Direct Numerical Simulations of Gas-liquid Flows in Subdomains of Structured Innovative Multiphase Chemical reactors

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Jahrestreffen der ProcessNet-Fachgruppen Computational Fluid Dynamics, 29.02 – 02.03, 2016, Bingen

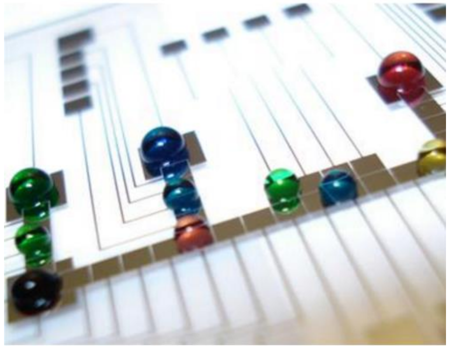
Outline

- Motivation & introduction
- Phase field method and *phaseFieldFoam* in OpenFOAM
- Simulations of single droplet **wetting dynamics**
- Interface-resolving simulations of two-phase flows in **foam structure**
- Simulations of rising bubble in **periodic open-cell structure**
- Summary & outlooks

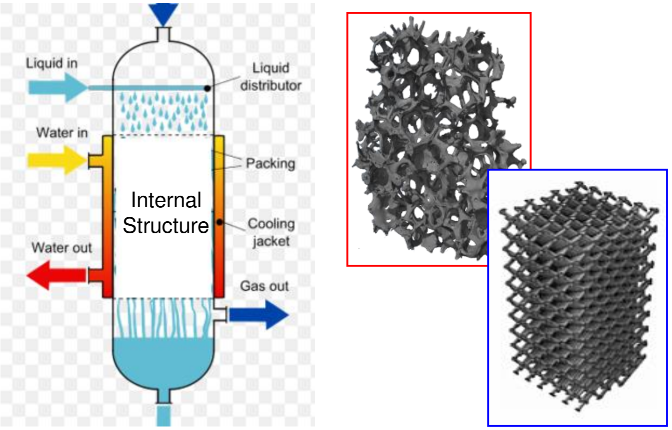
Motivation

- Understanding hydrodynamic interaction of gas-liquid flows with solid surface

Lotus effect
Credit: Wijesena

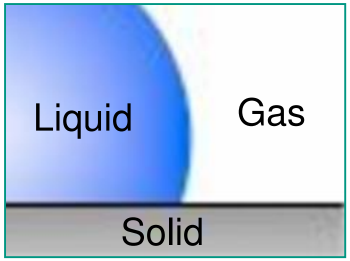


Microfluidic device
Credit: Wheeler



Mulitphase chemical reactor with
structured packings

- Local fluid dynamics features **motion of three-phase contact line**



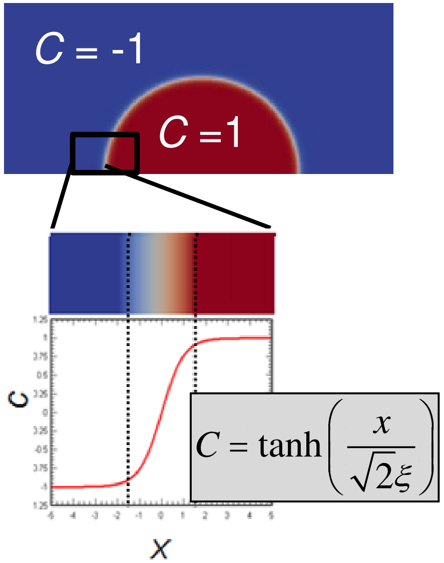
Classical paradox between:
•motion of contact line
•no-slip boundary condition

Volume fraction equation in VOF:

$$\frac{\partial F}{\partial t}+(\mathbf{u}\cdot\nabla)F=0$$

$\mathbf{u}=0$ on wall

Phase Field Method



$$C = \tanh\left(\frac{x}{\sqrt{2}\xi}\right)$$

- Phase field (C) as phase indictor
  - Smooth transition from -1 to 1 → **diffuse interface**
- Cahn-Hilliard equations for phase field evolution

$$\frac{\partial C}{\partial t} + (\mathbf{u}\cdot\nabla)C = \kappa\nabla^2\phi \quad \Longrightarrow$$

describes motion of contact line!

- Wetting boundary condition for static contact angle

$$\hat{\mathbf{n}}_s \cdot \nabla C = \frac{\sqrt{2}}{2}\frac{\cos\theta_e}{\varepsilon}(1 - C^2)$$

κ : mobility parameter
ε : mean-field thickness
Φ: chemical potential

- Single-field Navier-Stokes equation:

$$\rho_C\left(\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \nabla\cdot\left[\mu_C\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right)\right] - C\nabla\phi + \rho_C\mathbf{g}$$

- Mixture density and viscosity $\rho_C = \frac{1+C}{2}\rho_{\mathrm{L}} + \frac{1-C}{2}\rho_{\mathrm{G}} \quad \mu_C = \frac{1+C}{2}\mu_{\mathrm{L}} + \frac{1-C}{2}\mu_{\mathrm{G}}$

Numerical implementation and verification

- Phase field method is implemented in OpenFOAM (foam-extend-1.6 and 3.2)
  - As a novel top-level OpenFOAM solver ***phaseFieldFoam*** [1]
- Verification by a series of test cases against analytical solutions [2]

[1] H. Marschall, X. Cai, M. Wörner. **2016**, in preparation
[2] X. Cai, H. Marschall, M. Wörner and O. Deutschmann, *Chem. Eng. Technol.* **2015**, 38: 1985–1992

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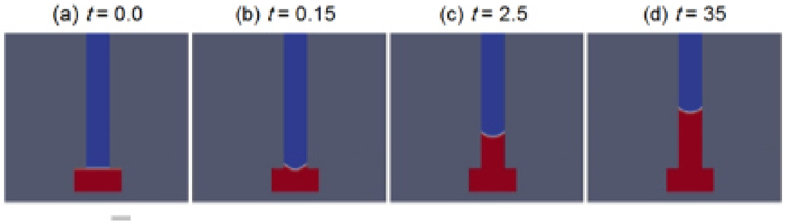
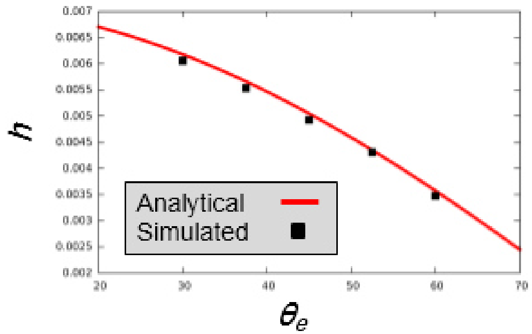
Capillary rise of liquid in narrow channel


(a) $t = 0.0$ (b) $t = 0.15$ (c) $t = 2.5$ (d) $t = 35$

Final column height VS. static contact angle



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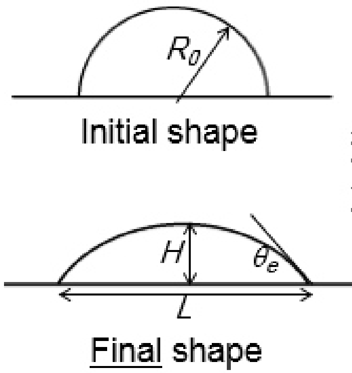
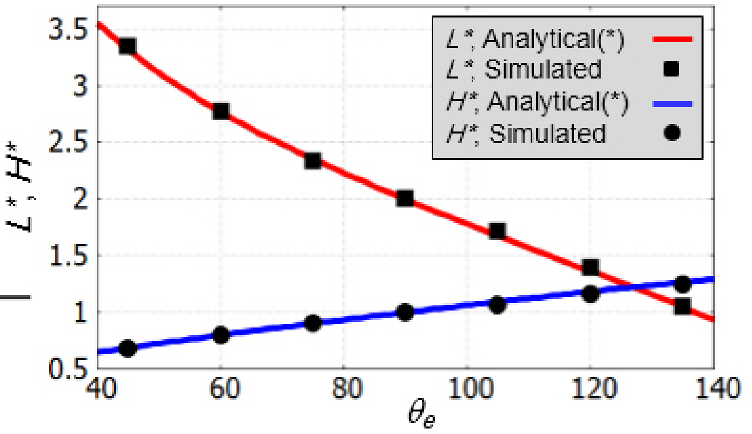
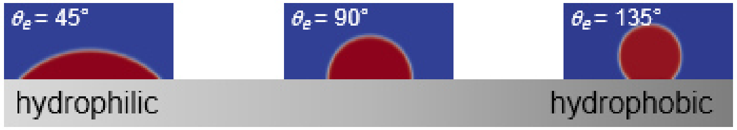
Capillary-driven wetting/dewetting of droplets





