Numerical simulation of drop impact and rebound phenomena on smooth and micro-structured hydrophobic surfaces

A. Stroh[1], V. Fink[1], X. Cai[1], R. Bernard[2], J. Kriegseis[1], B. Frohnapfel[1], H. Marschall[3], M. Wörner[1]

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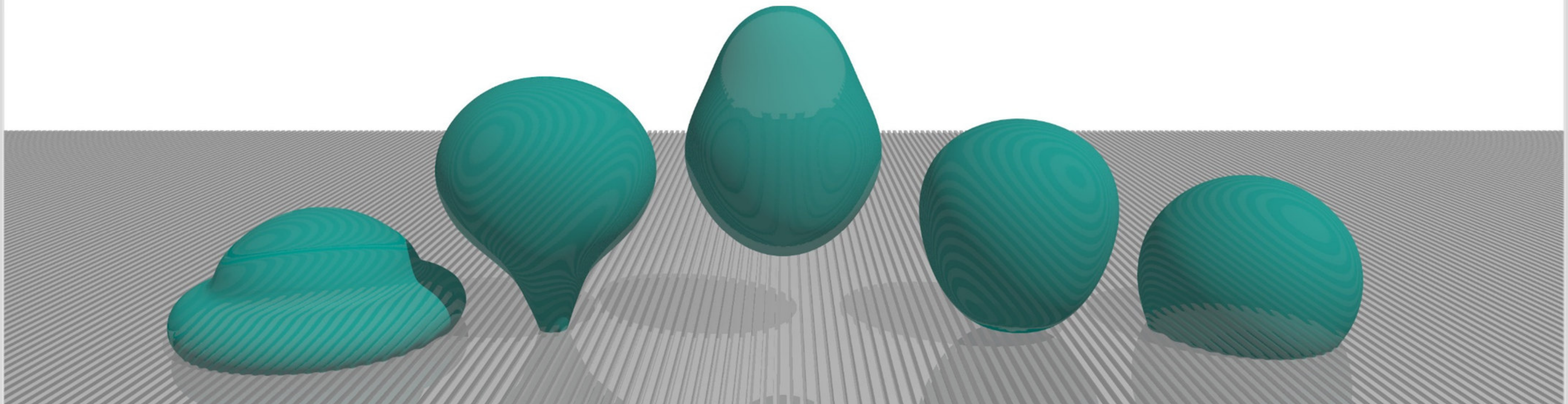
[1]*Karlsruhe Institute of Technology*, [2]*University of Stuttgart*, [3]*Technical University of Darmstadt*



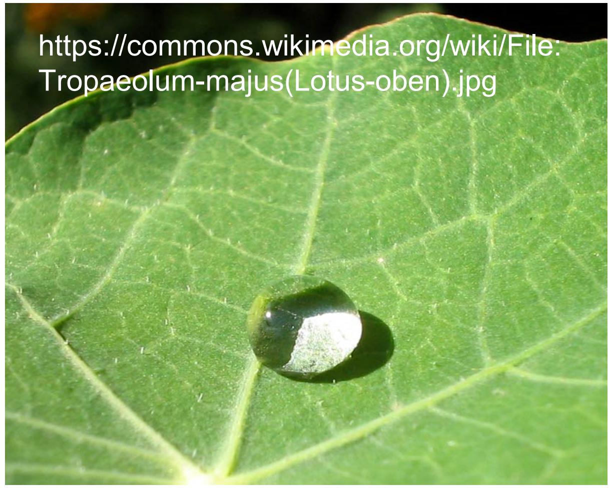
V. Fink, X. Cai, A. Stroh, R. Bernard, J. Kriegseis, B. Frohnapfel, H. Marschall, M. Wörner, *Int. J. Heat Fluid Flow* **70** (2018) 271-278

Agenda

- Introduction and motivation
  - Wettability and roughness
- Experiment
  - Drop impact on flat and micro-structured surfaces
- Numerical simulation
  - Phase field method in Open∇FOAM
  - Computational setup and code performance
  - Simulation results
- Summary and outlook

The lotus effect

- The **lotus effect**# refers to self-cleaning properties that are a result of **hydrophobicity** as exhibited by the leaves of the lotus flower
- Although known in Asia for a long time the underlying mechanism was explained only in the 1970s after the introduction of the scanning electron microscope
- The surface of the **lotus leave** is not smooth but **rough**



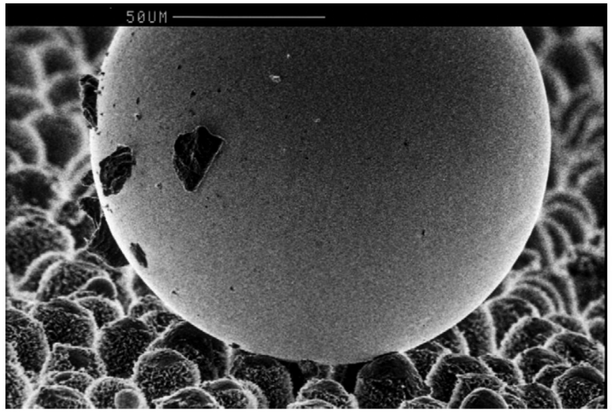


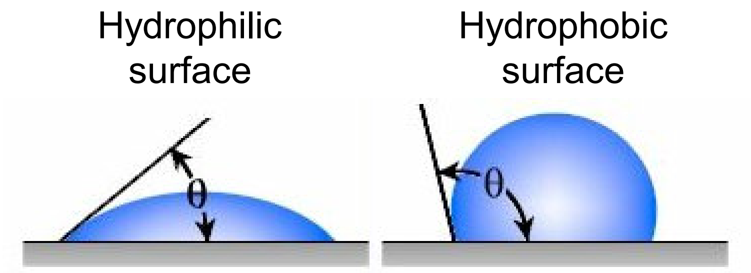
Figure 1. Droplet on a Lotus leaf. Particles adhere not to the leaf surface but to the droplet (Source: Barthlott and Neinhuis 1997).

