPa) [10]. The use of hydrogels is motivated by the application to tissue engineering. Hydogels have the advantage of biocompatibility, softness and porous nature [18]. Other materials commonly used for fabricating micropillars are hard polydimethylsiloxane (h-PDMS) (1 MPa) and polypropylene (PP) (150 MPa) [7]. These four materials vis epoxy, PP, h-PDMS and hydrogels, thus span a large range of flexural modulus. Interestingly it is known that the water holding property of h-PDMS is 20% larger than that of PP, suggesting that softer materials may exhibit greater pinning. However at high aspect ratio both materials displayed higher hydrophobicity. In buckled state, the PP pillars displayed lower hysteresis.

The large range of bending resistance we plan to consider, 100 kPa to 10 GPa, can be possible to simulate due to our simplification of the pillars to a single line of particles, with appropriate flexural modulus. How the time step restriction will affect the feasibility of our simulations needs to be found out. However, we are confident that a large range can be considered representing a variety of materials that are being used for micropillar fabrication today.

At the end of this WP, we plan to deliver the variation of wetting parameters across microstructure topology and material properties. We hope to identify optimal spots in the parameter space in terms of liquid hold up, reversibility and self cleaning properties.

c) Work package # 3 (WP3)
Effect of drop dynamics on aggregation of micopillars
Duration: 1 years
It is known that flexible micropillars aggregate due to capillary and other electrostatic forces. In this work package we plan to study the effect of drop deformation, either due to its flow dynamics, drop coalescence or due to evaporation of the drop. This is important for reusability of a surface that undergoes wetting. In this work package we plan to model evaporation of drop. SPH being a Lagrangian method makes it easy to model evaporation, as this amounts to losing particles at a desired rate. Marangoni convection may become important in this step. Our code is capable of simulating currents due to temperature gradients and this has been validated against analytical results. An evaporation sessile drop on a micopillar array of flexible pillars will be simulated to observe the feature width of aggregated pillars. Specifically we would like to observe how the droplet splits due to the various instabilities that may be inherent in the system and how each of these sub-droplets contribute to the self organization of the micro pillars.

We also plant to introduce other dynamic scenarios. Two 3D drops will be placed on a micropillar array to check for the underlying aggregation of pillars and how it affects the coalescence and possibility the jumping of these coalesced drops due to hydrophobicity [6].

A self cleaning scenario can be modeled using debris particles that lie between the hairs with a some static charge. The removal of these droplets during the rolling of a droplet can also be studied. Lastly we would like to study the aggregation and self assembly of hairs that are in the trail of a drop moving over the micropillar array. All these simulations will be performed on computers at the Friedrich-Alexander University of Erlangen, where we have simultaneous access to up to 500 compute nodes at a time.

Possible plan for extension to second phase

If granted, and provided the first phase of the project goes according to plan, the second phase of the project will focus on the effect of switching and tuning of the microstructure to control motion of droplets .

Year	1				2				3			
Quarter	1	2	3	4	1	2	3	4	1	2	3	4
WP1: Rigid pillars												
WP2: Flexible pillars												
WP3: Drop dynamics and pillar aggregation												

Table 0.1: The timeline planned for different work packages in the project

3.4 Data handling

The primary way to disseminate the results of our research will be through scientific publications in refereed journals. The computer code(s) we use for the simulations are currently version controlled through the version control software, GIT. This makes it easy for publishing the code as an open source project through websites such as github or bitbucket.

3.5 Other information

– not applicable

3.6 Explanations on the proposed investigations

3.6.1 Experiments involving humans or human materials

– not applicable

3.6.2 Animal experiments

– not applicable

3.7 Involvement of international cooperation partners

– not applicable

4 Bibliography

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5 Requested modules/funds

5.1 Basic Module

5.1.1 Funding for staff

With this proposal, the applicant requests funding for his own position (Temporary Position for Principal Investigator). Given on his experiences in the field of research obtained during his PhD research at the Indian Institute of Science in Bangalore and during his postdoctoral studies at the Institute for Multiscale Simulation at the University Erlangen-Nuremberg, the applicant is well prepared for performing the proposed research project.

The postdoctoral researcher, shall be supported by a student helper (WiHi with bachelor degree). The student helper will support the researcher with performing routine simulations, analyze the simulation results and care for Data Handling (see. 2.4).