$L^* = L / R_0$
$H^* = H / R_0$



(*) Chen et al. 2009

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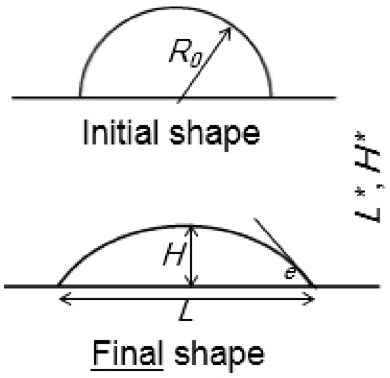
Gravitational effect on wetting droplet



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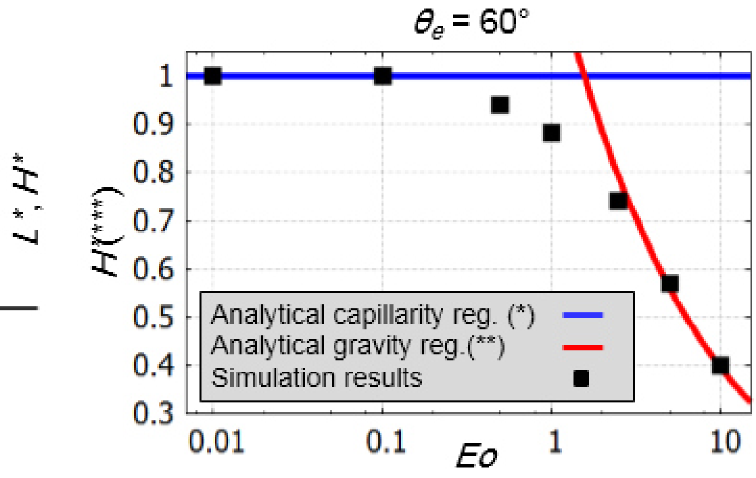

(*)Chen et al. 2009 (**)Dupont et al. 2007 (***) H': normalized height of droplet

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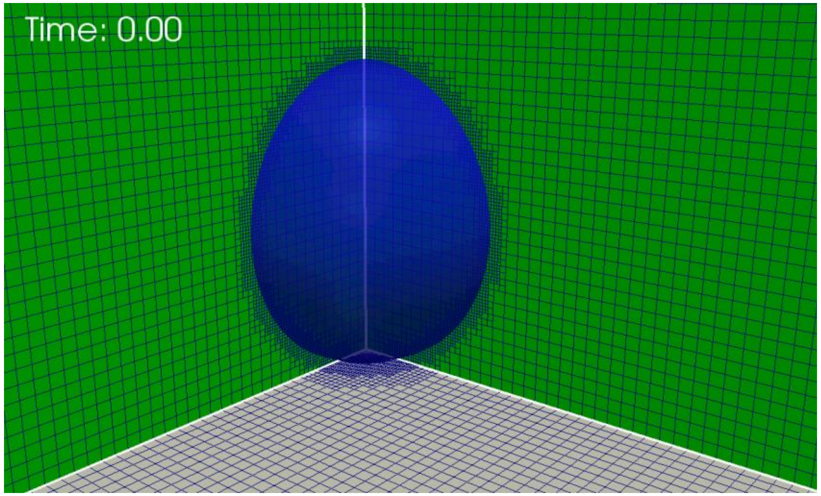
Single droplet wetting dynamics

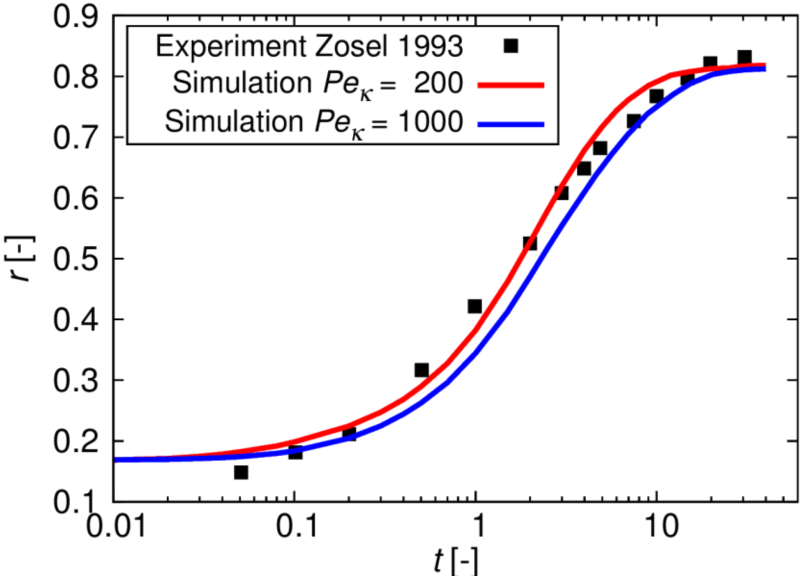
- Viscous droplet spreading

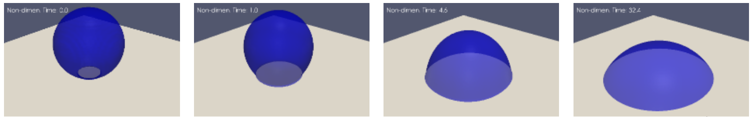
- Experiment by Zosel 1993
  - Diameter ≈ 3 mm
  - PIB solution μ = 25 pa·s
  - on smooth flat PTFE surface (θ_e = 58º)



Droplet spreading on flat surface
3D adaptive mesh refinement

Droplet base radius over time





time

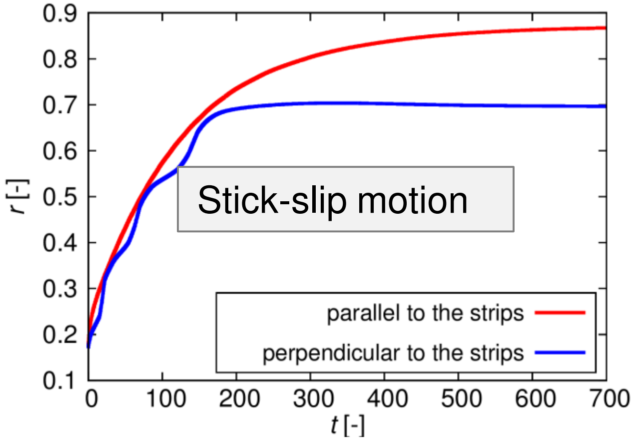
Reference: X. Cai, H. Marschall, M. Wörner and O. Deutschmann, *Chem. Eng. Technol.* **2015**, 38: 1985–1992