📖 W. Barthlott, C. Neinhuis, *Planta* **202** (1997) 1-8

"The Lotus Effect" is a registered trademark of STO SE & CO. KGAA (US Registration No. 2613850)

Wettability of a solid surface

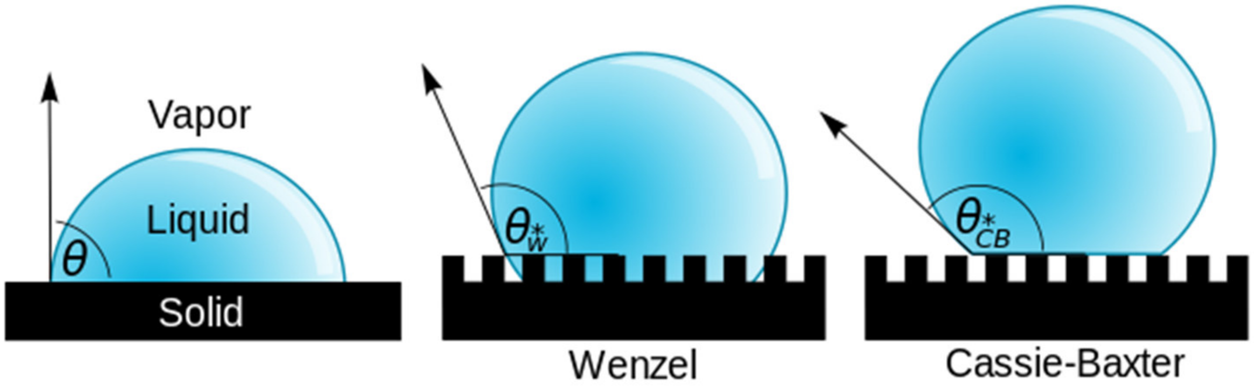
- The wettability is characterized by the **contact angle**



Source: www.ramehart.com/contactangle.htm

*The contact angle θ depends on the **surface energies** of the three phases (gas, liquid, solid)*

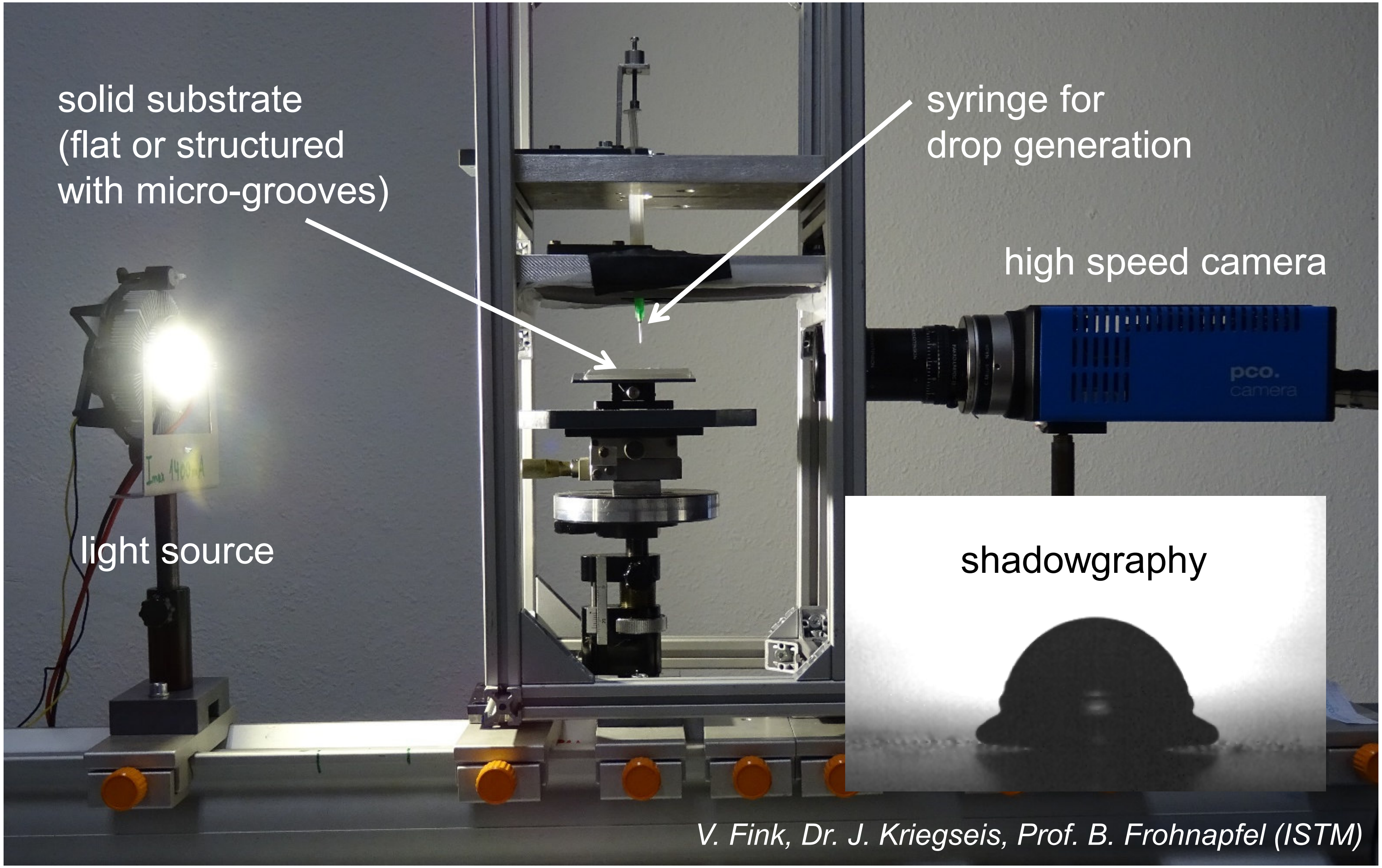
- Surface **roughness** reduces wettability / increases θ



Source: Wikipedia

- Surface structuring for anti-icing, **drag reduction**, etc.

