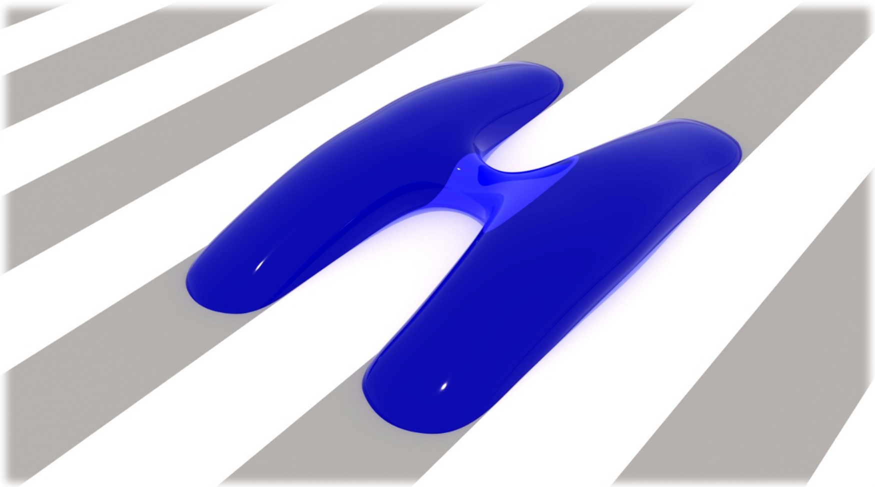
Wetting of Structured Surfaces: Modeling and Simulation

Mathis Fricke, Department of Mathematics,
Technical University of Darmstadt, Germany



Conference on Functional Materials Engineering,
Hasselt, October **2024**

UHASSELT

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Mathematical Modeling and Analysis

CRC 1194

- Please feel free to **take pictures** of the slides!
- Publications with more details are referenced with **QR codes.**
- The slides are available on my webpage: www.mathis-fricke.de/presentations

Thanks to my collaborators ..

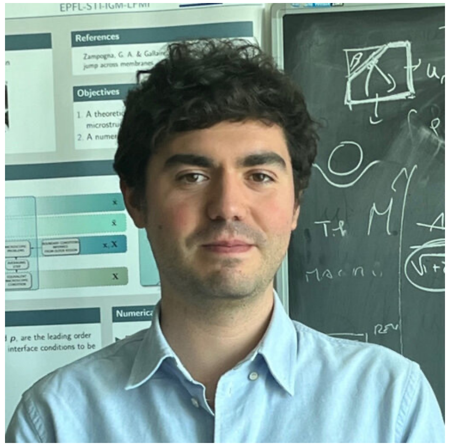

D. Bothe


T. Maric


J. De Coninck

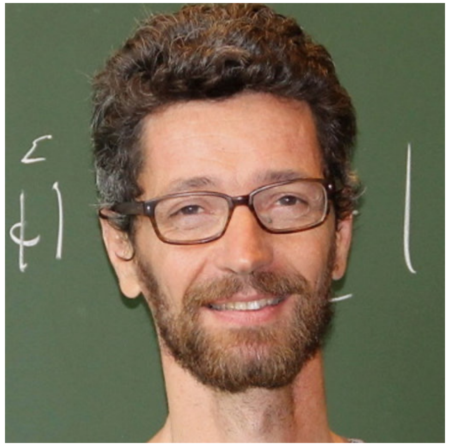

S. Raju


Z. Tukovic


T. Fullana

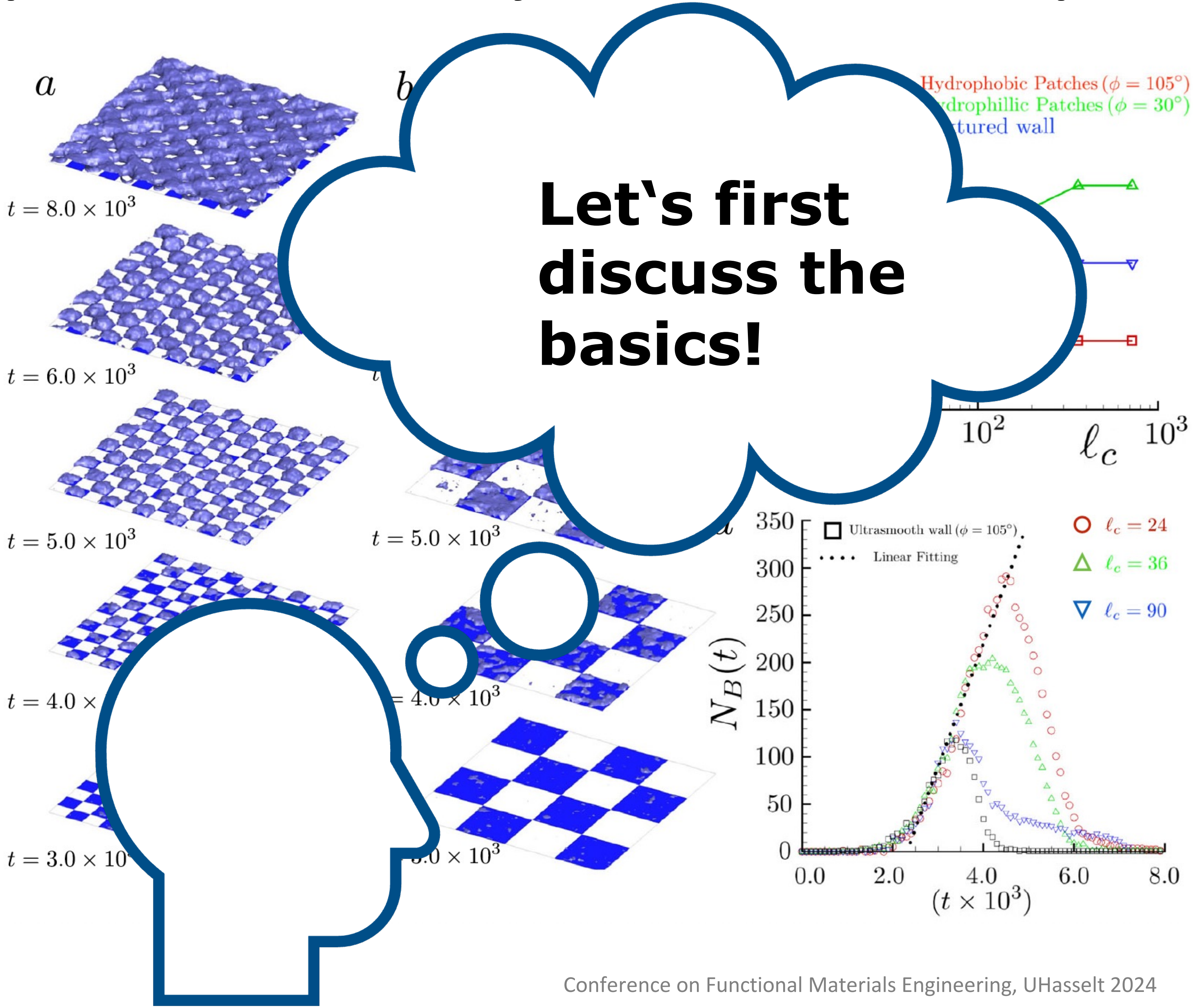

Y. Kulkarni


S. Afkhami


S. Popinet


S. Zaleski

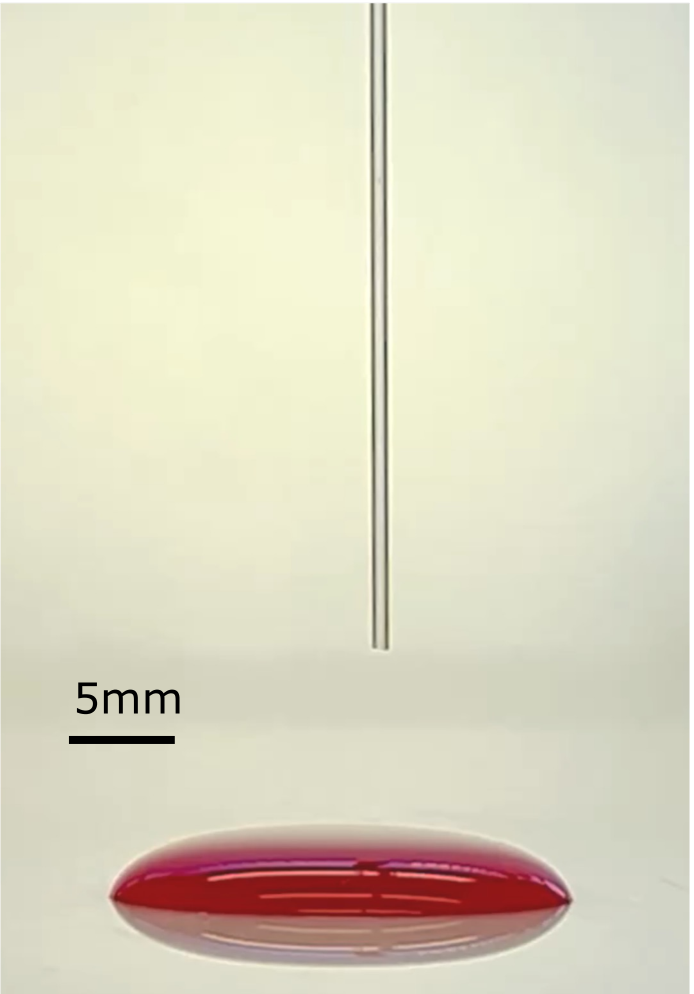
Recap: Surface Wettability and Structure can improve heat transfer



See yesterdays keynote by Joël De Coninck.

Gallo et al.,
Nat. Commun. 14, **2023**

Capillary Rise: A prototypical dynamic wetting process



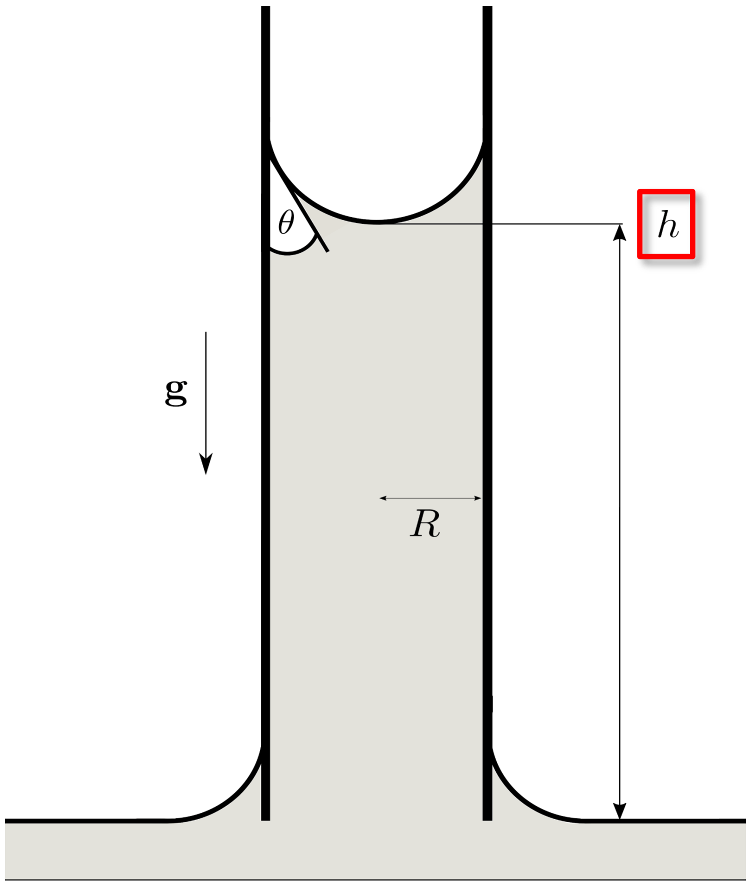
Why is this „simple“ process interesting?