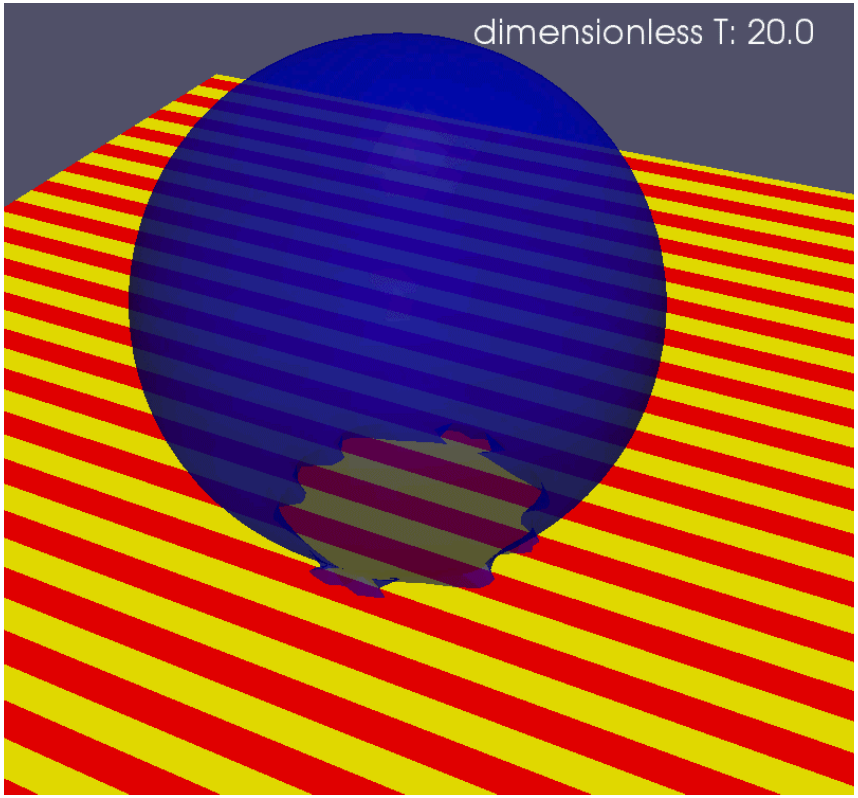
Single droplet wetting dynamics

- Droplet spreading on chemically-heterogeneous surface

- Experiment by Jansen et al. 2013
  - Glycerin droplet volume = 3 *m*L
  - Alternating stripes made of

SiO_2,	$\theta_e = 40°$
PFDTS,	$\theta_e = 106°$


Stick-slip motion



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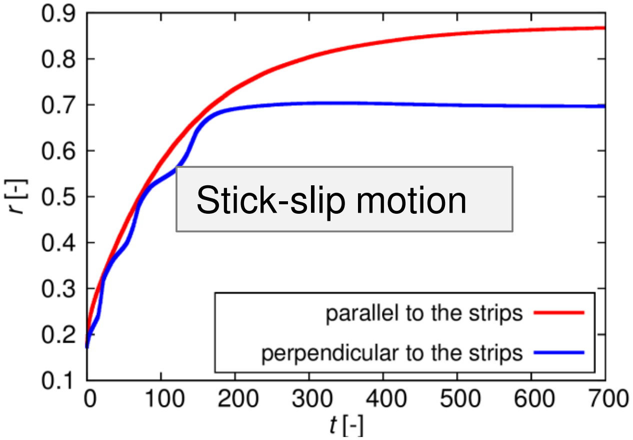

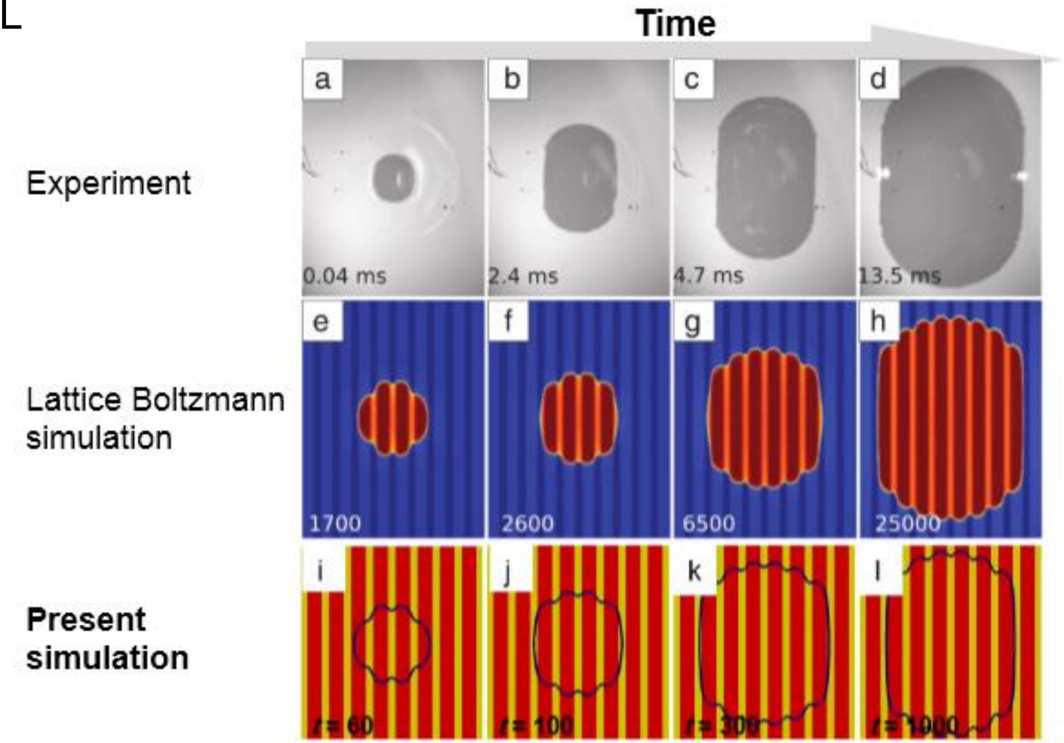

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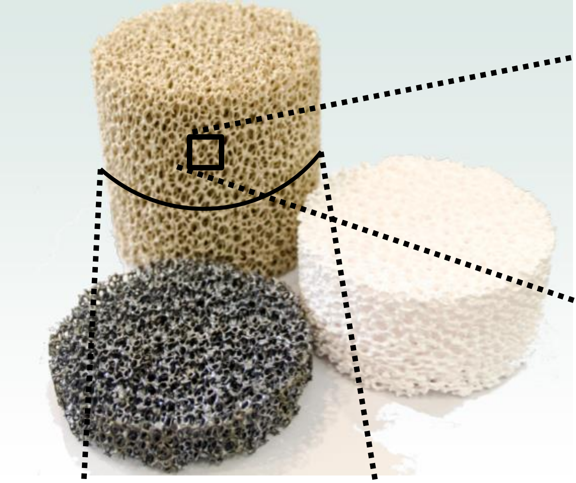
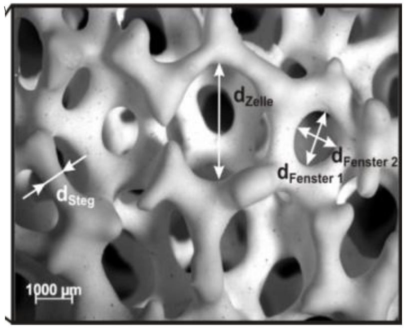
Interface-resolving for Two-phase Flow in Sponge

- Motivation of DNS
  - Characterization of local interfacial phenomena
  - Providing closure for Euler-Euler simulation

<u>Interface-resolving</u> for Two-phase Flow in Sponge

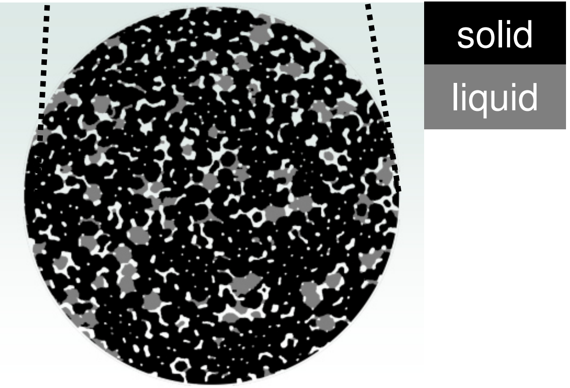
- Motivation of DNS
  - Characterization of local interfacial phenomena
  - Providing closure for Euler-Euler simulation
- Total Foam structure
  - Height: 25 – 100 mm
  - Φ: 100 mm
- Individual liquid jets
  - Approx. 1 – 10 mm
- Local gas-liquid interface
  - Approx. 0.1 – 1 mm
- **Disparity of length scale up to 10^2 or 10^3!**



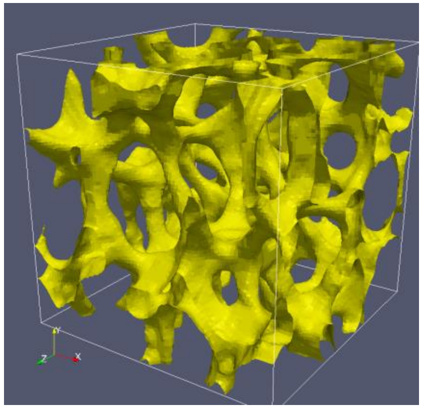


Representative Elementary Vol.