Experiment – setup

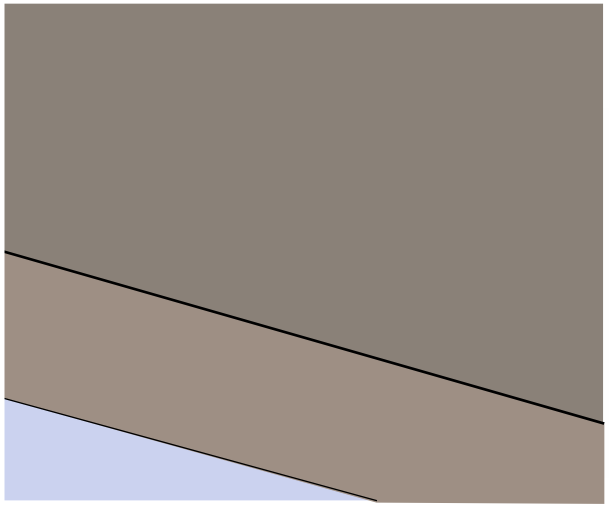


Experiment – impact outcomes

- Hydrophobic PDMS substrate
  - Flat surface: θ = 100.3°, mean roughness depth 0.56 µm
- Water drop with diameter D_0 = 2.1 mm
- Drop impact velocity U_0 = 0.62 m/s (Re = 1300, We = 11)

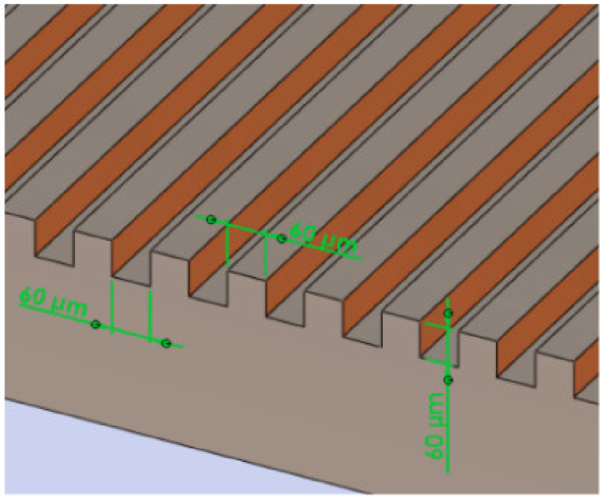
Flat Surface

Deposition



Surface with micro-grooves (60 µm)

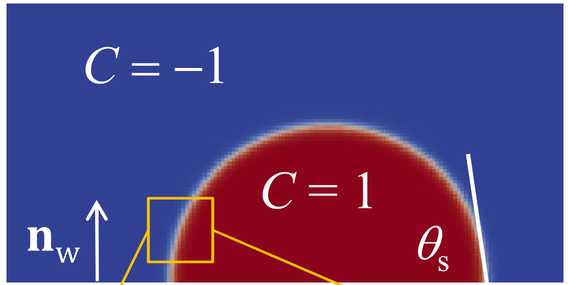
Rebound

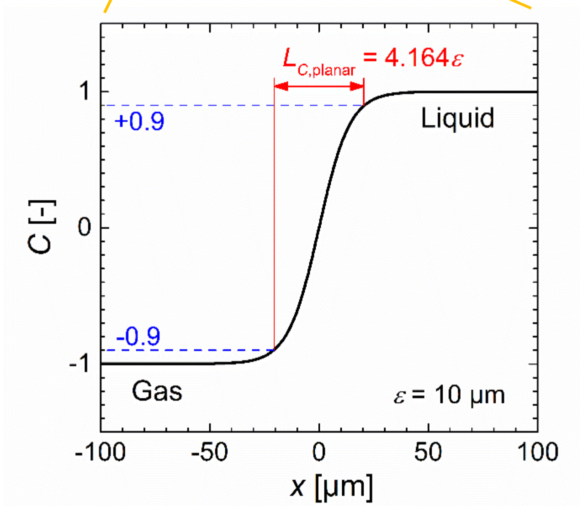


Can this distinct behaviour be reproduced numerically?

Phase field method

- Diffuse interface representation
  - Order parameter $-1 \le C \le 1$
  - Smooth transition layer between phases
  - Interface thickness parameter $\varepsilon > 0$





- Evolution equation for C

$$\frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla) C = M \nabla^2 \phi(C) \qquad \phi = \frac{\lambda}{\varepsilon^2} C(C^2 - 1) - \lambda \nabla^2 C$$

  - ϕ = chemical potential [J/m^3]
  - λ = mixing energy parameter [J/m]
  - M = mobility [m^{3}s/kg]

- Wetting boundary condition
  - θ_s = static (equilibrium) contact angle

$$\mathbf{n}_\mathrm{w} \cdot \nabla C = \frac{1 - C^2}{\sqrt{2}\varepsilon} \cos \theta_\mathrm{s}$$

📖 J.W. Cahn, J.E. Hilliard, *J. Chem. Phys.* **28** (1957) 258–267

Navier-Stokes equations

Karlsruhe Institute of Technology

- Two incompressible Newtonian fluids

$$\nabla \cdot \mathbf{u} = 0$$

$$\partial_t(\rho_C \mathbf{u}) + \nabla \cdot (\rho_C \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu_C \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}} \right) \right] + \rho_C \mathbf{g} + \mathbf{f}_\sigma$$

$$\rho_C = \frac{1+C}{2}\rho_{\mathrm{L}} + \frac{1-C}{2}\rho_{\mathrm{G}}, \quad \mu_C = \frac{1+C}{2}\mu_{\mathrm{L}} + \frac{1-C}{2}\mu_{\mathrm{G}}, \quad \mathbf{f}_\sigma = -C\nabla\phi$$