Therefore, we request the following funding for staff:

Temporary Position for Principal Investigator

– Dr. Prapanch Nair (TV-L E13 Stufe 2 bis E14 Stufe 1), 100%
– duration: 36 months
– requested funds: 36 months $\times$ 5 825 € (per month) = 209 700 €

5.1.1.1 Student helper (WiHi)

– N.N. 80 hours/month : €2262.5 per month)

– duration: 36 months

– requested funds: 36 months $\times$ €2262.5 (per month) $=$ €81450

Total requested funding for staff: €291150

5.1.2 Direct project costs

5.1.2.1 Equipment up to €$10,000$, software and consumables

1.	data storage (hard discs), $1\,000$ € p.a.	$3\,000$€
	Total	$3\,000$€

5.1.2.2 Travel Expenses

1.	2 conferences oversees, each one 1200 € transport, 500 € hotel, 600 € conference fee	4600€
2.	2 conferences in Germany and Europe, each one 700 € transport and hotel, 300 € conference fee	2000€
	Total	6600€

5.1.2.3 Visiting Researchers

– not applicable

5.1.2.4 Expenses for Laboratory Animals

– not applicable

5.1.2.5 Other costs

– not applicable

5.1.2.6 Project-related publication expenses

– 750€ p.a. = 2250€ for 3 years

5.1.2.7 Instrumentation

– not applicable

Total requested funding for direct project costs: €$12,350$

6 Project requirement

6.1 Employment status information

The applicant, Dr. Prapanch Nair, is currently employed as a postdoctoral fellow at the Institute for Multiscale Simulation at the Friedrich Alexander Universit"at Erlangen-Nuremberg, Department for Biological and Chemical Engineering (CBI). The current contract ends October 31, 2019.

6.2 First time proposal data

– not applicable

6.3 Composition of the project group

The proposed research will be performed at the Institute for Multiscale Simulation. With the following colleagues from this institute exist collaborations or concrete plans for collaboration in relation with the current proposal:

– Prof. Dr. T. Pöschel (head of the institute)

– Prof. Dr. M. Engel (particle simulation)

– Dr. P. Müller - permanent staff member (particle-fluid coupling)

– Dr. Daniel Nasato - DFG-SFB-funded (DEM simulation)

– Dr. Christopher Robert Windows-Yule - non-permanent staff member (Statistical mechanics of particle systems)

– Dr. Mubashir Hussain - non-permanent staff member (particle based fluid simulations)

– Dipl.-Ing. Sebastian Mühlbauer - DFG-funded (chemical reaction kinetics)

6.4 Cooperation with other researchers

6.4.1 Researcher with existing cooperation agreement for the present project

For the priority programme SPP 2171, we plan to collaborate with other projects in the program that fall under the following categories:

– Experimental research focused on measurement of contact angles on substrates made of soft/elastic material microstructure.

– Experimental research focused on dynamic measurement of receding contact angles, as we intend to simulate and measure the same.

– Simulations that model drop motion at the macro scale which could couple our micro scale findings for larger simulations.

– Experimental research that characterizes substrate topology.

Apart from the researchers from the Institute for Multiscale Simulations and other groups participating in SPP 2171, there is ongoing collaboration with

– Prof. Dr. J. Harting, FAU Erlangen, Institute for Complex Fluids and Interfaces
– Prof. Dr. U. Rüde, FAU Erlangen, Institute for Computer Science

6.4.2 Researcher with whom collaboration was done in the past three years (only fields related to the current research project)

Prof. N. Brilliantov (Univ. Leicester); Prof. A. Formella (Univ. Vigo); Prof. J. Harting (Univ. Erlangen); Prof. J. Gallas (Univ. Joao Pessoa); Dr. P. Nair (Univ. Erlangen); Prof. S. Roy (IIT Delhi, India); Prof. G. Tomar (IISc Bangalore, India).

6.5 Scientific equipment

The Institute for Multiscale Simulation has a medium size Linux cluster with about 800 cores which can be used for simulations. Larger simulations shall be performed at the computer center of the university (RRZE-Regionales Rechenzentrum Nürnberg) where the institute has a contingent of computer time.

6.6 Project-relevant cooperation in commercial enterprises

– not applicable

6.7 Project-relevant participation in commercial enterprises

– not applicable

7 Additional information

– No funding request for this project has been previously submitted to any third party. In case such a request is submitted, the German Research Foundation will be immediately informed.
– The DFG Liaison Officer has been informed of this application