(µ)CT & Reconstruction
S. Meinicke, KIT-TVT



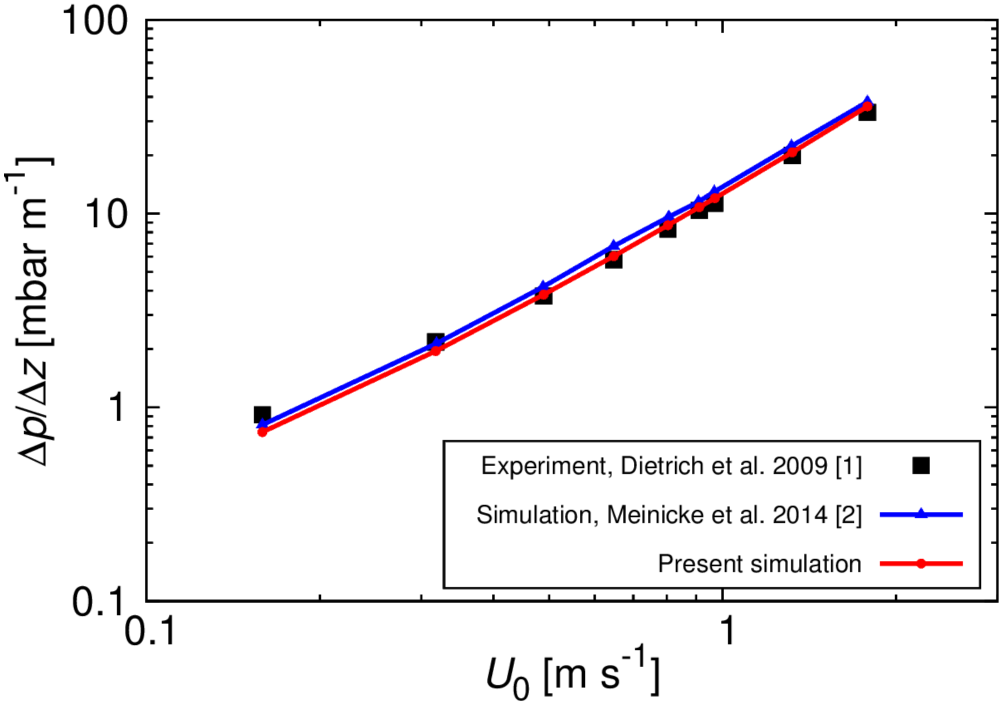
Source: Wallenstein et al. 2015



STL geometry for CFD

Validation for Hydrodynamics of Gas Flow

- Apply the solver for gas flow through sponge structure
- Compare simulated pressure drop versus superficial velocity against:
  - experimental results (Dietrich et al. 2009*)
  - CFD results using “simpleFoam” (Meinicke et al. 2014**)



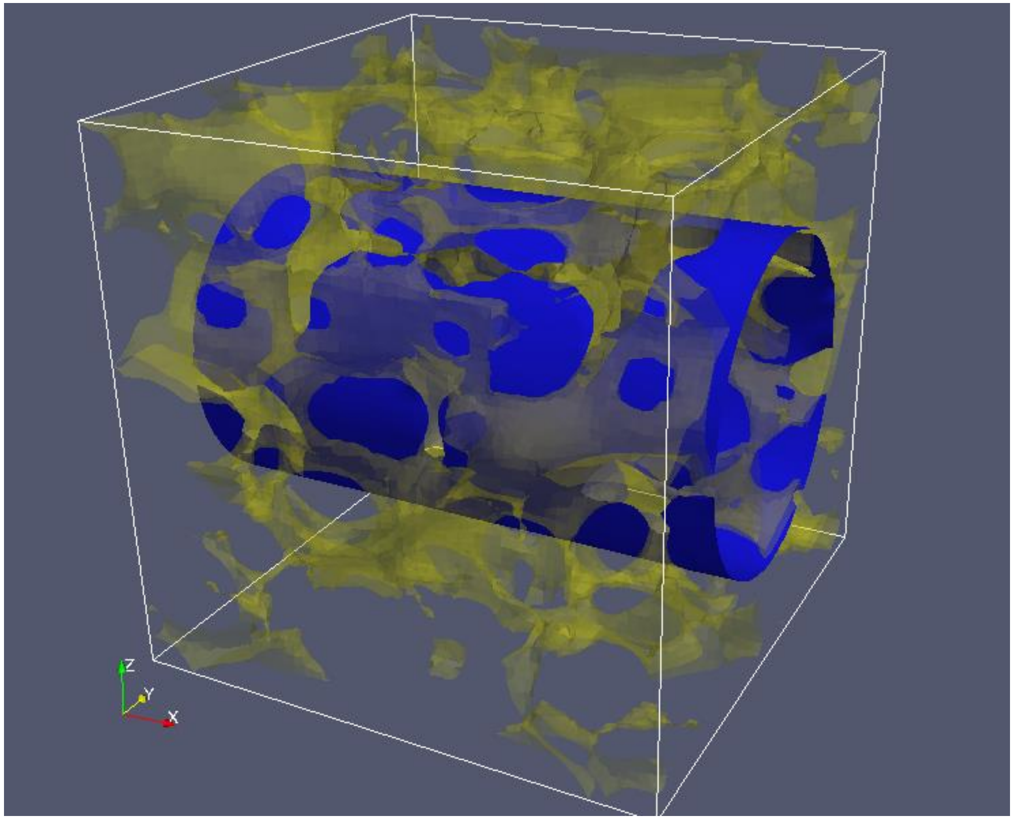
- U_0: superficial gas velocity
- $\Delta p / \Delta z$: pressure drop per unit length

[1] B. Dietrich, W. Schabel, M. Kind, H. Martin. Pressure Drop Measurements of Ceramic Sponges - Determining the Hydraulic Diameter. Chem. Eng. Sci. 64 (16), 3633-3640. 2009

[2] S. Meinicke, Th. Wetzel, B. Dietrich. CFD modelling of single-phase hydrodynamics and heat transfer in solid sponges, 11th Int. Conf. on CFD in the Minerals & Proc. Industries, Conference Proceedings, Melbourne, 2015

Interface-resolving for Two-phase Flow in Sponge

- REV → difficult to get inlet liquid distribution from exp.
- Mirroring geometry + periodic boundary conditions



SiSiC foam, 20 ppi, 85% porosity

Interface-resolving for Two-phase Flow in Sponge

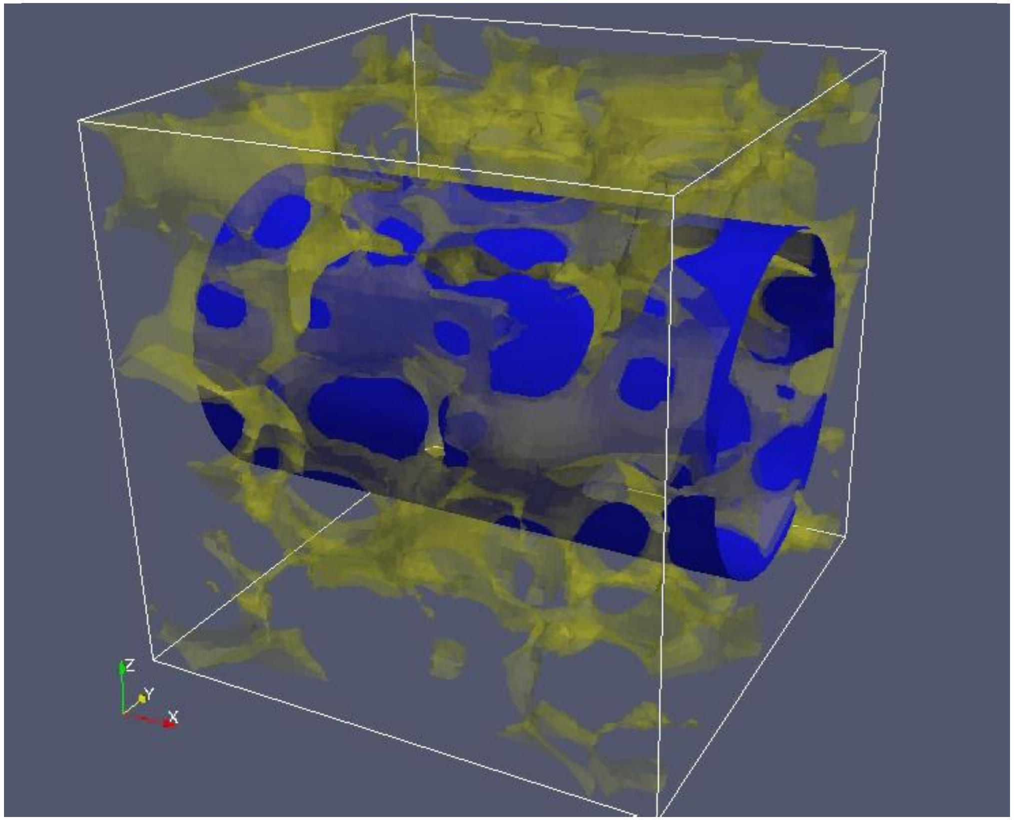
- Conventionally:
  inlet flow rate → pressure drop