- Determining the PF method related parameters ε, λ, M
  - Cahn number $Cn = \varepsilon / D_0 \approx 0.01$
    - D_0 = droplet diameter
  - Mixing energy parameter $\lambda = 3\varepsilon\sigma / \sqrt{8}$
  - Mobility parameter $M = \chi\varepsilon^2$
    - Proportionality factor χ [m·s/kg] $\chi = O(0.1-10)$

📖 D. Jacqmin, *J. Comput. Phys.* **155** (1999) 96-127
📖 J. Kim, *Commun. Comput. Phys.* **12** (2012) 613-661

Computer code *phaseFieldFoam*

- Code development
  - Dr. Xuan Cai (KIT)
  - Dr. Holger Marschall (TU Darmstadt)
- Implementation in Open∇FOAM
  - **C++ toolbox** for the development of customized numerical solvers for solution of continuum mechanics problems including **computational fluid mechanics** (CFD)
  - foam-extend-1.6, foam-extend-3.2, foam-extend-4.0
- Validation and application for various test cases
  - Present computations: V. Fink, A. Stroh, R. Bernard

🕮 X. Cai, H. Marschall, M. Wörner, O. Deutschmann, *Chem. Eng. Technol.* **38** (2015) 1985–1992

🕮 X. Cai, M. Wörner, H. Marschall , O. Deutschmann, *Catalysis Today* **273** (2016) 151–160

🕮 X. Cai, M. Wörner, H. Marschall, O. Deutschmann, *Emission Control Science and Technology* **3** (2017) 289-301