- Numerous **applications** (e.g. porous media, microfluidics,….)
- **Prediction** of the dynamics is non-trivial!
- Axial symmetry → **Simplified models** available

Two major challenges

- **Predictive** models → only use well-defined material parameters
- **Multiscale** character → very high computational costs

Capillary Rise: A prototypical dynamic wetting process



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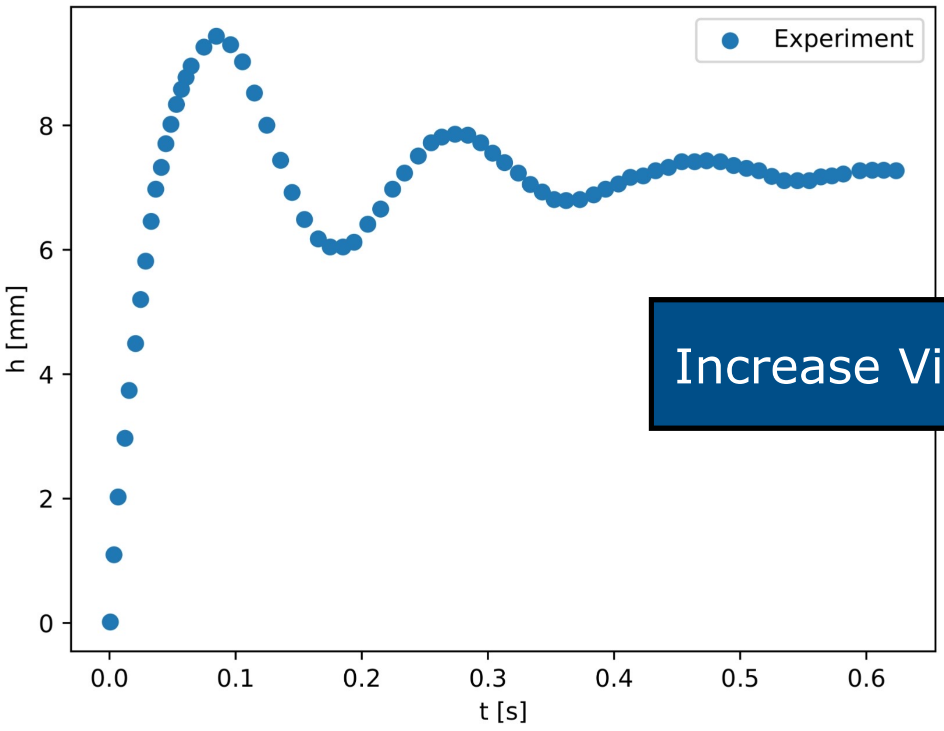
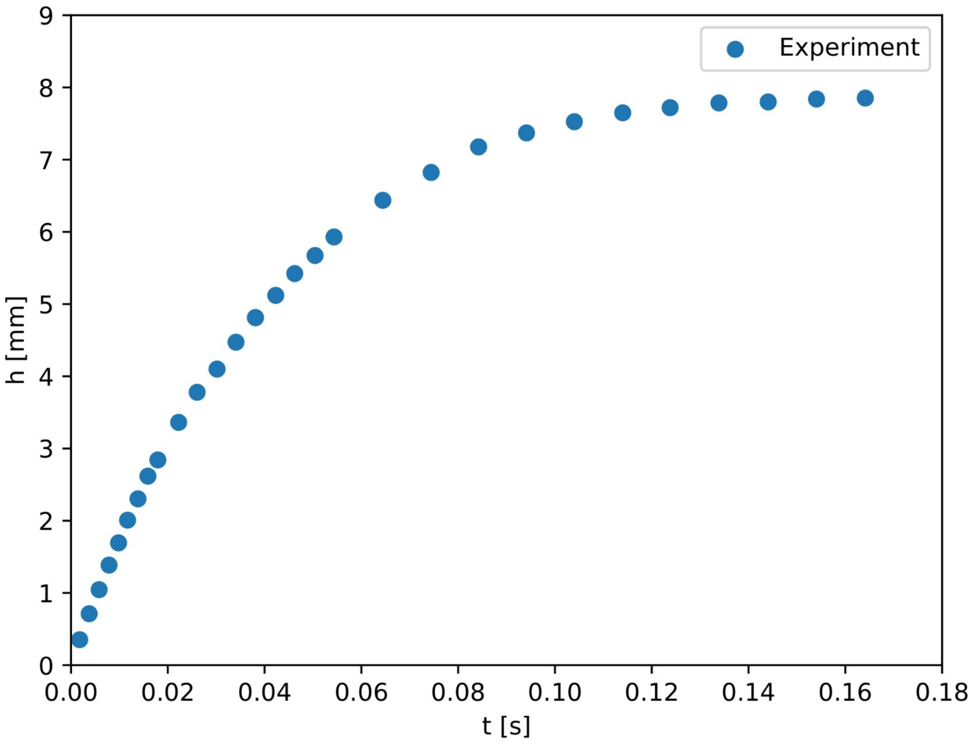
Goal: Predict rise height h=h(t)

Experiments: Monotonic vs. Oscillatory Rise (Quéré, 1997)

- Experimental data for glass capillaries with radius $R = 689\mu\text{m}.$



Increase Viscosity



Ether: $\eta = 0.3\,\text{mPa}\cdot\text{s}$

Low viscosity

Ethanol: $\eta = 1.17\,\text{mPa}\cdot\text{s}$

High viscosity

Experiments: Monotonic vs. Oscillatory Rise (Quéré, 1997)

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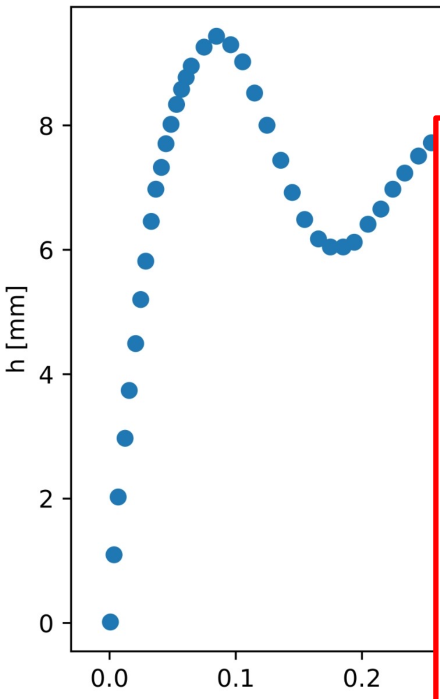
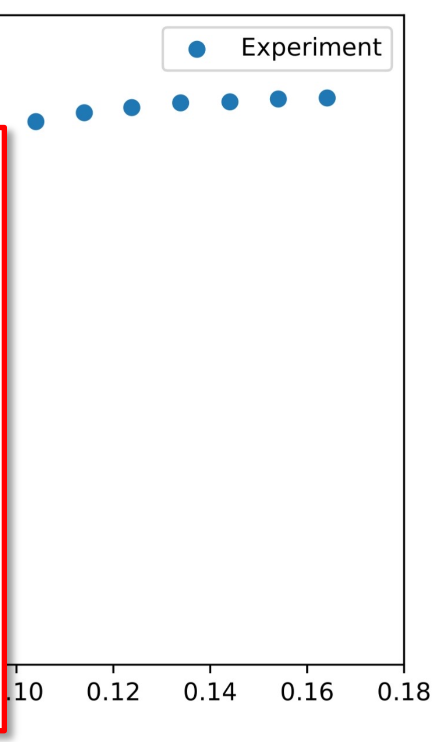




Warning:

Predicting these curves is actually far from trivial!

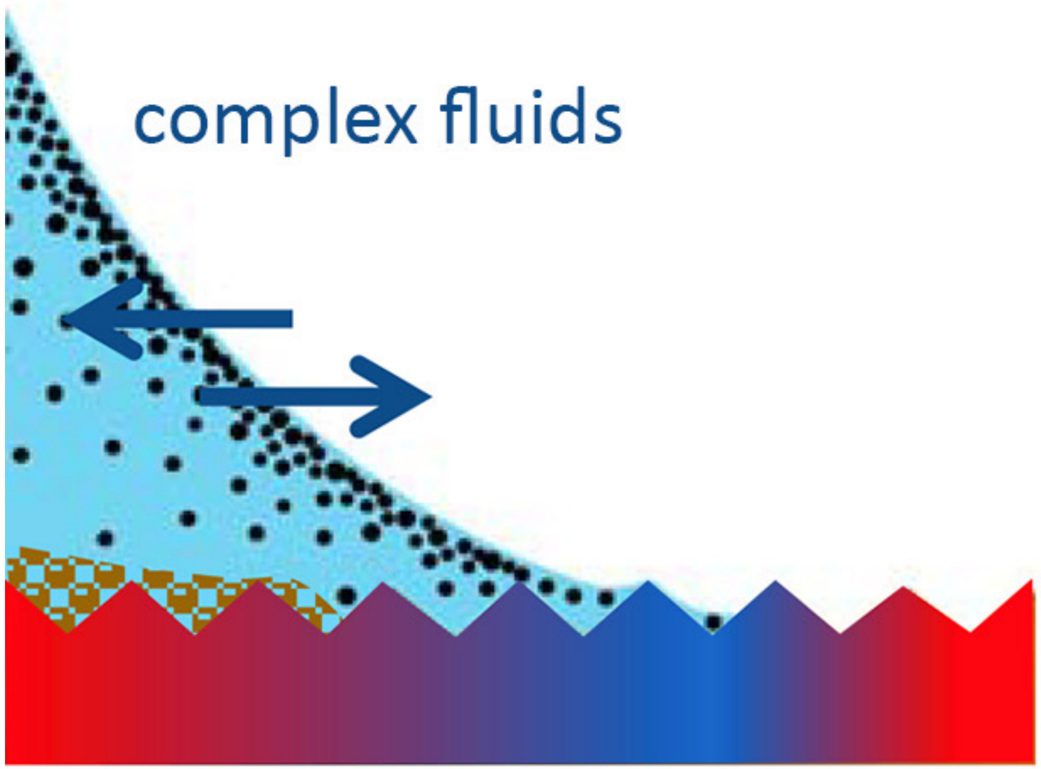
Ether: $\eta = 0.3\,\text{mPa}\cdot\text{s}$

Low viscosity

Ethanol: $\eta = 1.17\,\text{mPa}\cdot\text{s}$

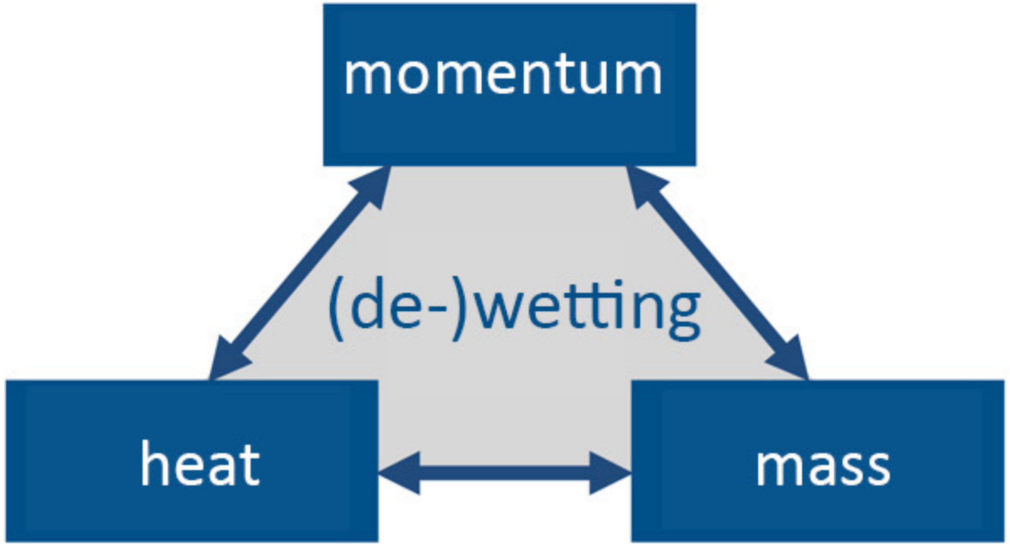
High viscosity

Collaborative Research Center on Wetting and Transport Phenomena



complex surfaces

transport/transfer



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Collaborative Research Center on Wetting and Transport Phenomena

Production engineering

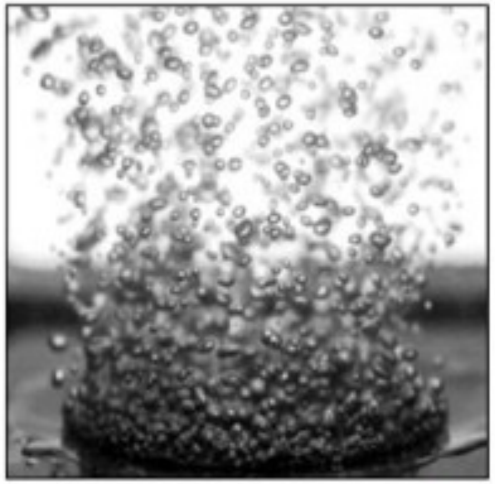
Dörsam

Coating and printing technology

↓

Faster printing, less fluid, improved print quality, ...

Energy technology



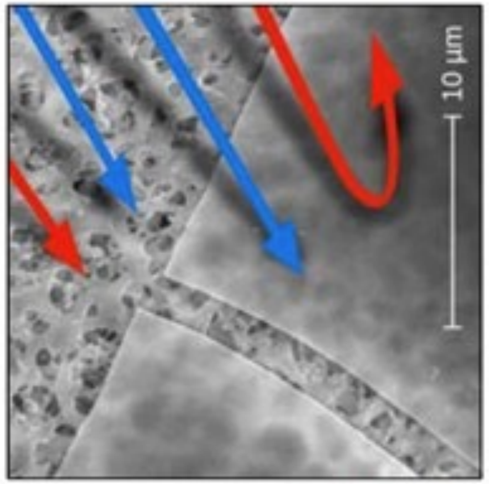
Stephan

Evaporators, condensers

↓

Improved heat transfer, higher heat flux density, ...

Process engineering



Andrieu-Brunsen

Microfluidics & separation

↓

Higher mass flux density, higher degree of selectivity, ...