- **In current periodic domain:**
  pressure drop → inlet/domain flow rate

$$p \equiv P - \frac{\overline{p_0} - \overline{p_{L_x}}}{L_x} \cdot \mathbf{x} = P - \mathbf{f}_x \cdot \mathbf{x}$$

$$-\nabla p = -\nabla P + \mathbf{f}_x$$

- Input to DNS:
  - liquid saturation *ß*
  - Pressure drop $\Delta p/\Delta x$
- Output from DNS
  - gas-liquid interfacial area
  - Providing closure for Euler-Euler (future steps)

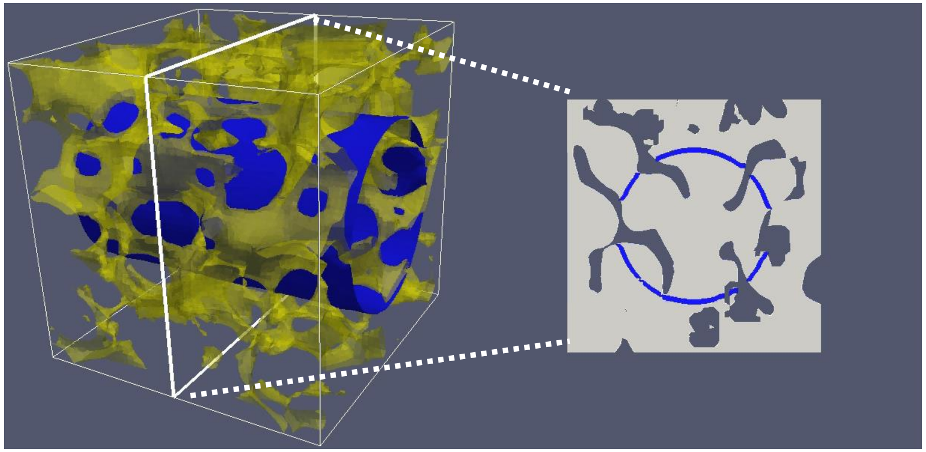


SiSiC foam, 20 ppi, 85% porosity

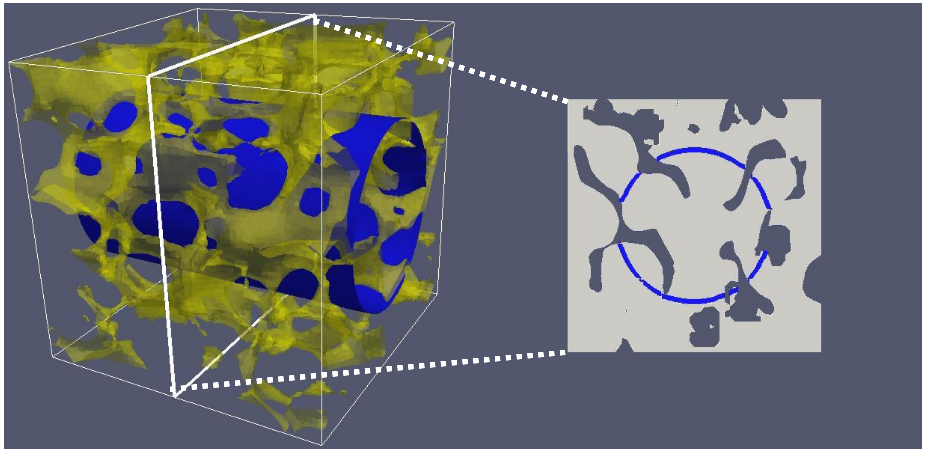
Interface-resolving for Two-phase Flow in Sponge

- Effect of equilibrium contact angle wettability
- Air-water on SiSiC

θ_e = 20° - 80°



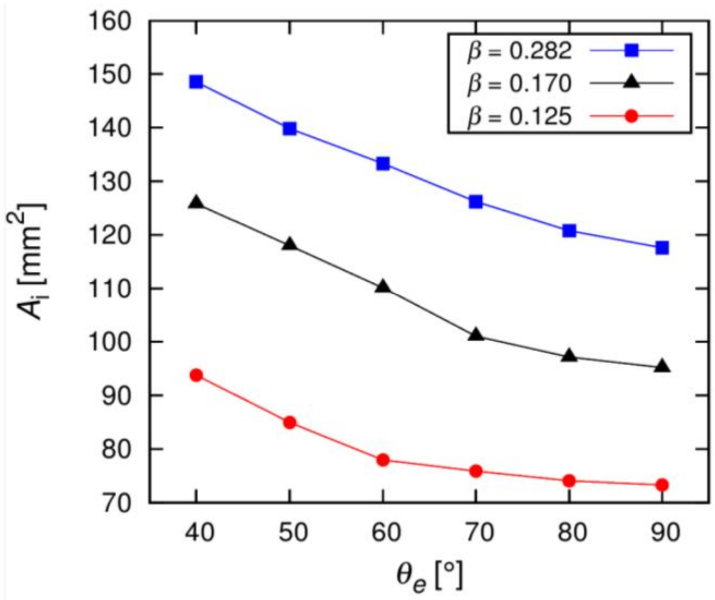
θ_e = 40°



θ_e = 80°

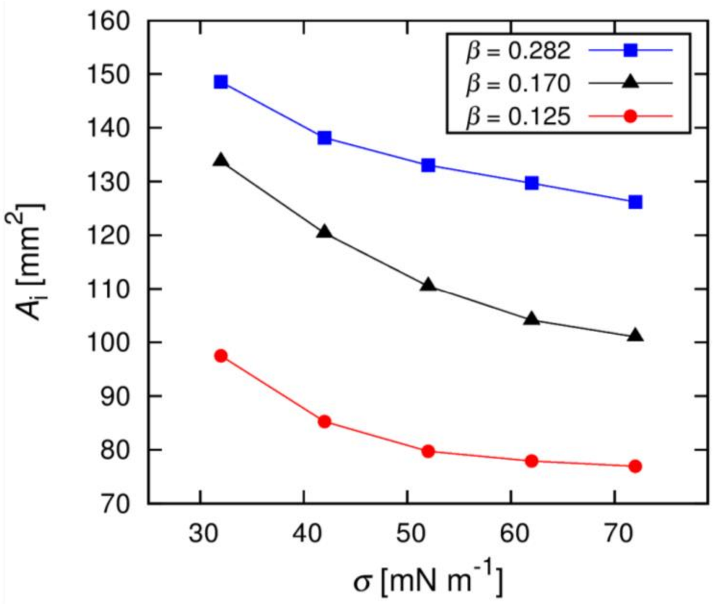
Interface-resolving for Two-phase Flow in Sponge