Numerical setup

$h = 10\,\mu\text{m}$

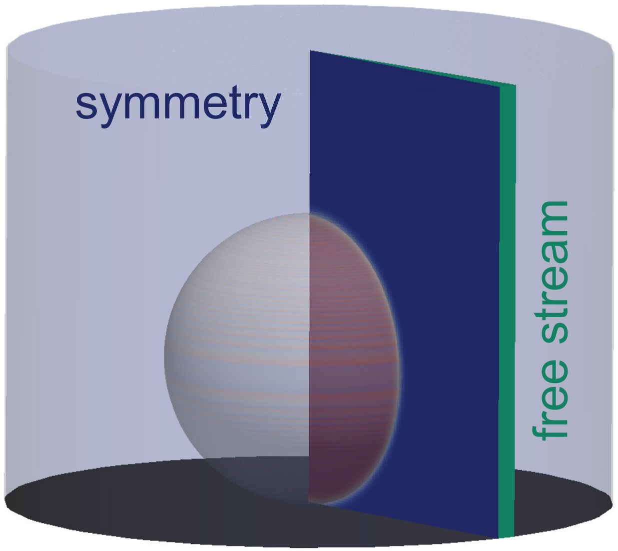
$\varepsilon = 22\,\mu\text{m}$

$\chi = 1\,\text{m} \cdot \text{s/kg}$

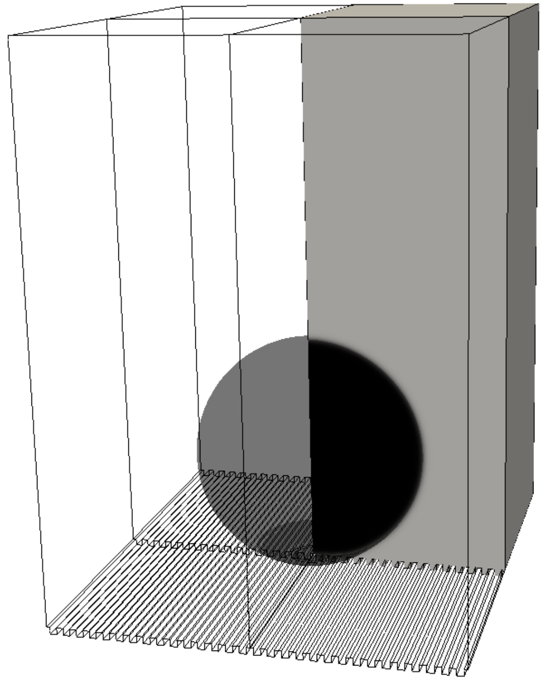
$4\varepsilon / h = 8.8$

$D_0 / h = 210$

$Cn = 0.0105$



no-slip wall, θ_s=100.3°

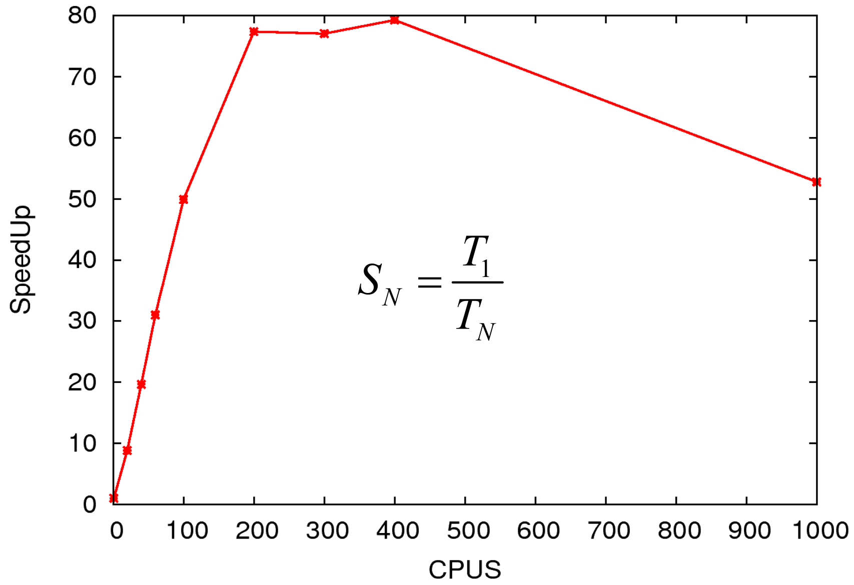


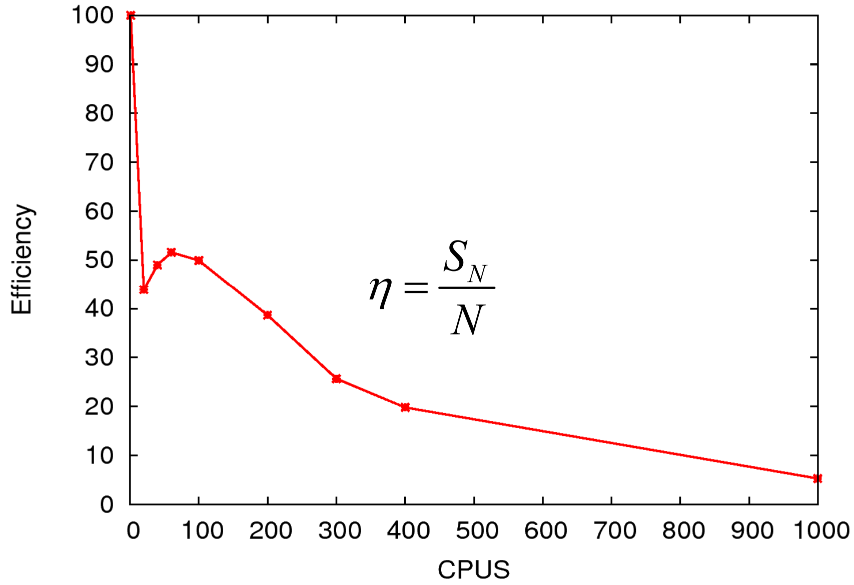
	2D axisymmetric	3D with quarter symmetry
Domain size	$2.1R_0 \times 3.1R_0$	$1.9R_0 \times 1.7R_0 \times 4.8R_0$
No. mesh cells	72,600	18,000,000
No. time steps	10^6	10^7
HPC system	bwUniCluster, ISTM cluster	ForHLR II

Code performance

OpenFOAM 3.2-extend, OpenMPI 1.6.5, Scotch 6.0 domain partitioning library

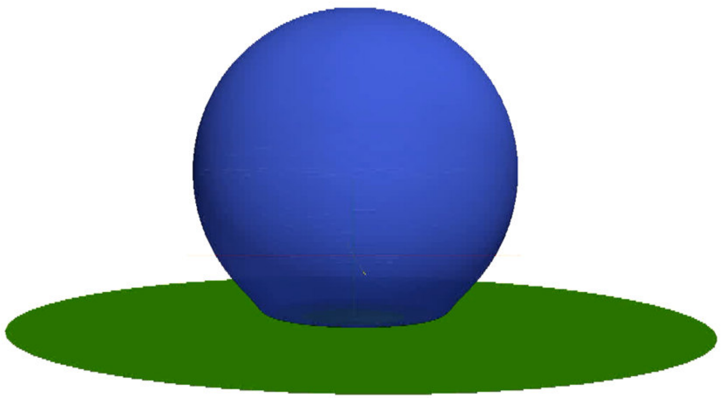
	bwUniCluster	ForHLR II
No. mesh cells	500,000	18,000,000
No. cores	32	500
Time-to-solution	2 days	60 days





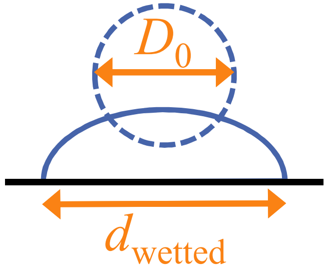
Impact on flat surface (SIM)