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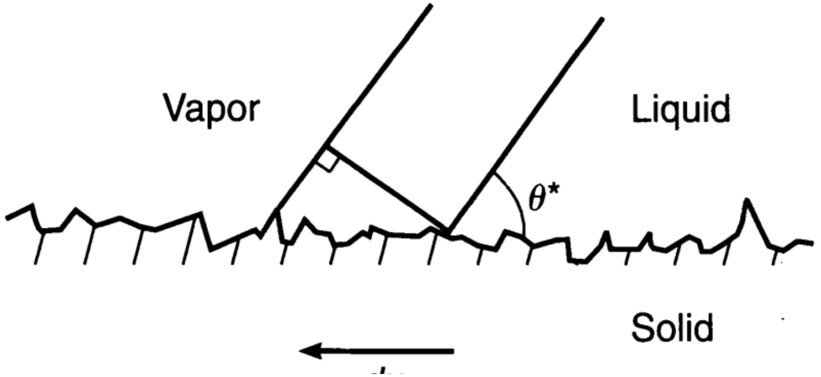
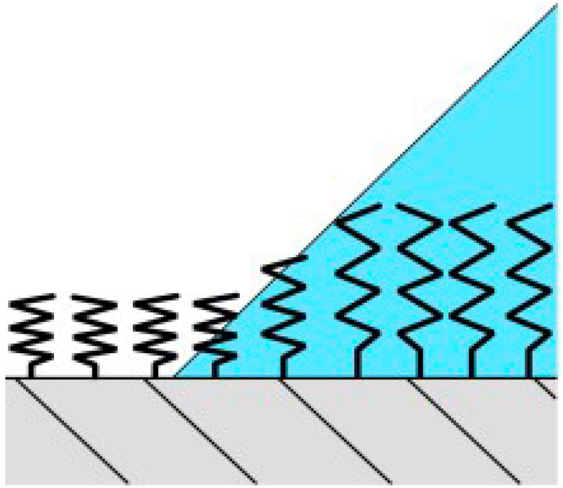
Examples: Wetting of complex surfaces

- **Rough** surfaces

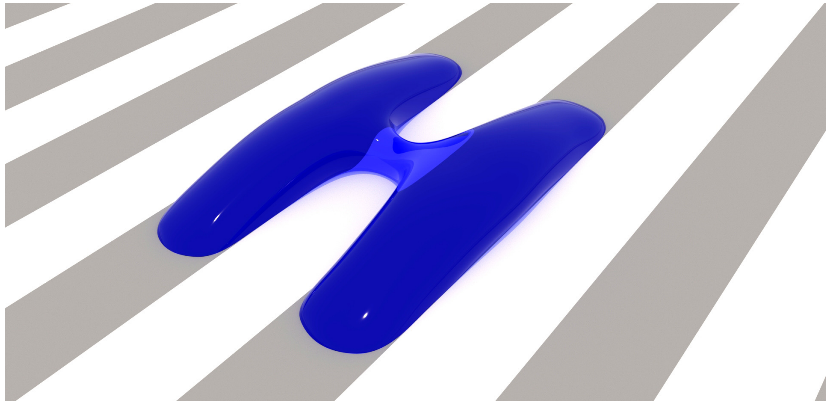


- **Complex coatings**
  (here Polymer Brushes**)**

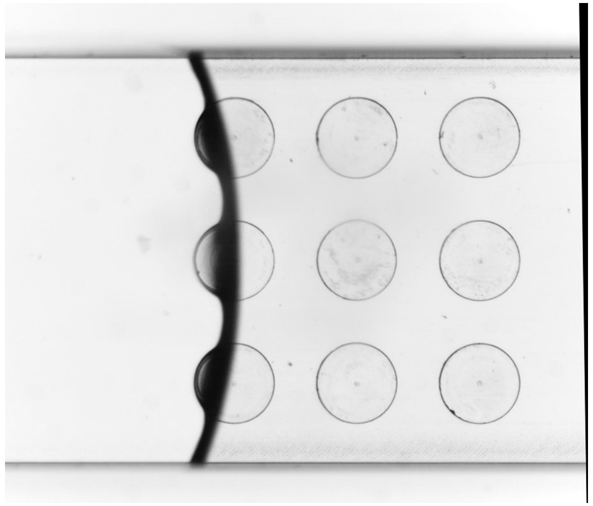
→ **Adaptive** wetting



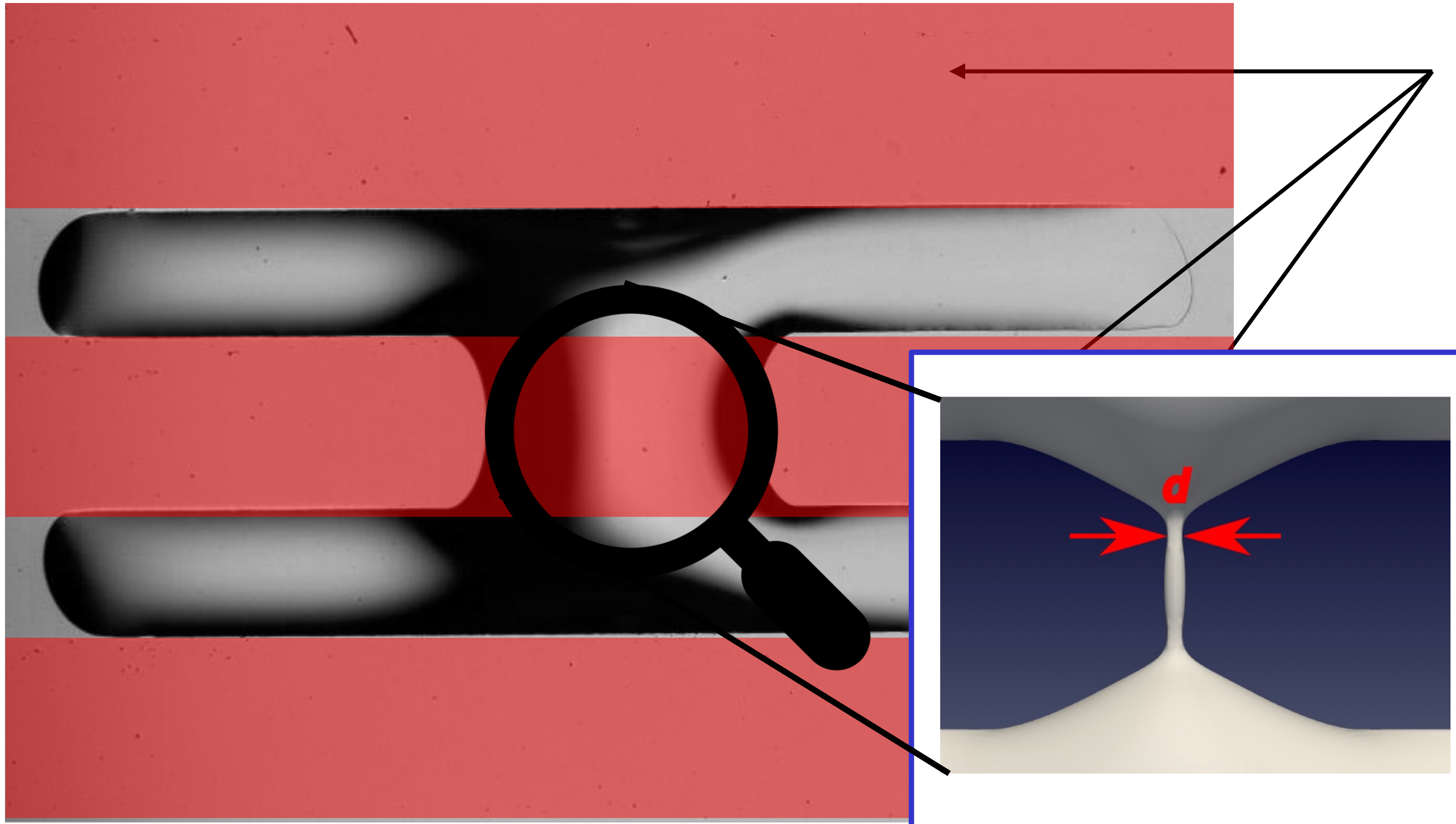
- **Chemical** heterogeneities



- Complex **topography**
  (here cavities)



Simulations give more insights – Breakup of a liquid bridge

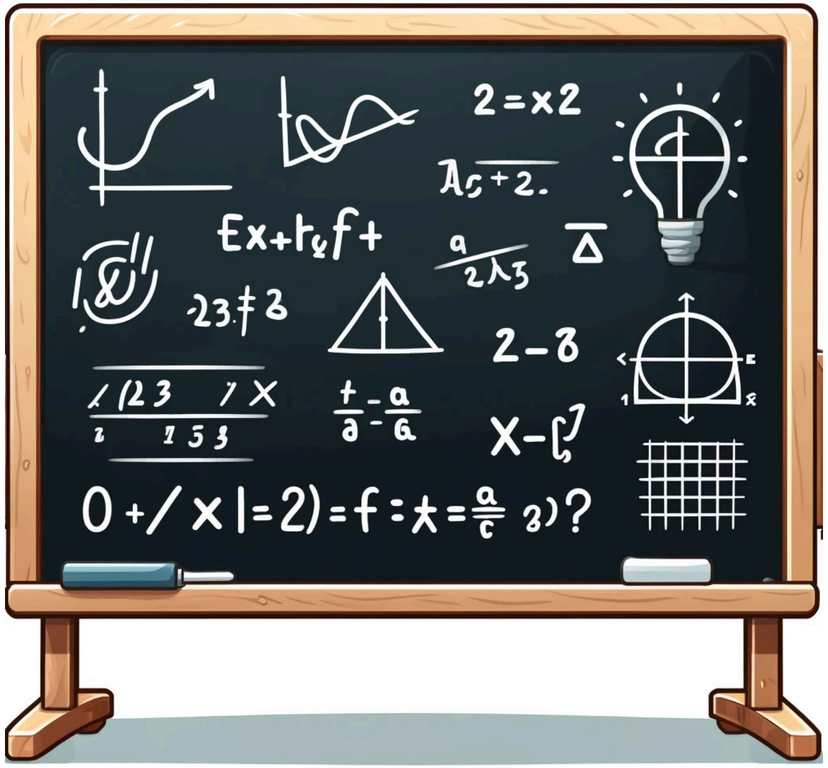


Structured surface:

Hydrophobic part of the substrate

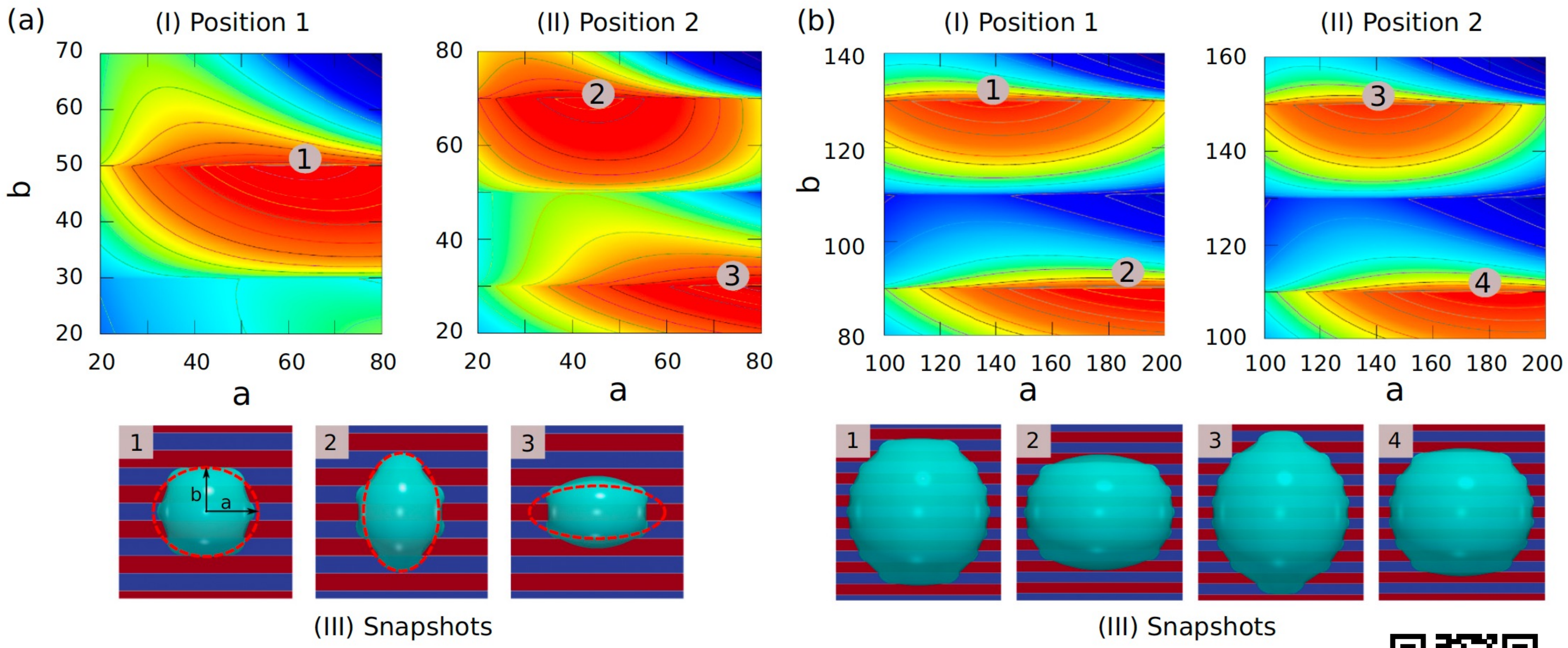
Breakup is **too fast** for the high-speed camera! Simulations help!