Effect of Solid Surface wettability



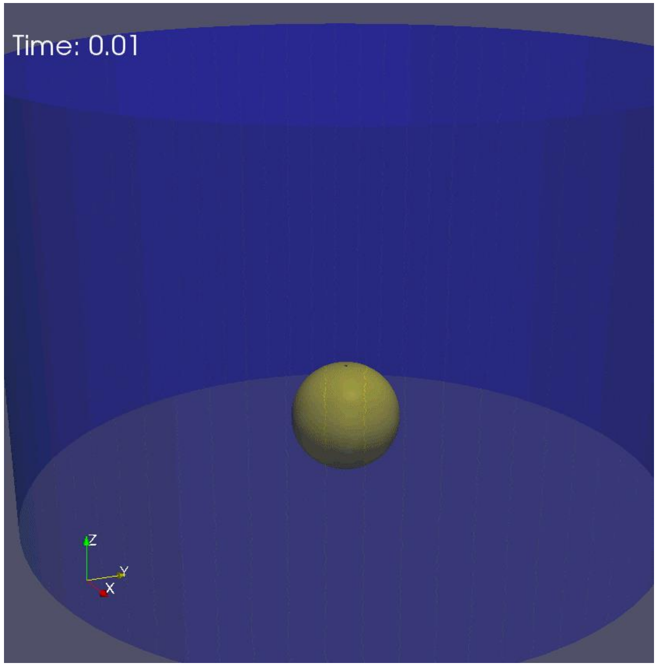
Gas-liquid interfacial area A_i vs. contact angle θ_e for different liquid saturation β

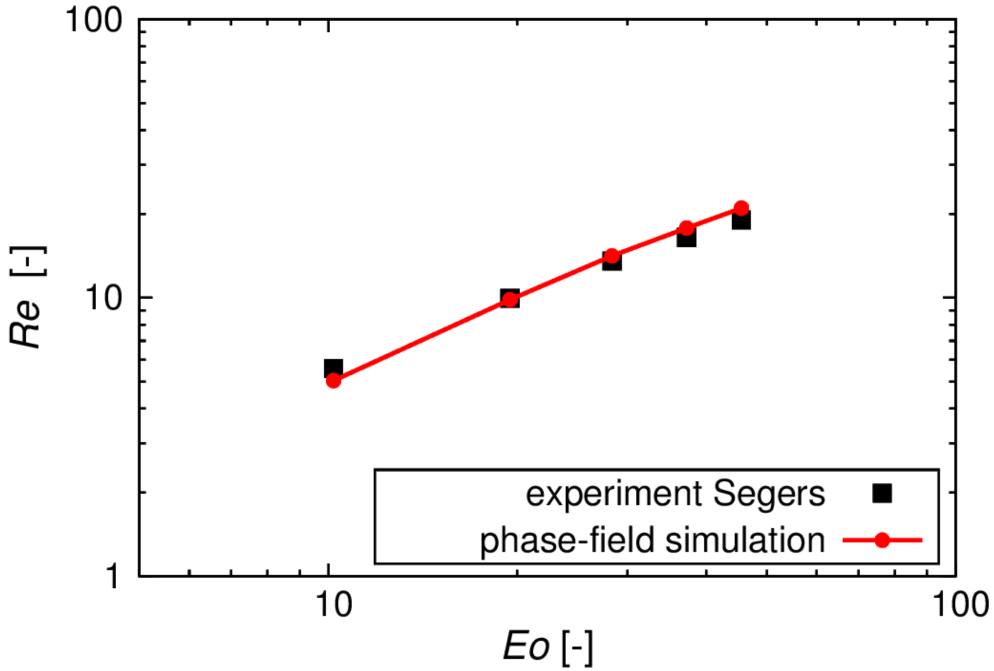
Effect of interfacial tension



Gas-liquid interfacial area A_i vs. contact angle θ_e for different liquid saturation β

Validation for bubble terminal rise velocity





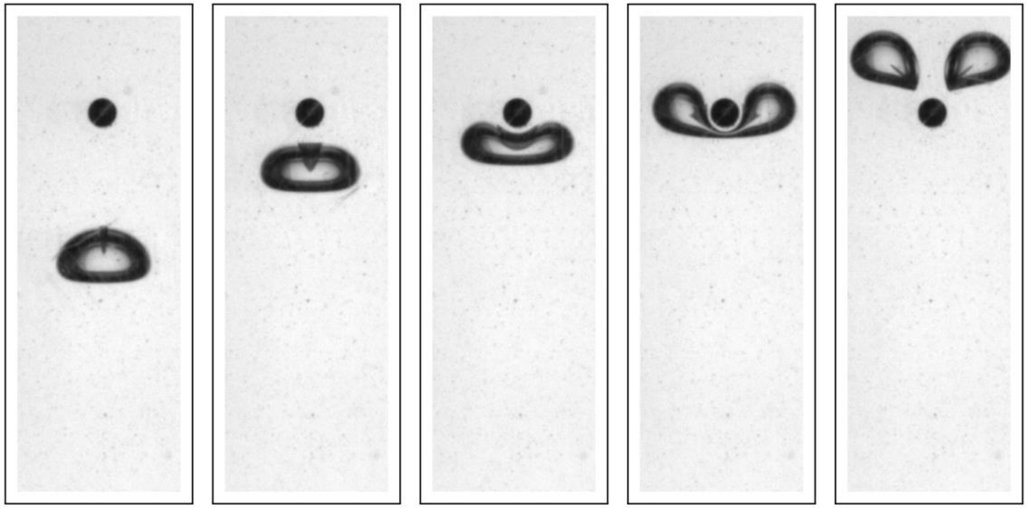
- Air bubble rising glycerin liquid
- **Morton number = 0.064**

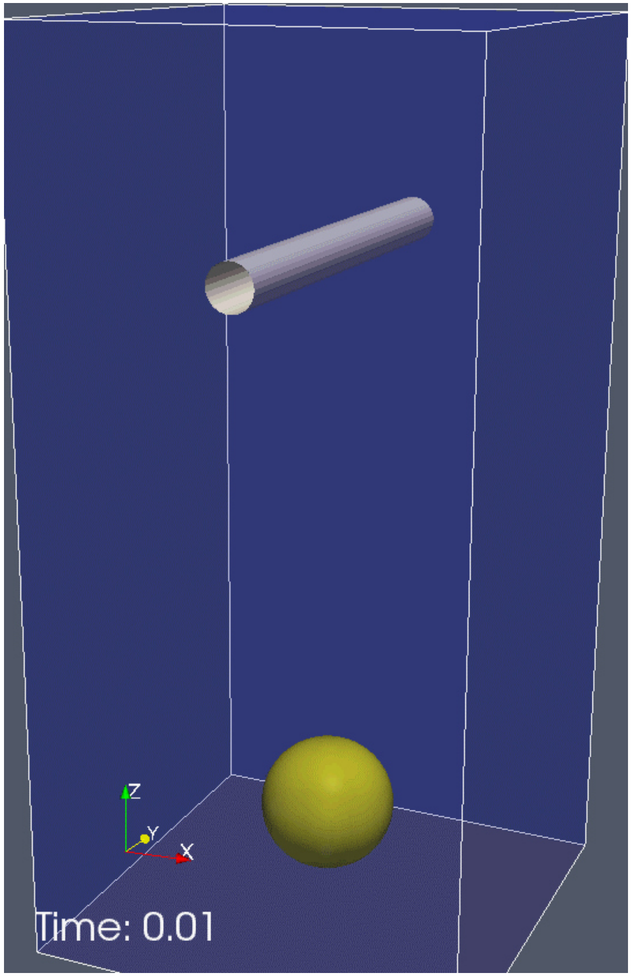
- Re = $\rho U D / \mu$
- Eo = $\Delta \rho g D^2 / \sigma$

- U : terminal velocity
- D : bubble diameter

Validation on cylinder-induced bubble breakup

- Experiment from Segers PhD thesis 2015
  (Group of Prof. Kuipers and Prof. Deen, TU Eindhoven)



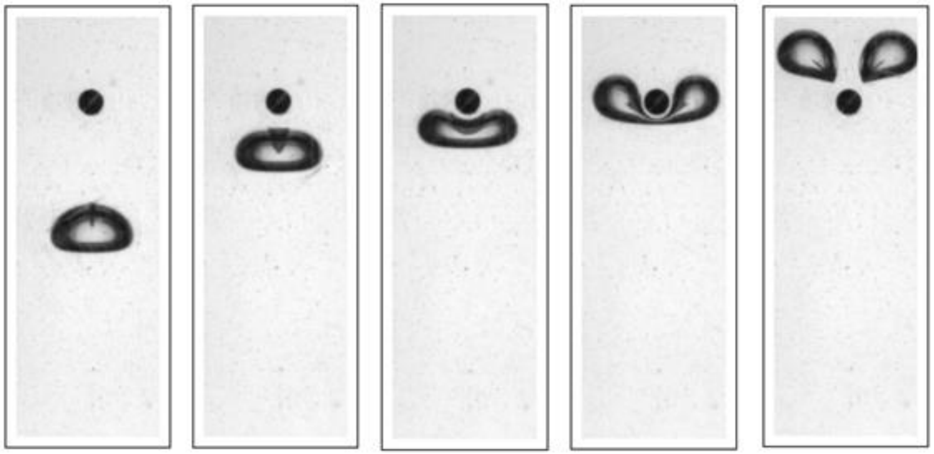


- Cross-sectional diameter of cylinder = 3.1 mm
- Equivalent diameter of bubble = 9.1 mm

Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2015**, submitted

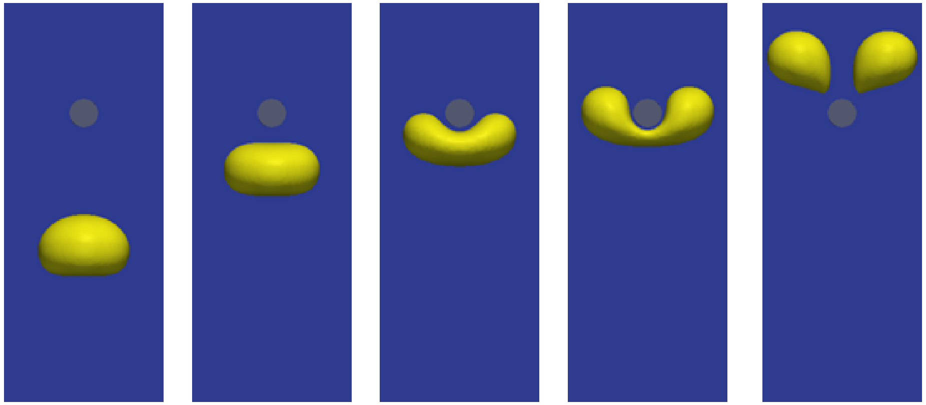
Validation on cylinder-induced bubble breakup

Experiment Segers
stainless steel cylinder



(a) 0 s (b) 0.065 s (c) 0.09 s (d) 0.13 s (e) 0.18 s

Phase-field Simulation
θ_e = 60°



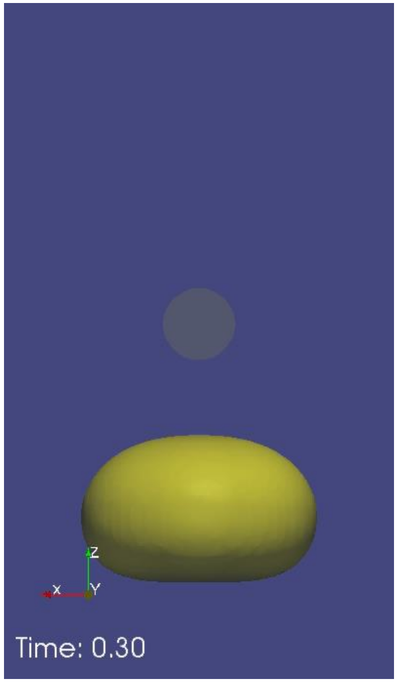
(f) 0 s (g) 0.08 s (h) 0.105 s (i) 0.153 s (j) 0.21 s

Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2015**, submitted

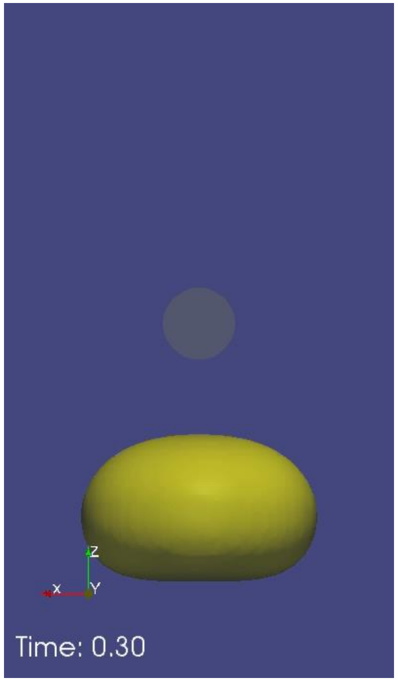
Validation on cylinder-induced bubble breakup

- Effect of surface wettability

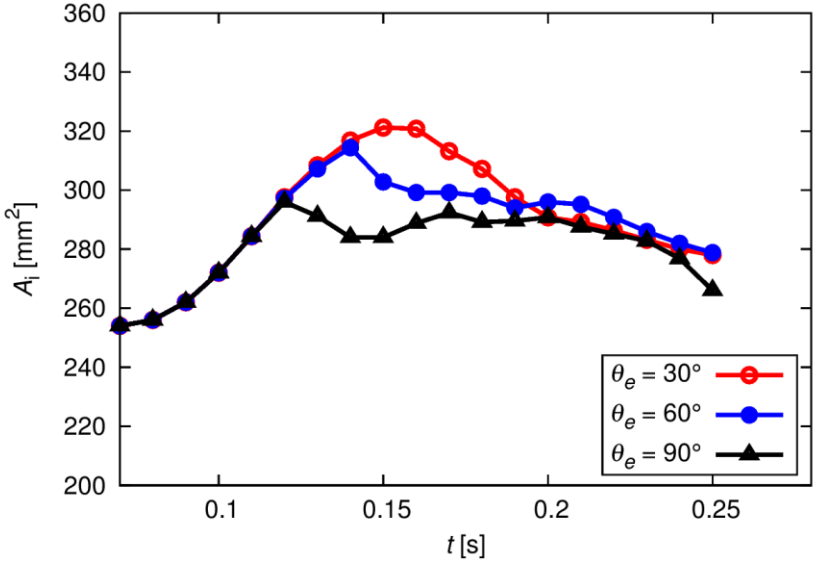
$\theta_e = 30°$



$\theta_e = 90°$



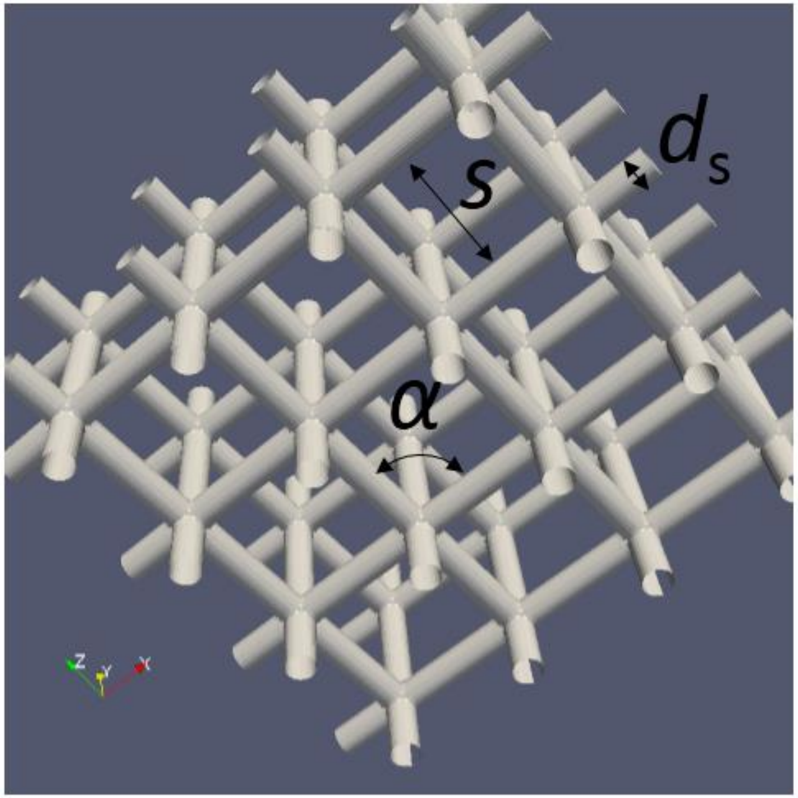
Time evolution of bubble surface area A_i



Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2015**, submitted

Periodic Open Cell Structure (POCS)

- SEBM-manufactured by FAU Erlangen(*) (Prof. W. Schwieger, Prof. H. Freund)
- STL geometry for CFD provided by C.O. Möller, TUHH (Prof. M. Schlüter)
- Geometry parameters
  - Window size *s* = 4 mm
  - Strut diameter d_s = 1 mm
  - Grid angle = 90°