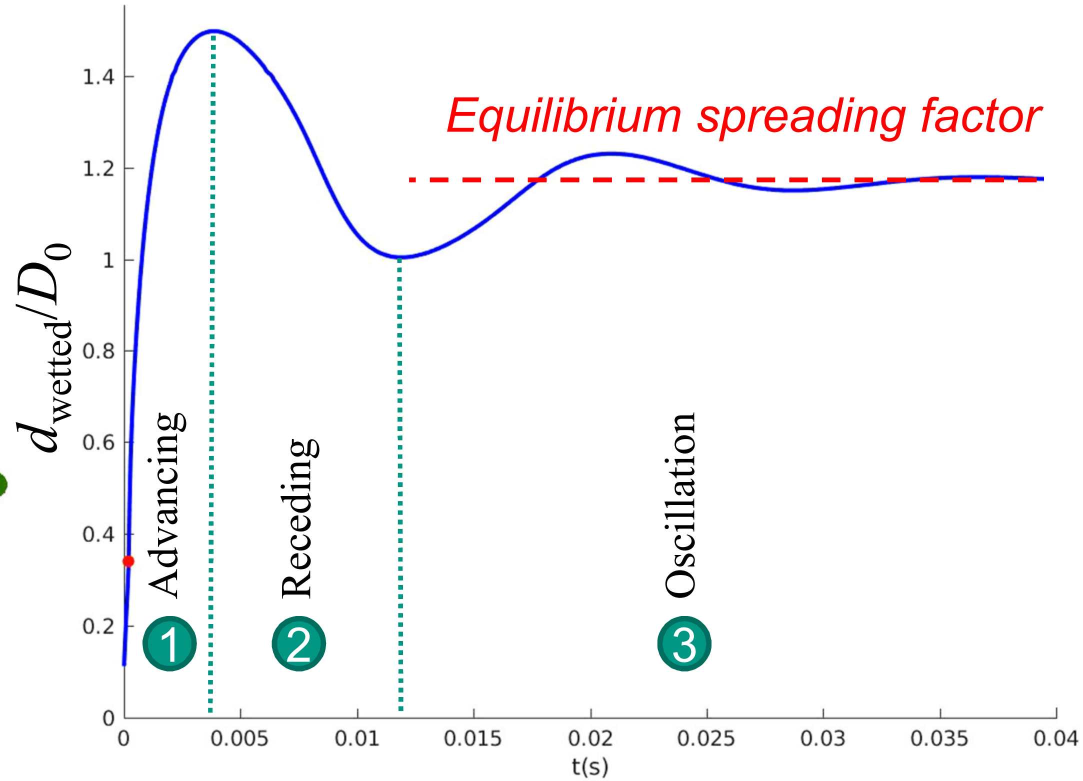
- Drop shape



- Spreading factor

d_{wetted}/D_0



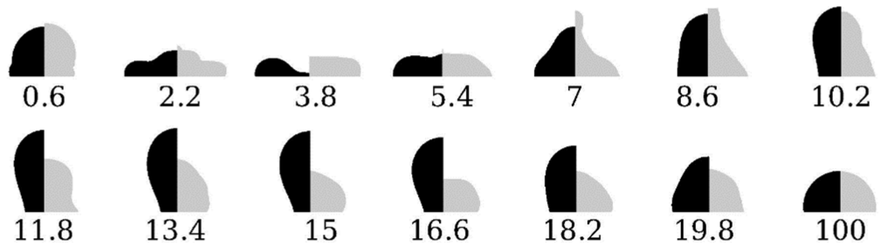


Flat surface – comparison

Simulation

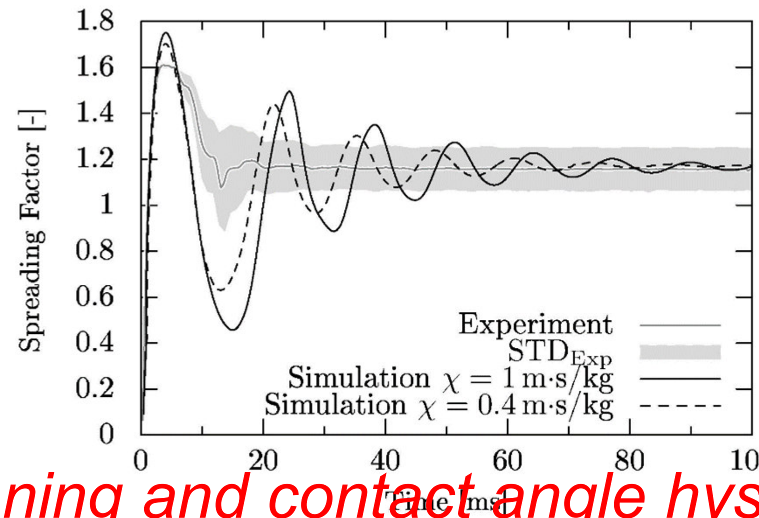
Experiment

- Instantaneous drop shape



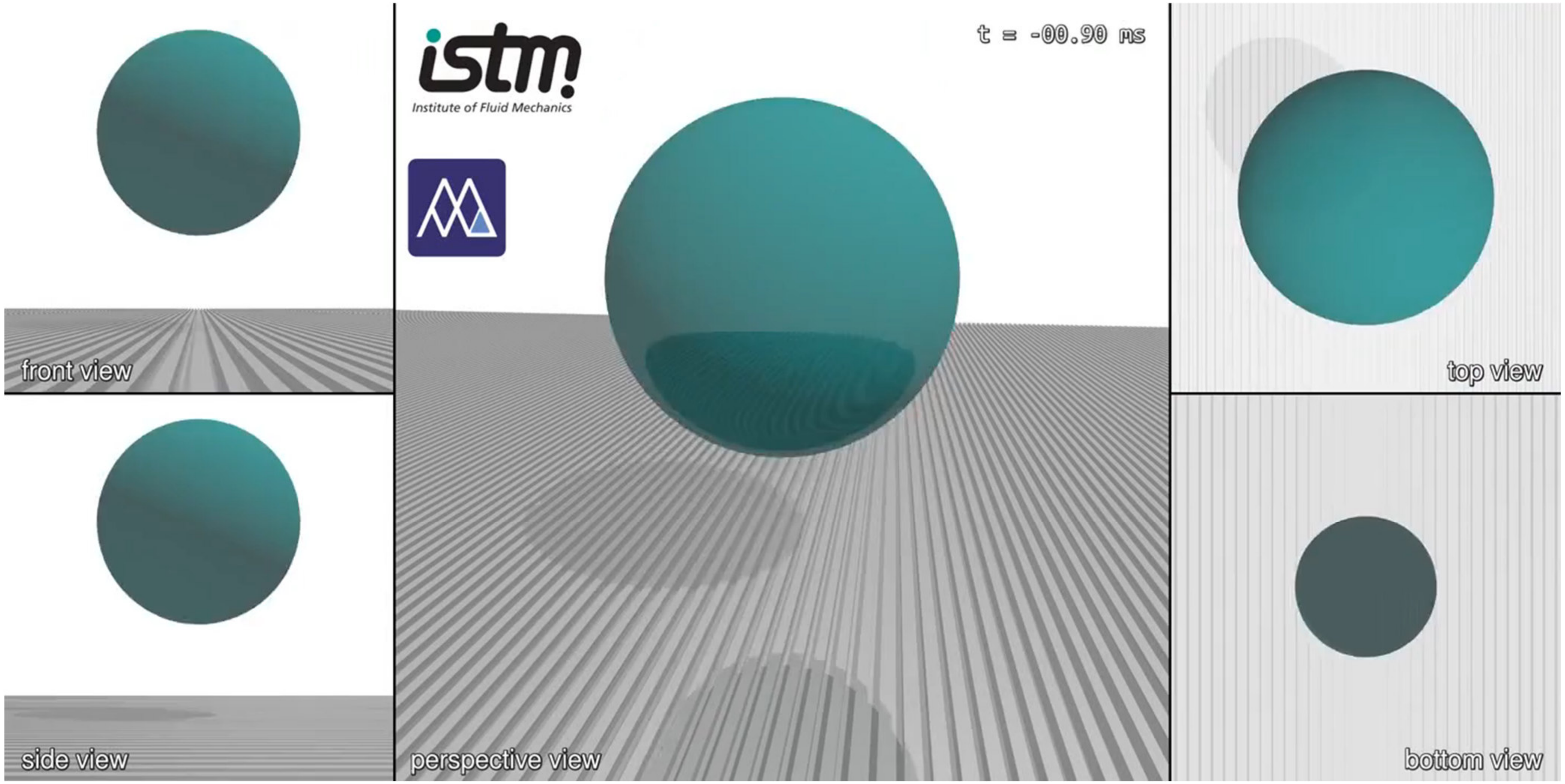
time in milliseconds

- Spreading factor

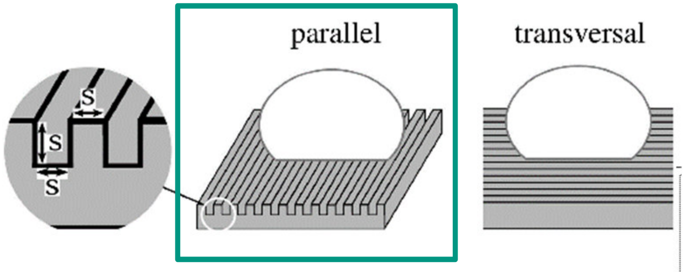