Hartmann, Fricke et al.:*Breakup dynamics of capillary bridges on hydrophobic stripes*, International Journal of Multiphase Flow 140, DOI:10.1016/j.ijmultiphaseflow.2021.103582, **2021**



Modeling Fundamentals

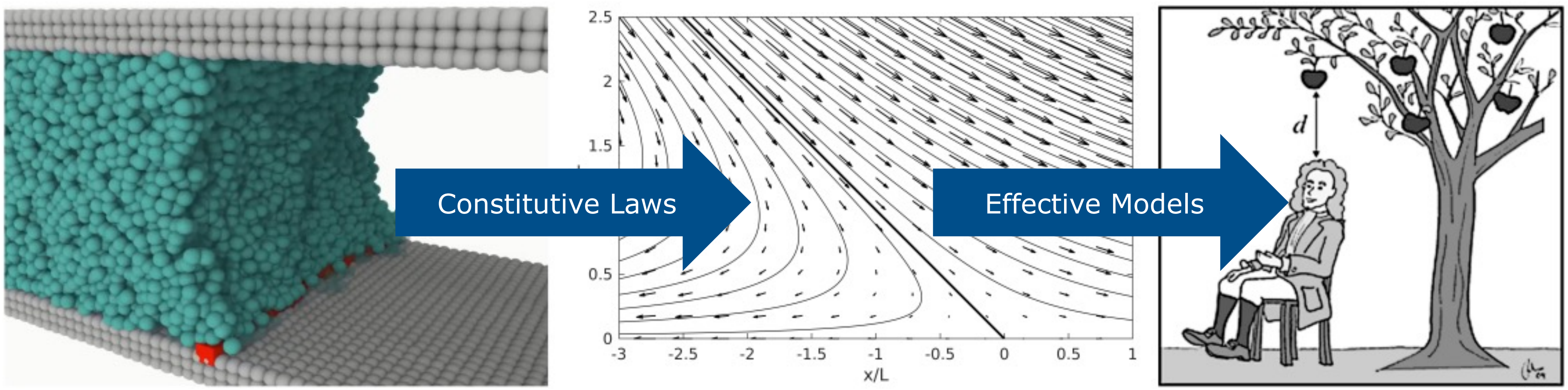
Static Wetting → Minimization of the free energy



Wu, Wang, Selzer and Nestler, Physical Review E 100, **2019**

Modeling Hierarchy for Wetting Dynamics

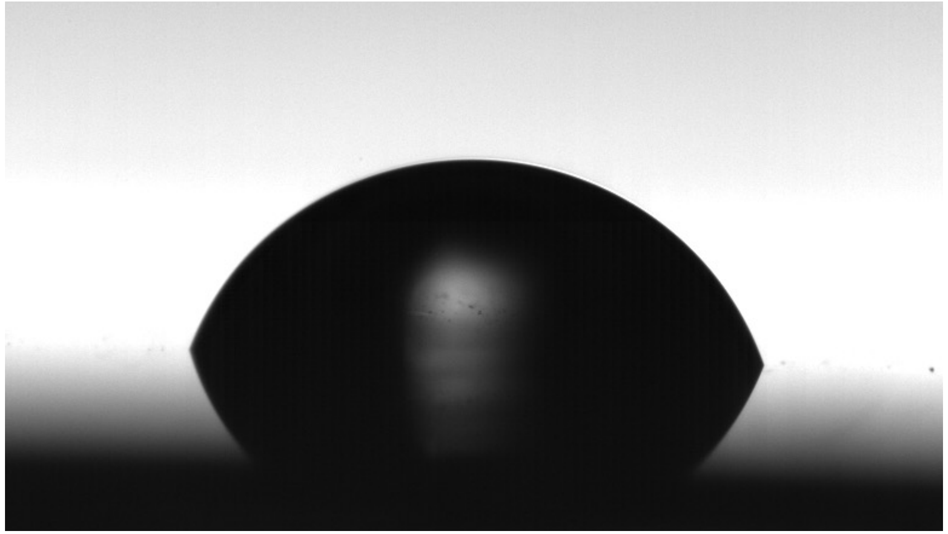
- **Molecular Dynamics (MD):** Modeling from first principles, highly accurate, limited in terms of time and length scales.
- **Continuum mechanics (Navier Stokes):** Inherits knowledge from MD in form of constitutive laws and boundary conditions, still costly.
- **Simplified models (typically ODEs):** Fast to solve, Taylor-made, basis for optimization!



(a) Molecular dynamics. (b) Continuum mechanics. (c) Simplified models.

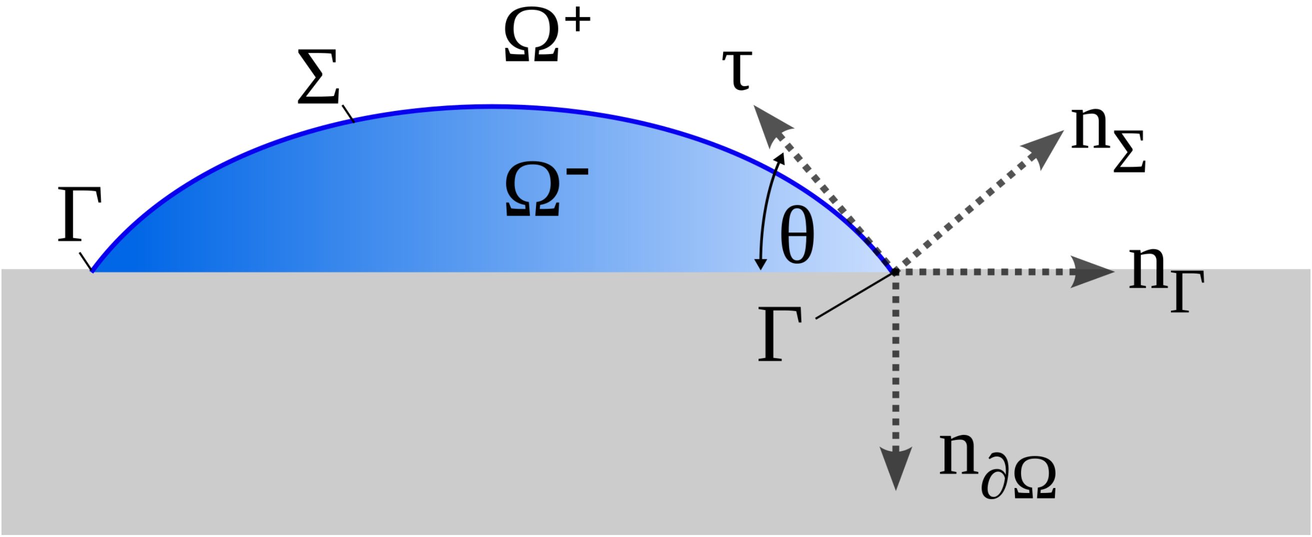
Complexity in Modeling & Simulation of Dynamic Wetting

- Real surfaces are **rough**,
- may have chemical or topographical **defects** or **structure,**
- Interfaces may be **contaminated** (e.g., surfactants).



Real droplet on a surface.

- **Simplify** the system as much as possible.
- Approximate interfaces as **sharp.**
- Treatment of surface defects with effective **boundary conditions**?
- **Initial conditions** sometimes unclear.

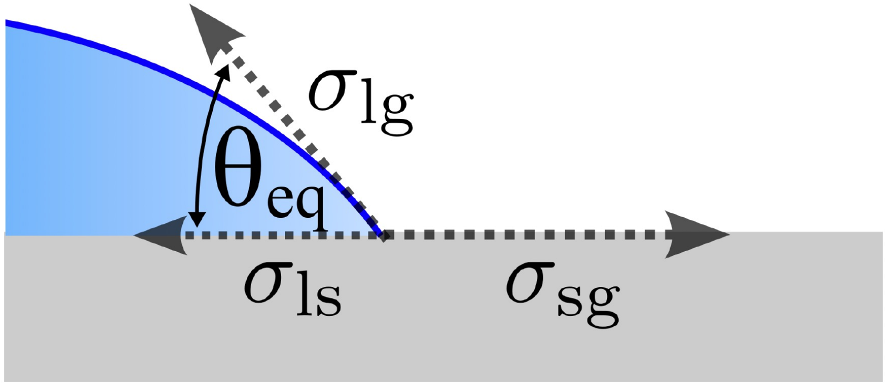


Mathematical model.

Static Wetting – The Young & Cassie-Baxter equation

- The contact angle on an **ideal** surface is governed by a balance of surface tension forces (Young equation):

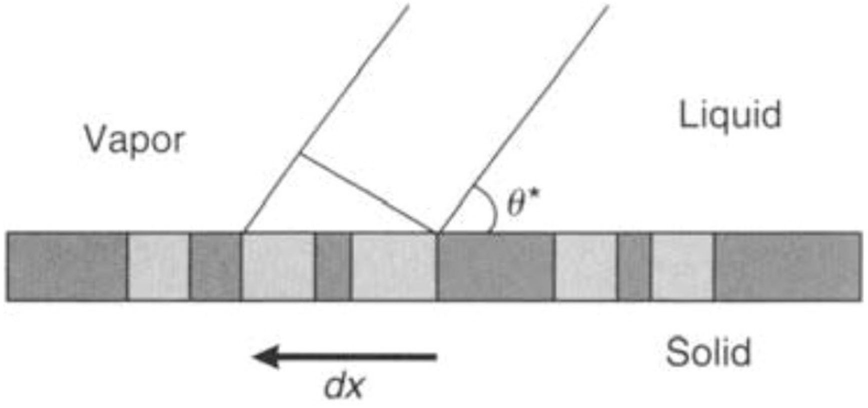
$$\sigma_{\mathrm{lg}} \cos \theta_0 + \sigma_{\mathrm{sl}} - \sigma_{\mathrm{sg}} = 0$$



Ideal surface

- Model for the **static** contact angle on **chemically textured** surface (Cassie-Baxter equation):

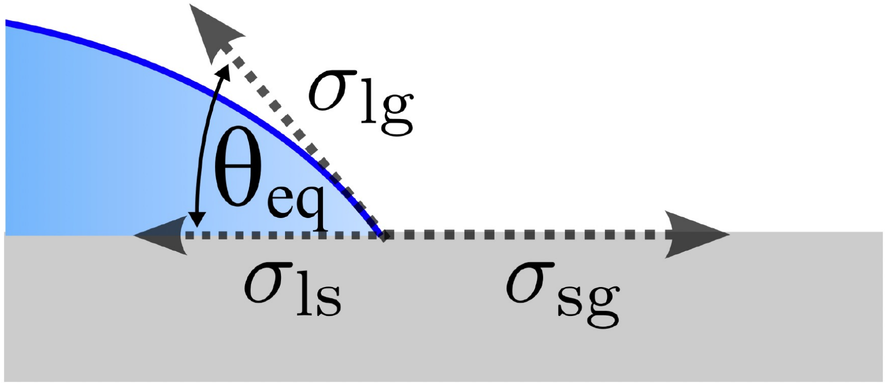
$$\cos \theta_{\mathrm{CB}} = r_1 \cos \theta_1 + r_2 \cos \theta_2$$



Chemically textured surface

Static Wetting – The Young & Cassie-Baxter equation

Can the Cassie-Baxter equation also be applied for **dynamic** cases?



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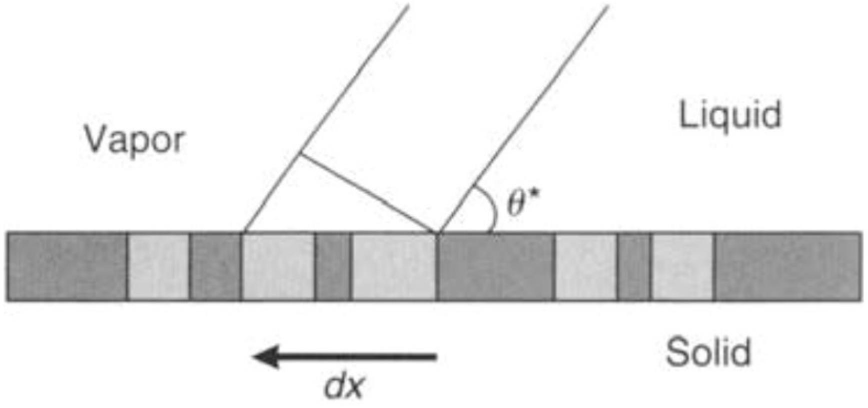


Chemically textured surface

Two-phase Navier-Stokes Wetting „Standard Model"

(incompressible, Newtonian, isothermal, sharp-interface)

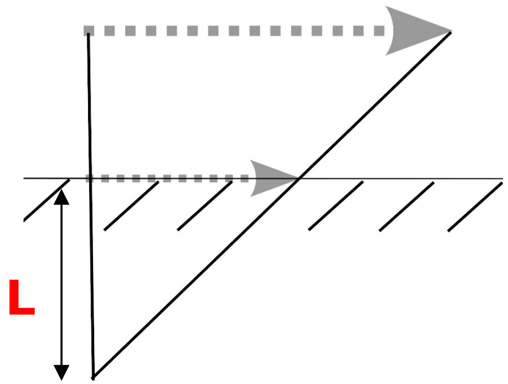
- Mass balance: $\nabla \cdot \mathbf{v} = 0$
- Interface Kinematics: $V_\Sigma = \mathbf{v} \cdot \mathbf{n}_\Sigma$
- Momentum balance:

$$\partial_t(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p = \eta \Delta \mathbf{v} + \rho \mathbf{g} + \mathbf{f}_\Sigma$$

- Surface tension force: $\mathbf{f}_\Sigma = \sigma \kappa_\Sigma \mathbf{n}_\Sigma \delta_\Sigma$

- Boundary conditions at the solid wall (slip!)

$$\mathbf{v}_\perp = 0$$



- Contact angle boundary condition:

$$-\zeta U_{\mathrm{cl}} = \sigma \left(\cos\theta - \cos\theta_{\mathrm{e}}\right)$$

Contact line friction: $\zeta \geq 0$

Contact line speed: U_{cl}

Two-phase Navier-Stokes Wetting „Standard Model“

(incompressible, Newtonian, isothermal, sharp-interface)

- Mass balance: $\nabla \cdot \mathbf{v} = 0$
- Interface Kinematics: $V_\Sigma = \mathbf{v} \cdot \mathbf{n}_\Sigma$
- Mome
- Surfac
- Bound

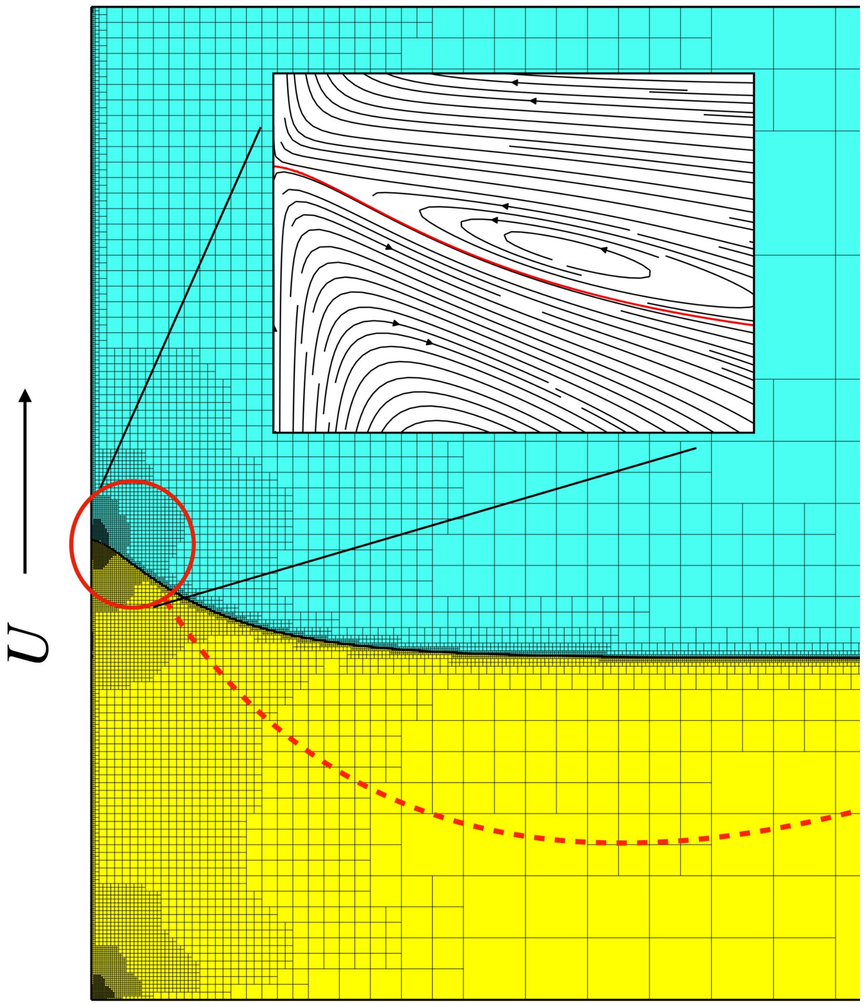
$\mathbf{v}_\perp =$

Contact line speed: U_{cl}

Recent developments in modeling:

Fullana, Kulkarni, Fricke et al.:
A consistent treatment of dynamic contact angles in the sharp-interface framework with the generalized Navier boundary condition, Preprint, **2024**

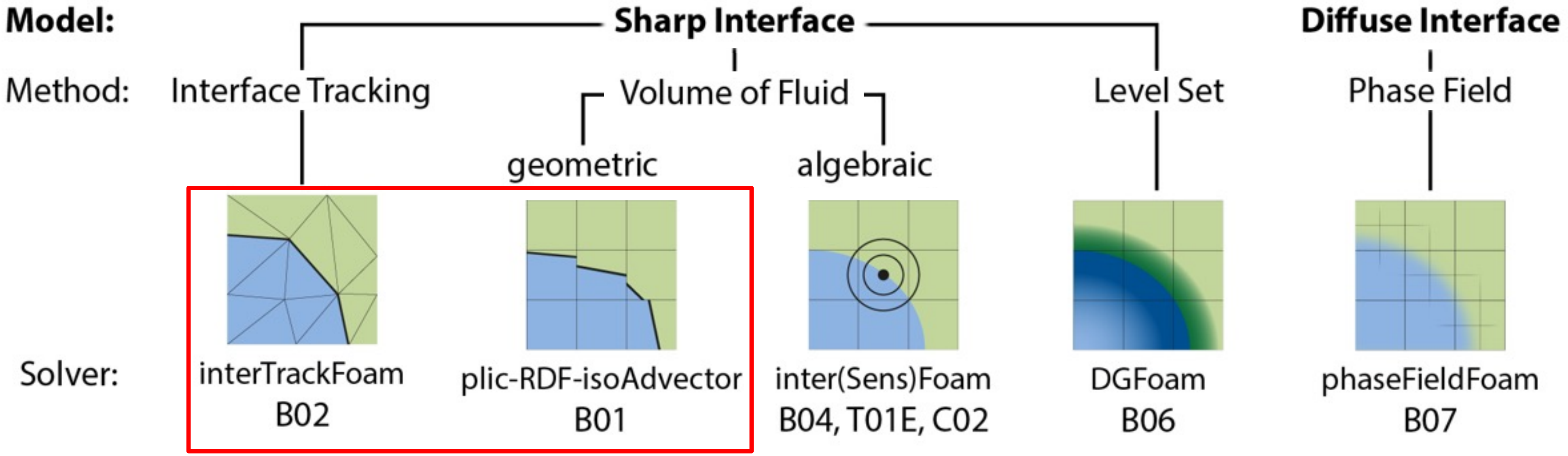
DOI: 10.5281/zenodo.10142047



Numerical Simulation Fundamentals

Our approach to CFD simulation

- There is no single method suitable for every problem!
- We develop diverse numerical methods for two-phase flows in the **OpenFOAM** library.
- Specific methods to tackle, e.g., topological changes, surfactant transport, evaporation, …



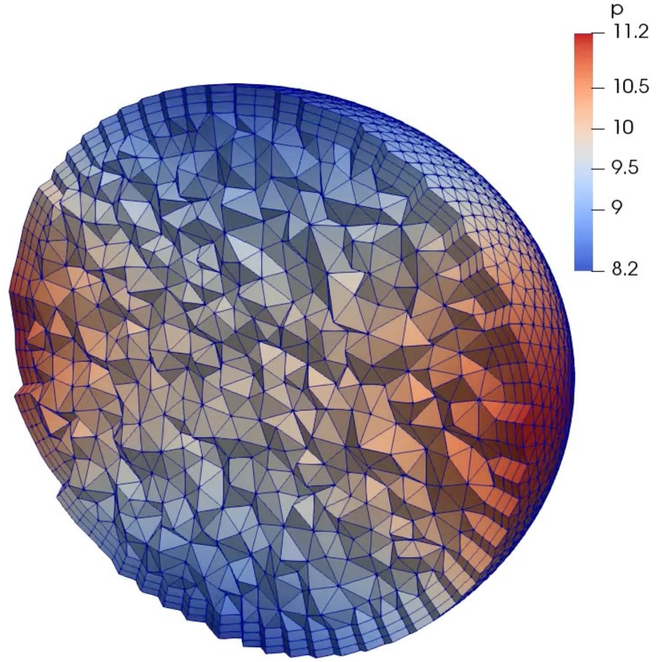
Deutsche Forschungsgemeinschaft

Tracking the fluid interface (Finite Volume based methods)

- We need to follow the **evolution of the interface** $\Sigma(t)$ and the bulk phases:

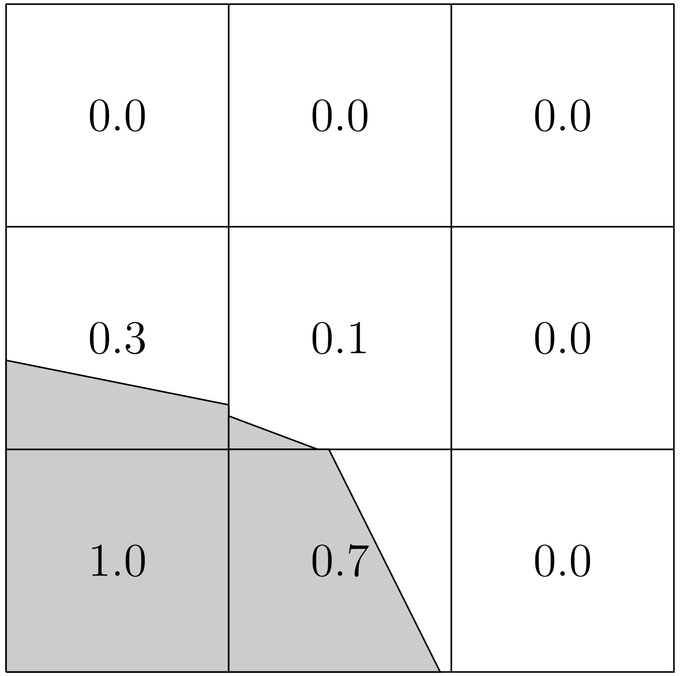
$$\Omega = \Omega_l(t) \ \cup \ \Omega_g(t) \ \cup \ \Sigma(t)$$

Arbitrary Lagrangian Eulerian (ALE) Method in OpenFoam



Dissertation
D. Gründing

Volume-of-Fluid Method (Eulerian)



Dissertation
M. Fricke

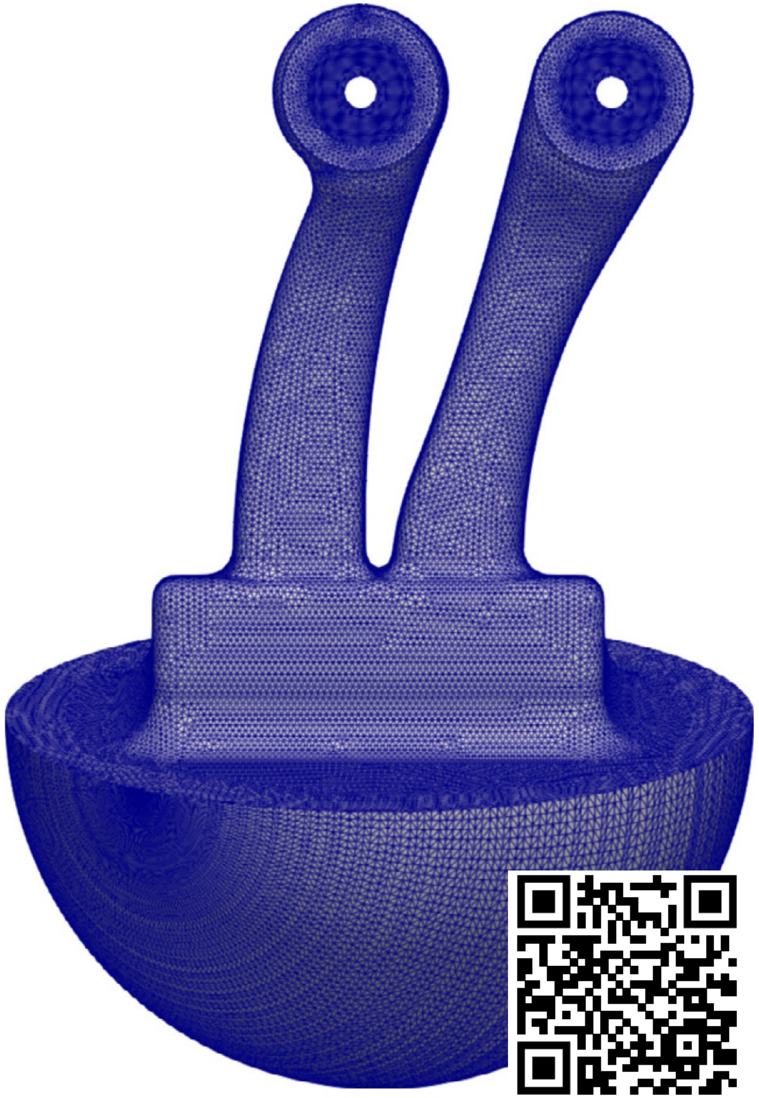
How to simulate two-phase flows in complex geometries?