Pinning and contact angle hysteresis

Impact on structured surface (SIM)



Structured surface – comparison



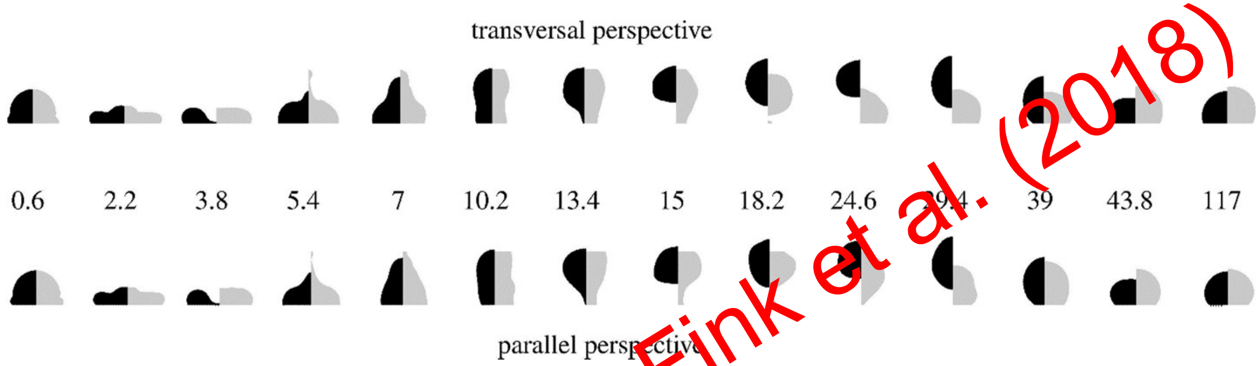
Simulation

Experiment

Structured surface – comparison

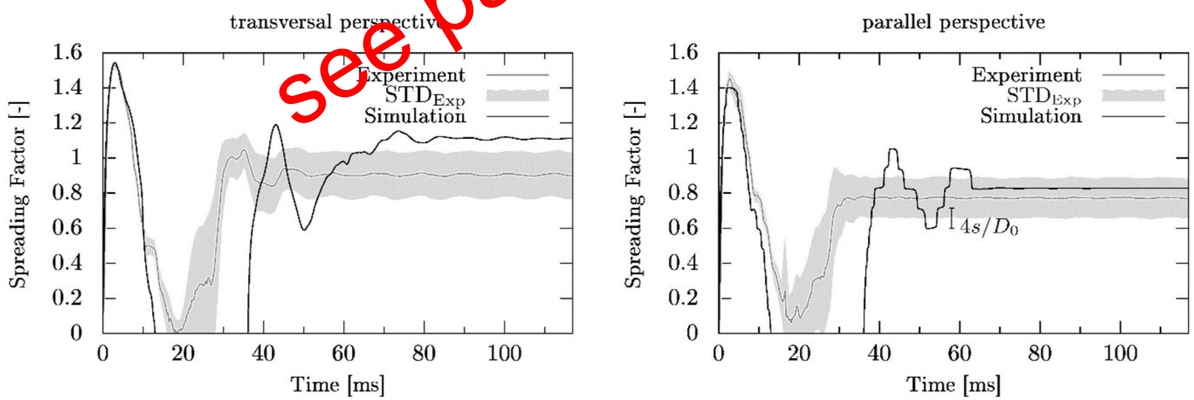
Karlsruhe Institute of Technology

- Instantaneous drop shape



see paper Fink et al. (2018)