A GeoVOF method for wetting in complex geometries

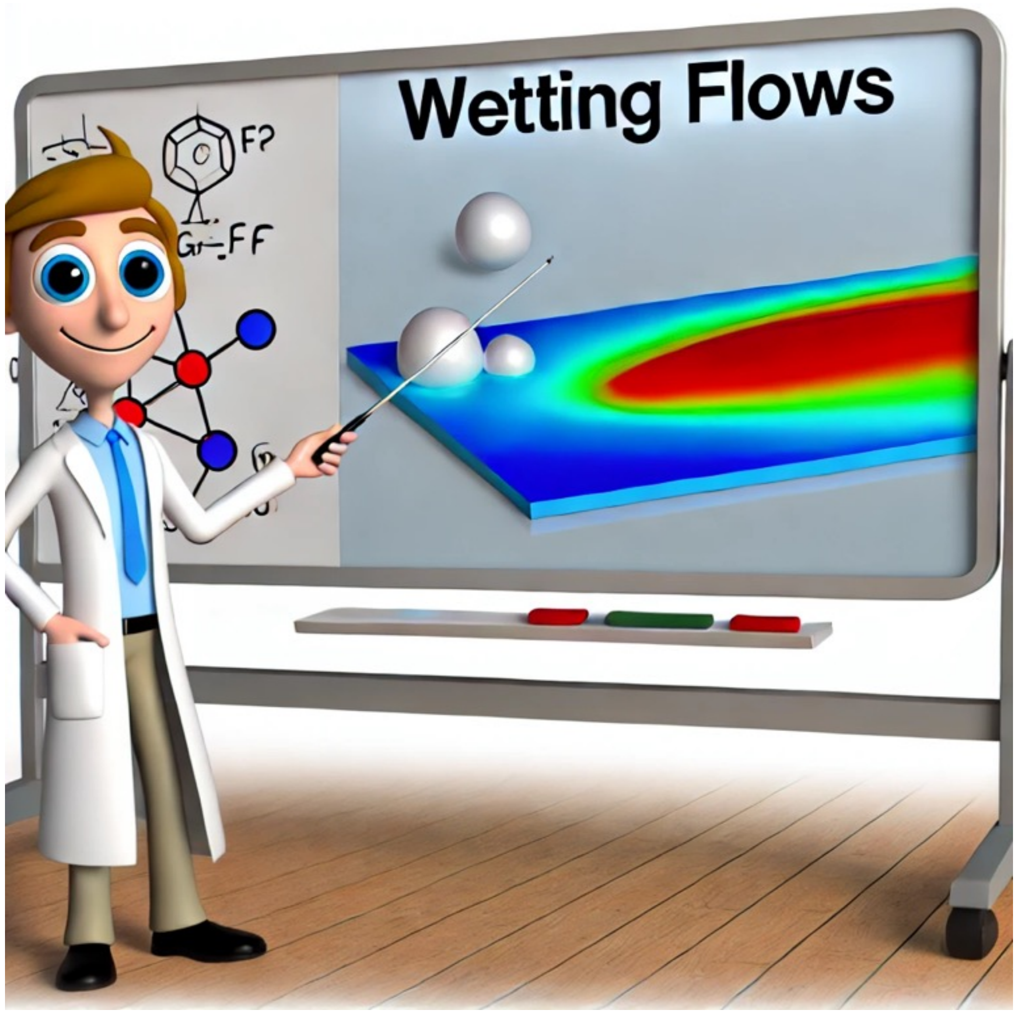
The mesh matters!

T. Maric (TU Darmstadt)

We are developing a Geometric Volume-if-Fluid on **unstructured meshes** based on the **IsoAdvector** method by J. Roenby.

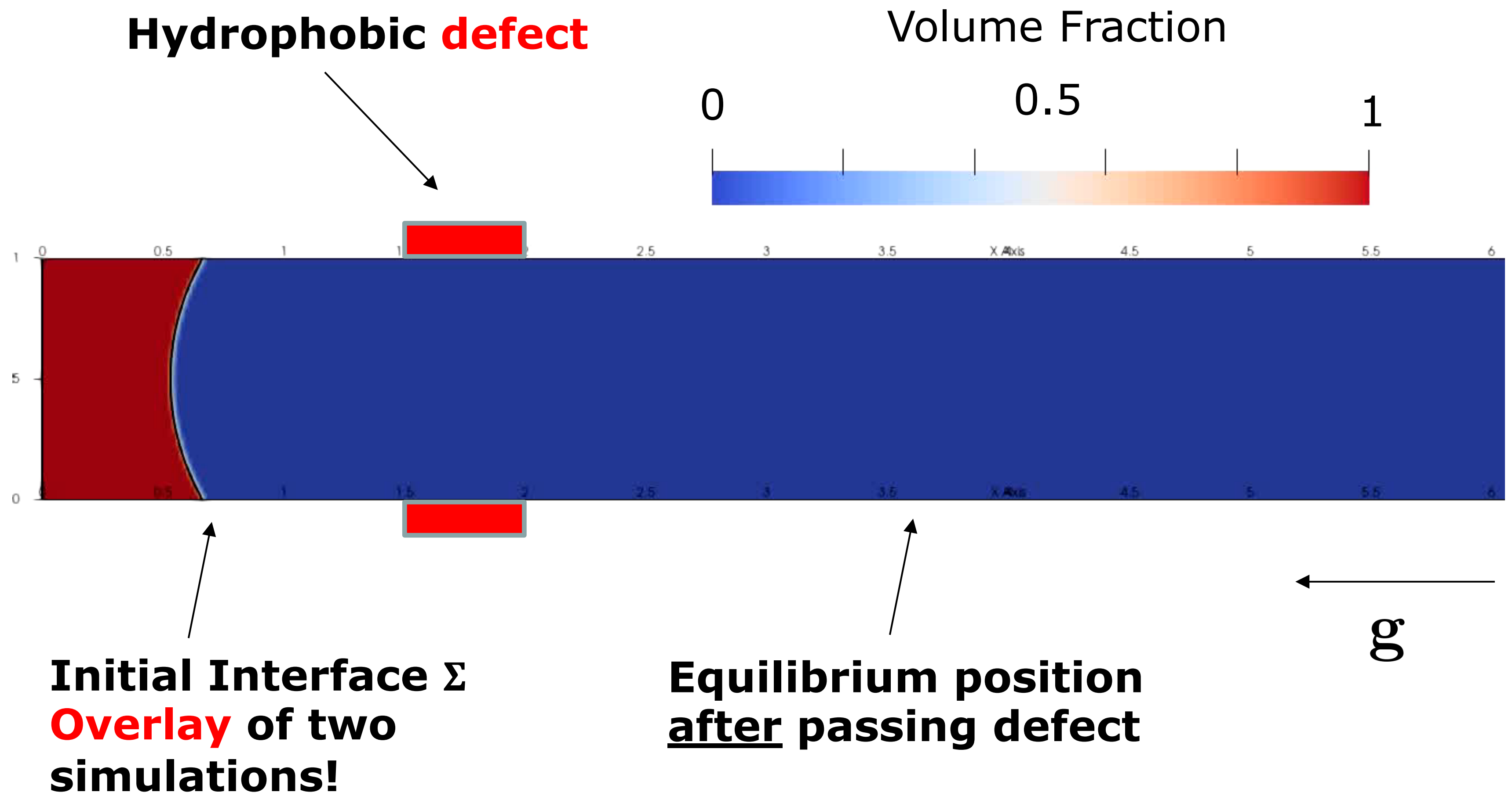


arXiv:2302.02629

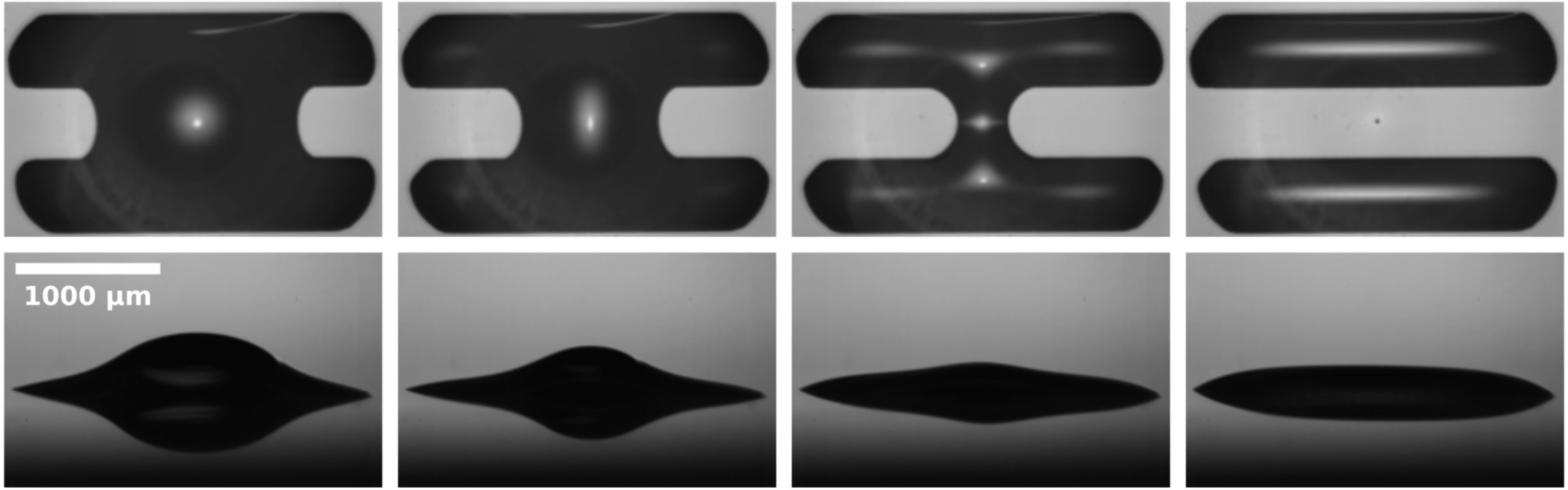


Examples: Wetting of Structured Surfaces

Example 1: Trapping of a meniscus - VOF simulations



Example 2: Evaporation & Breakup on a Structured Surface

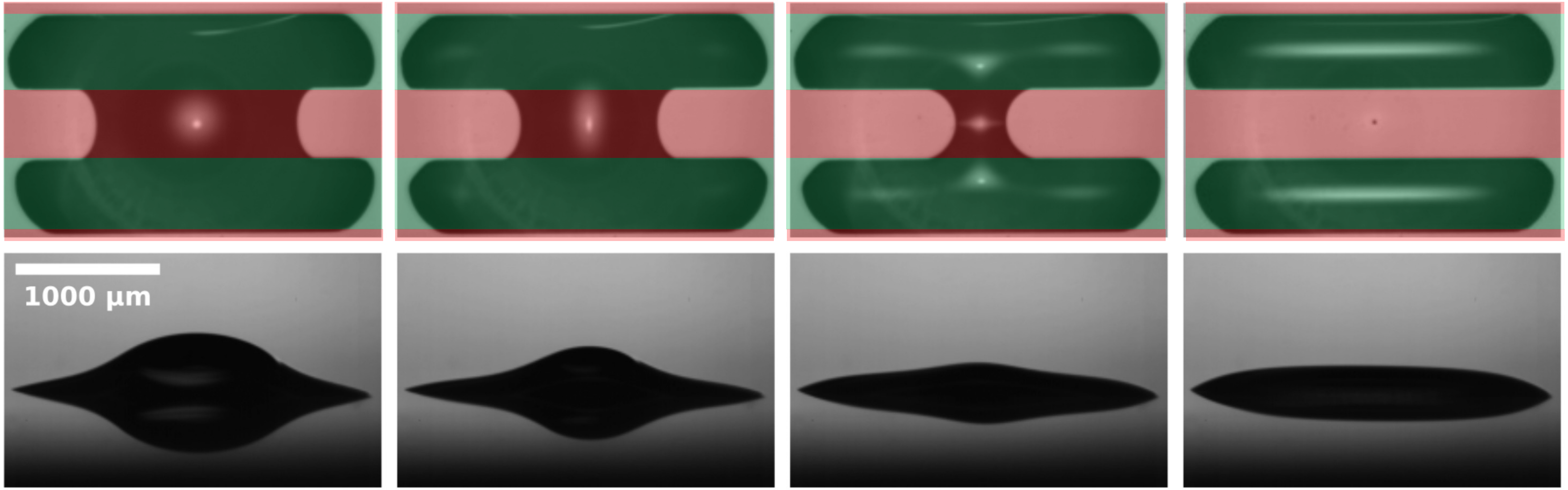


Top

Side

Hartmann, Fricke et al.:*Breakup dynamics of capillary bridges on hydrophobic stripes*, International Journal of Multiphase Flow 140, DOI:10.1016/j.ijmultiphaseflow.2021.103582, **2021**

Example 2: Hydrophobic & Hydrophilic Stripes



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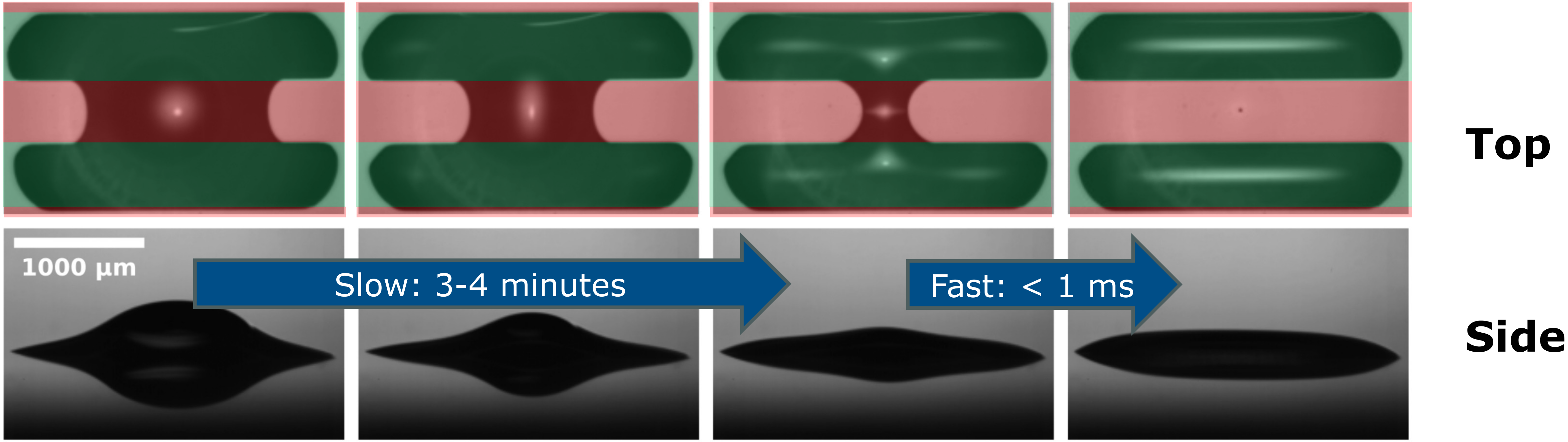
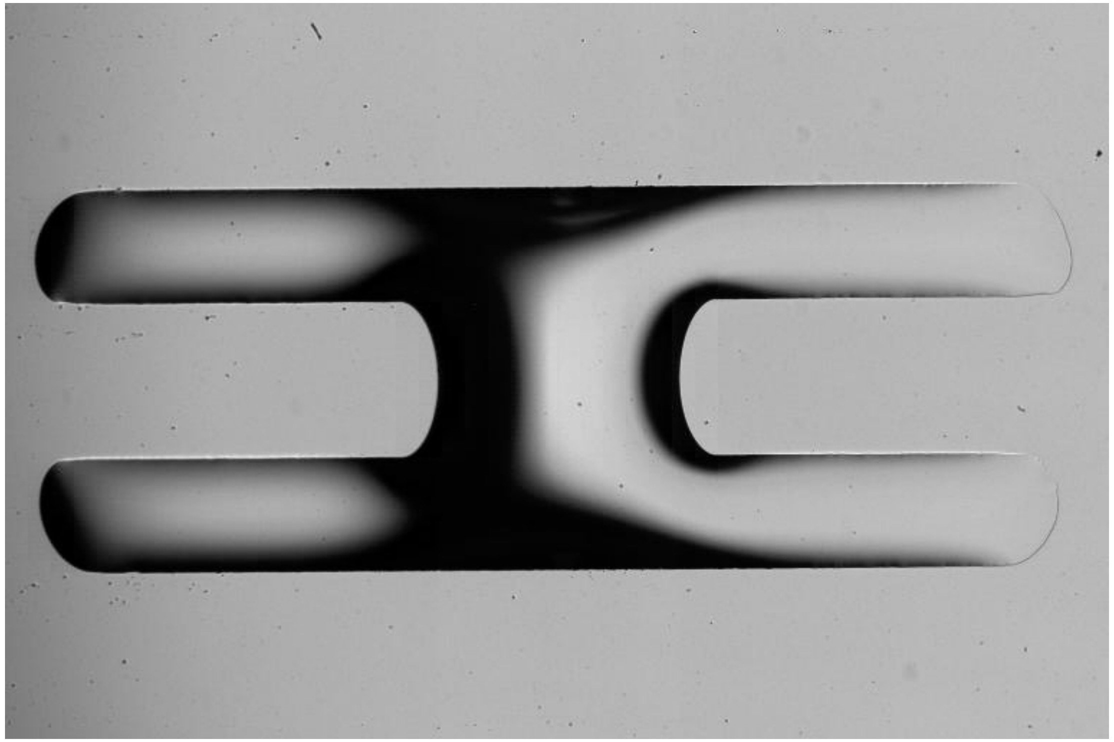
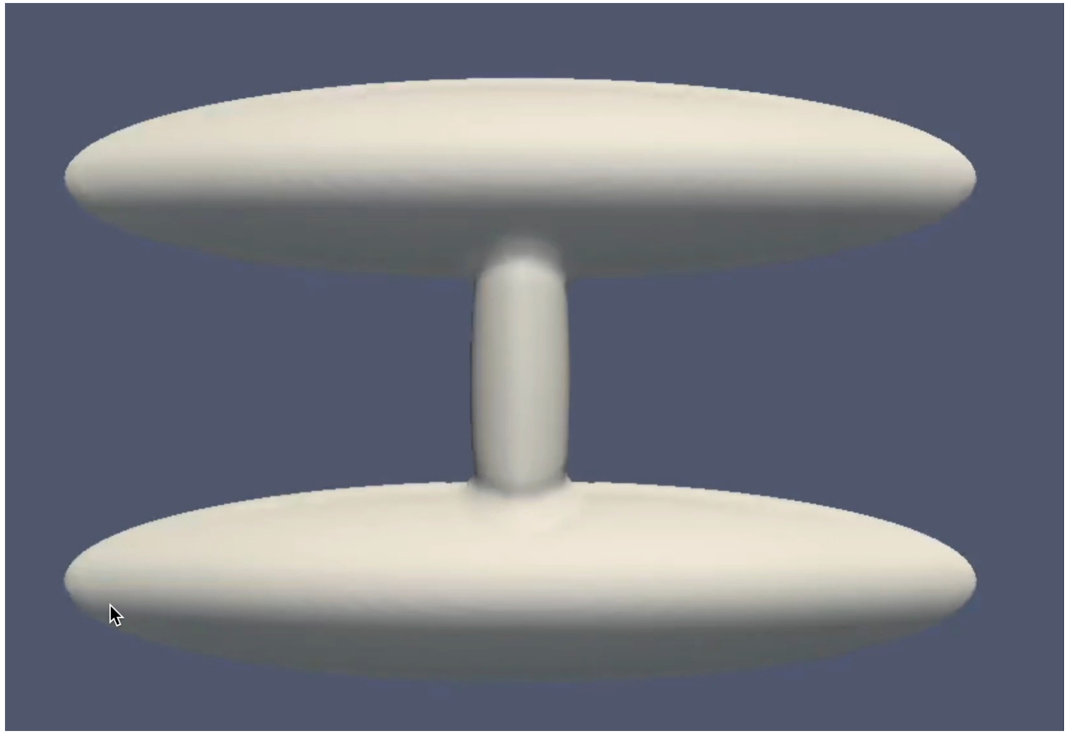


Hartmann, Fricke et al.:*Breakup dynamics of capillary bridges on hydrophobic stripes*, International Journal of Multiphase Flow 140, DOI:10.1016/j.ijmultiphaseflow.2021.103582, **2021**

Example 2: First naive attempts



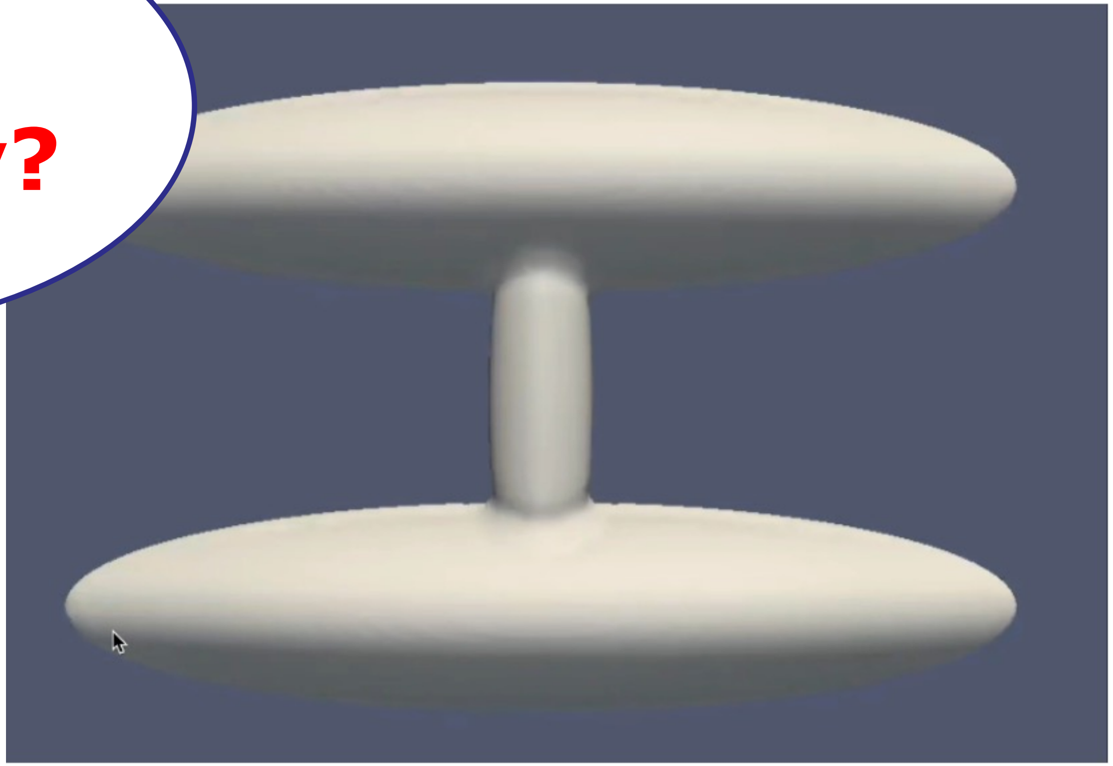
Experiment



Simulation

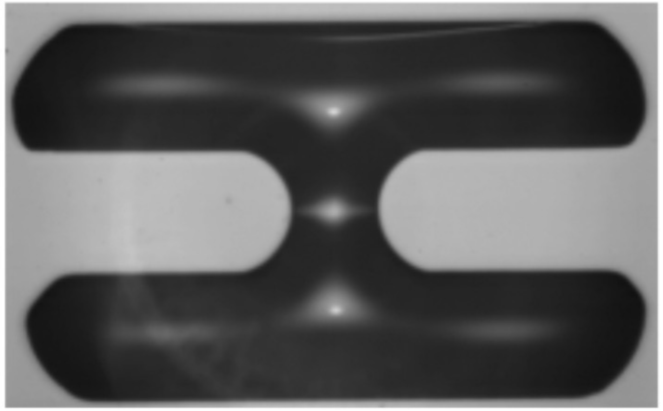
Example 2: First naive attempts

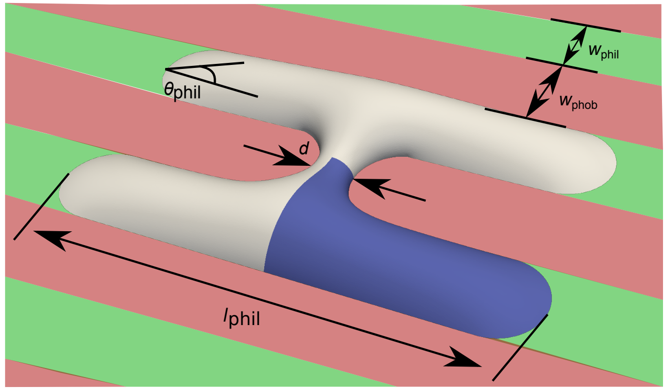
Initial geometry?