- Spreading factor



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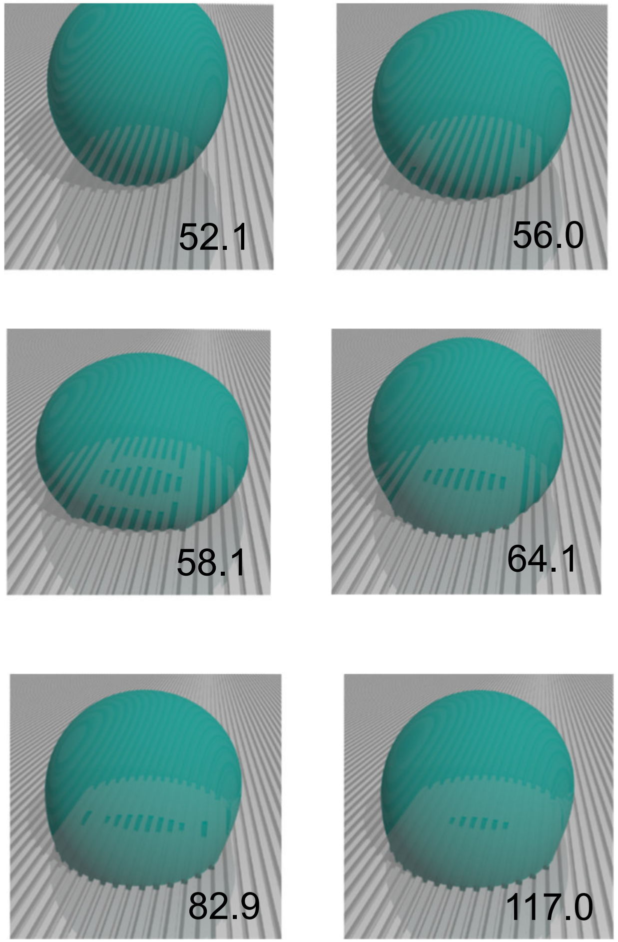
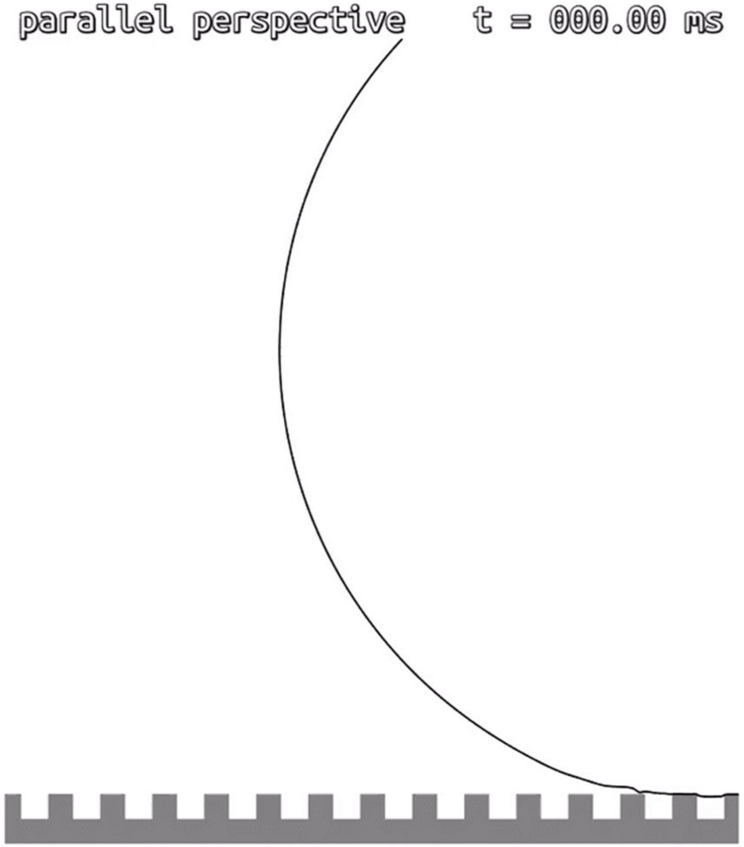
Cassie-Baxter → Wenzel state (SIM)



time in milliseconds

Drop midplane

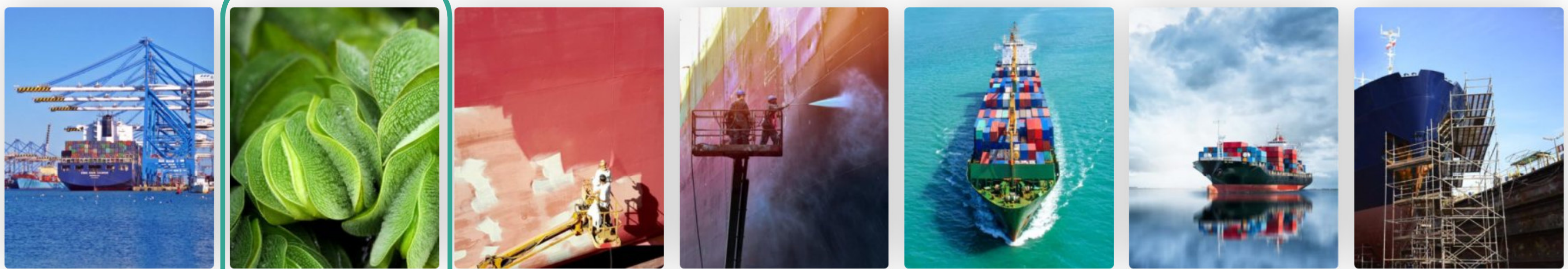


Summary and outlook

- Experiment: drop deposits on flat hydrophobic surface but bounces from surface structured by micro-grooves
- Phase field simulations with **identical parameter set** reproduce different impact outcomes on both surfaces
- Instantaneous drop shape and spreading factor
  - Good agreement for advancing and begin of receding phases
  - Reasons for deviations experiment/simulation at later stages
    - Finite surface roughness in exp. $\leftrightarrow$ ideally smooth surface in simulation
    - Cahn number should be based on groove dimension instead drop diameter
- Further advancement of *phaseFieldFoam*
  - Contact angle hysteresis $\rightarrow$ pinning as observed in experiment
  - Adaptive mesh refinement $\rightarrow$ reduced computational costs

Outlook – drag reduction

- EU project **Air Induced friction Reducing ship COATing**
  - https://aircoat.eu/, started May 2018
  - Passive **air lubrication technology** for ship-coating to reduce energy consumption
  - Inspired by **Salvinia floating fern** which keeps a permanent layer of air under water
  - WP 2 lead by KIT (Prof. Th. Schimmel, AP)



WORK PACKAGE #1	WORK PACKAGE #2	WORK PACKAGE #3	WORK PACKAGE #4	WORK PACKAGE #5	WORK PACKAGE #6	WORK PACKAGE #7
COORDINATION & PROJECT MANAGEMENT	OPTIMISATION OF AIRCOAT SURFACE (SMALL-SCALE)	EXPERIMENTAL & NUMERICAL TESTING (SMALL-SCALE)	AIRCOAT FOIL PRODUCTION PROCESSES (LARGE-SCALE)	DEMONSTRATION OF EFFICIENCY GAIN (LARGE & FULL-SCALE)	ECONOMIC & ENVIRONMENTAL VIABILITY (FULL-SCALE)	COMMUNICATION, DISSEMINATION & EXPLOITATION

Questions?