Simulation

Example 2: <u>Properly</u> separate slow and fast





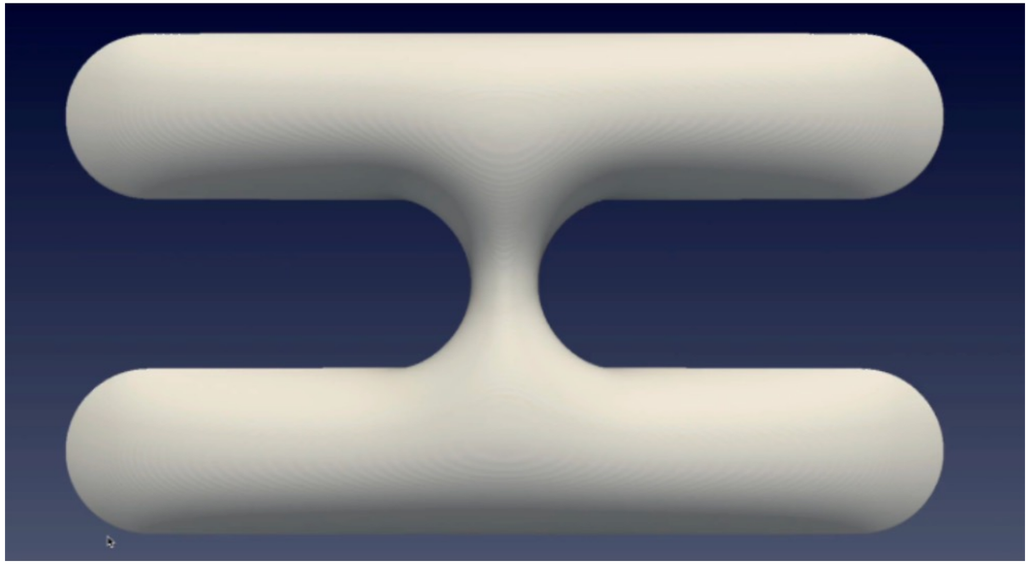
Surface Evolver until onset of breakup (find minimal surfaces)

Transfer Geometry

Tolle et. al, 2021

Hartmann et. al, 2021

Volume-of-Fluid Two-Phase Flow



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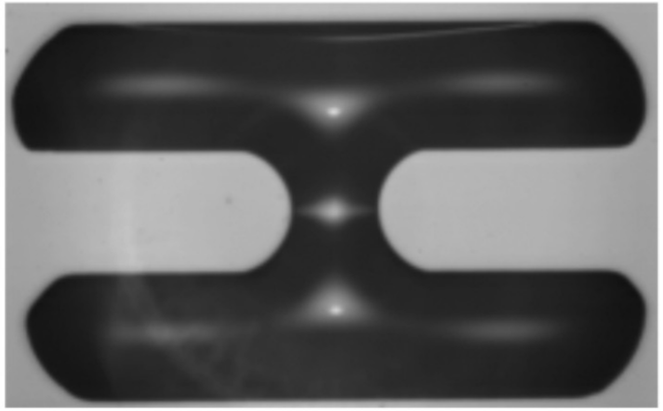

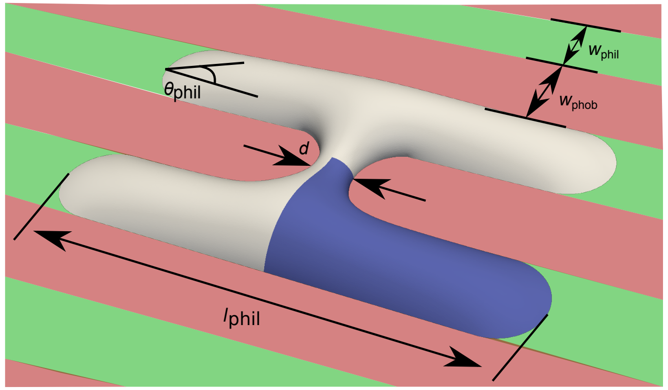

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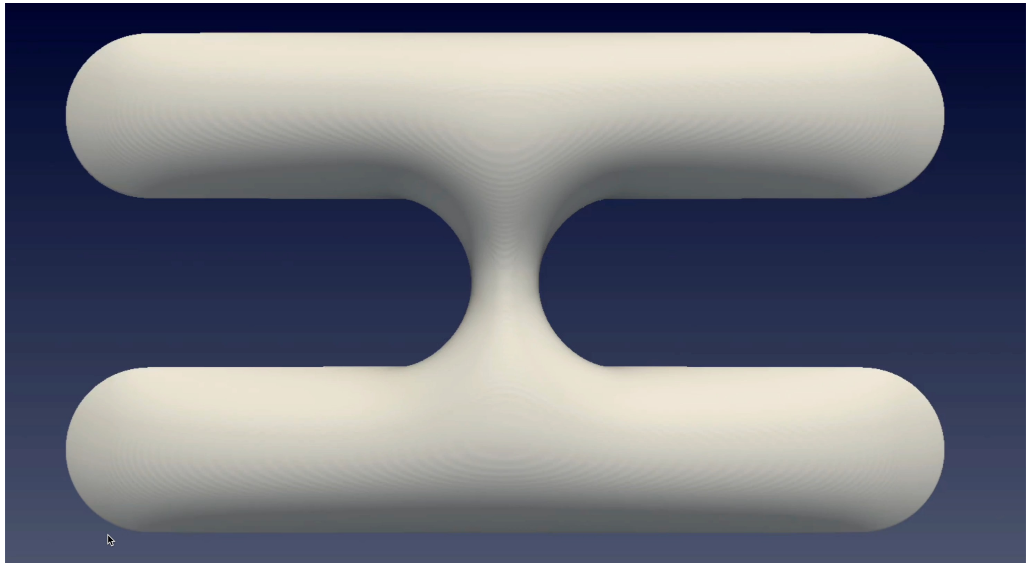
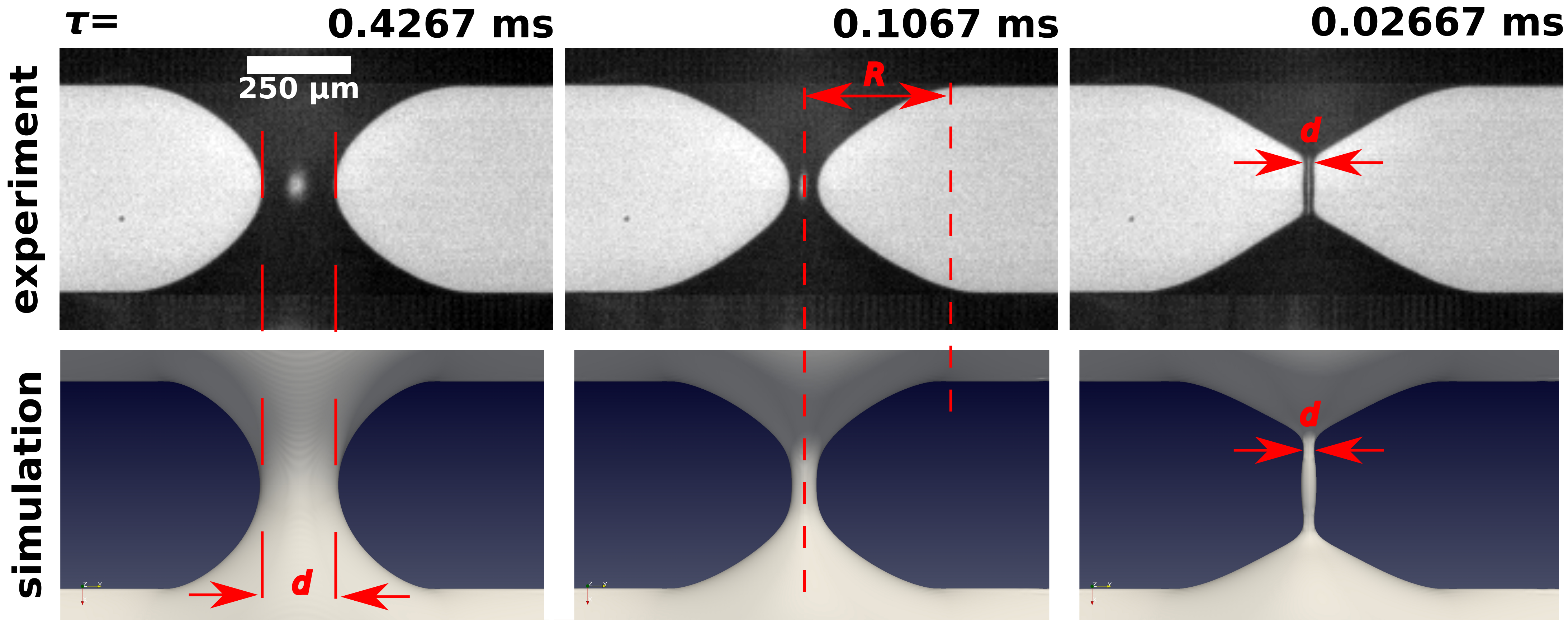


Example 2: Problem solved! ✅

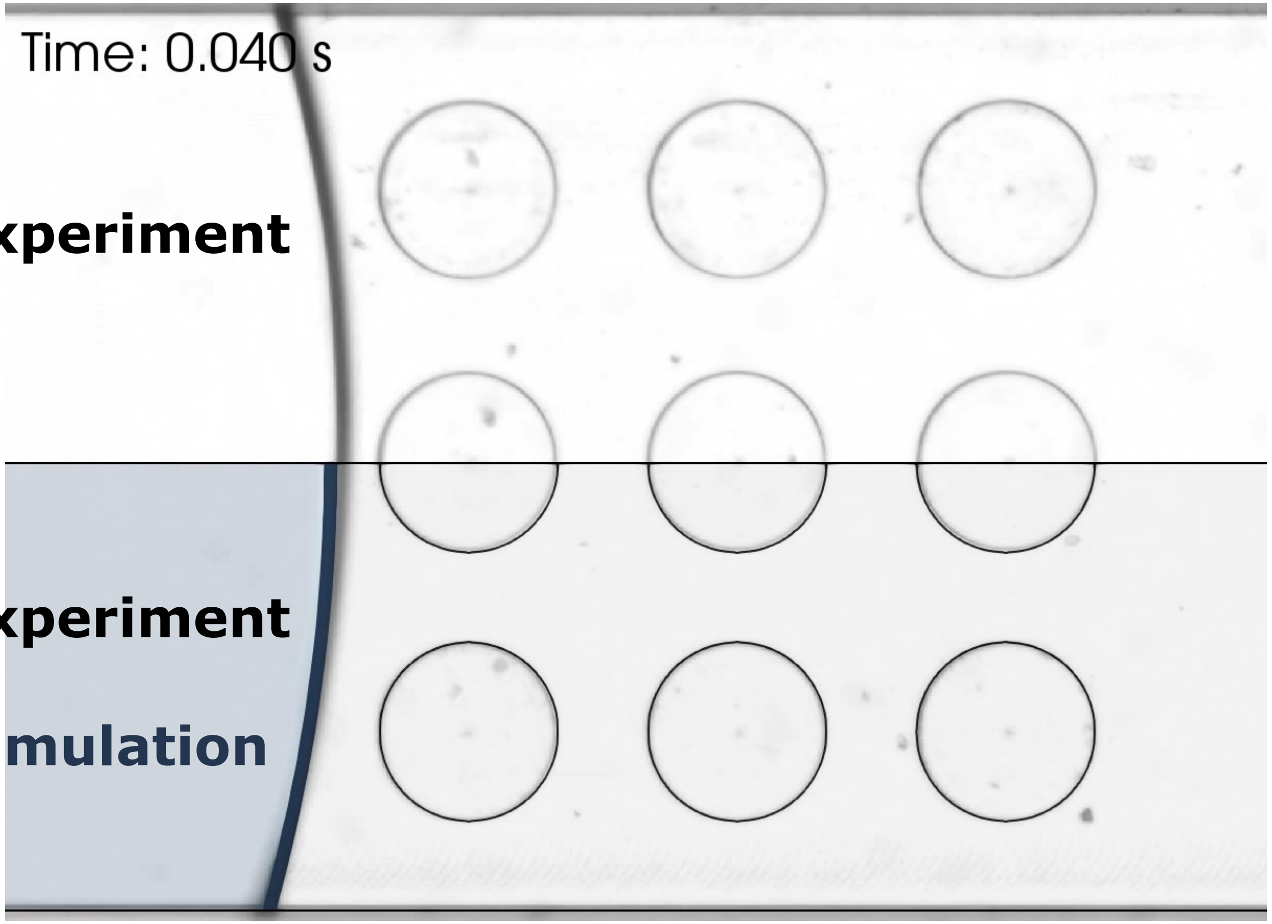


Hartmann et. al, 2021

Example 3: Meniscus passing over microcavities (air-water system)

Collaboration: **Lab-on-a-chip** research @ Robert Bosch GmbH
(lead by T. Maric, TU Darmstadt)

T. Maric



- Inlet velocity 10 mm/s
- Simulations with OpenFoam using unstructured grids
- Pinning at cavity edges
- PhD work by Luise Nagel (Bosch)

arXiv:2407.18068

Thank you very much for your attention!

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