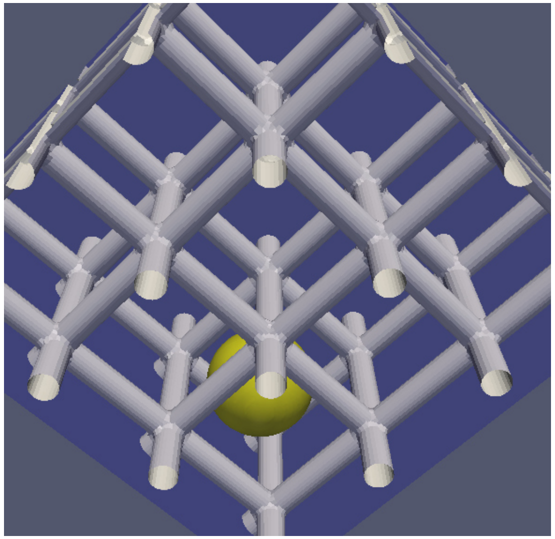


(*) M. Klumpp, A. Inayat, J. Schwerdtfeger, C. Körner, R.F. Singer, H. Freund, W. Schwieger, *Chem Eng J*, 242 (2014) 364-378.

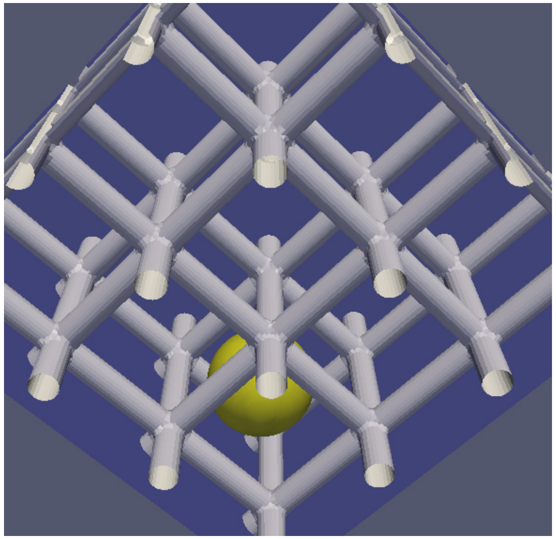
Bubble Rising in Periodic Open Cell Structure

- Air bubble ($D = 4$ mm) rising in quiescent water within a titled POCS

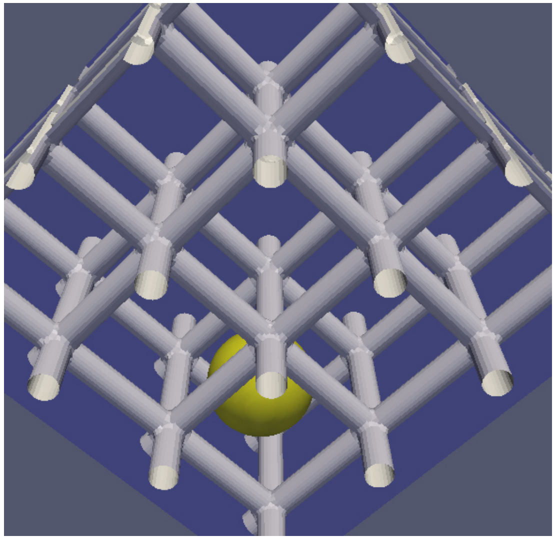
$\theta_e = 0°$



$\theta_e = 90°$



$\theta_e = 120°$



decreasing wettability (increasing contact angle) →

Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2015**, submitted

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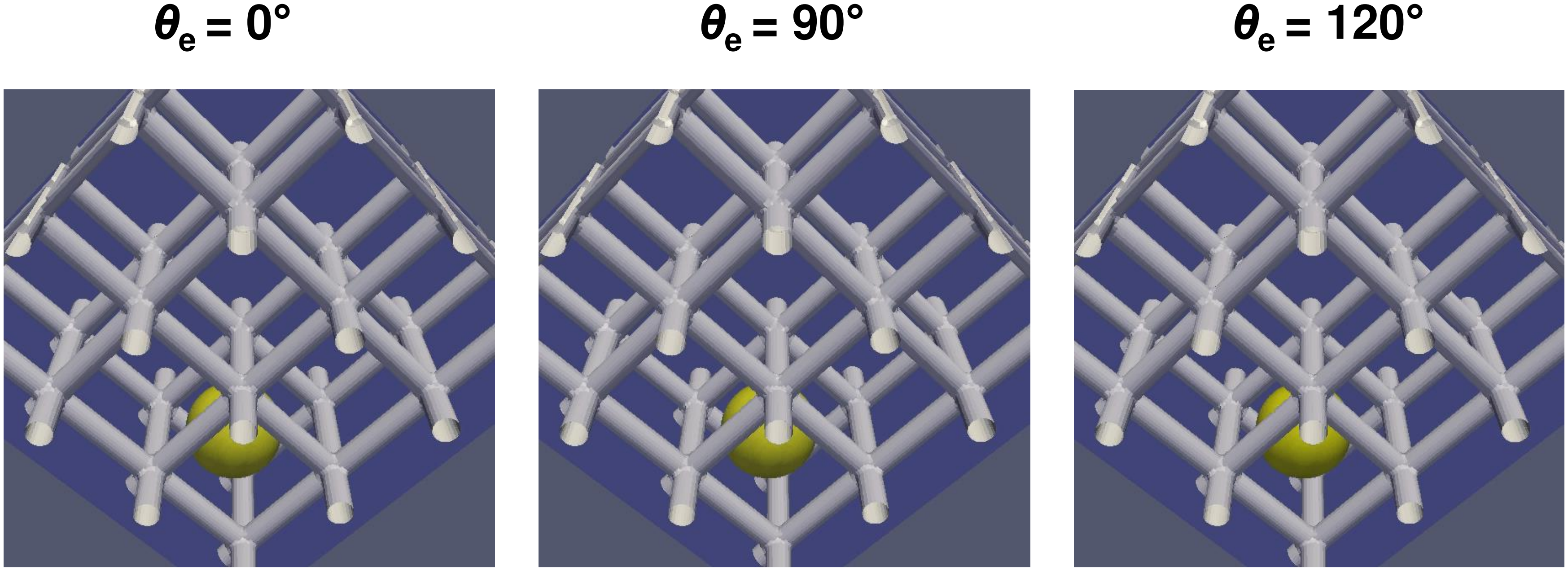

decreasing wettability (increasing contact angle)

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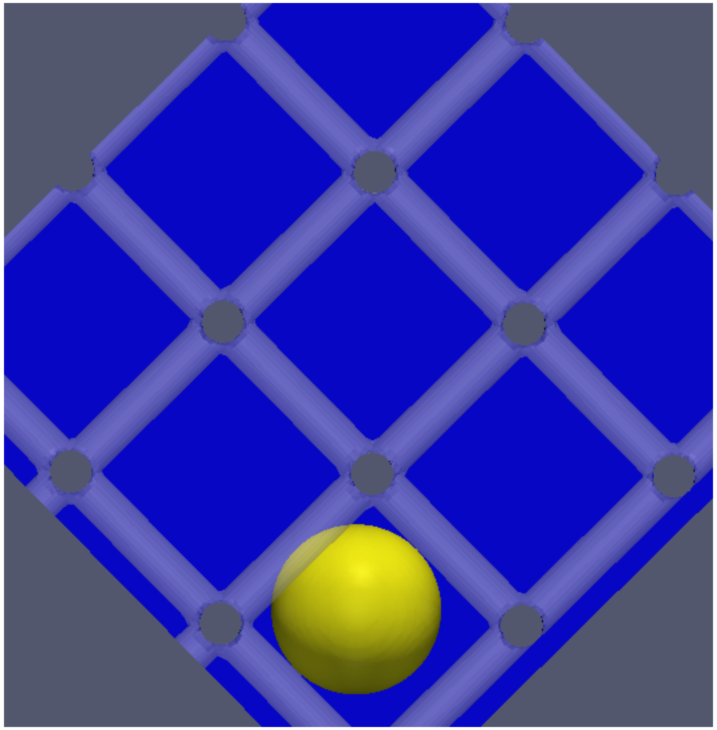
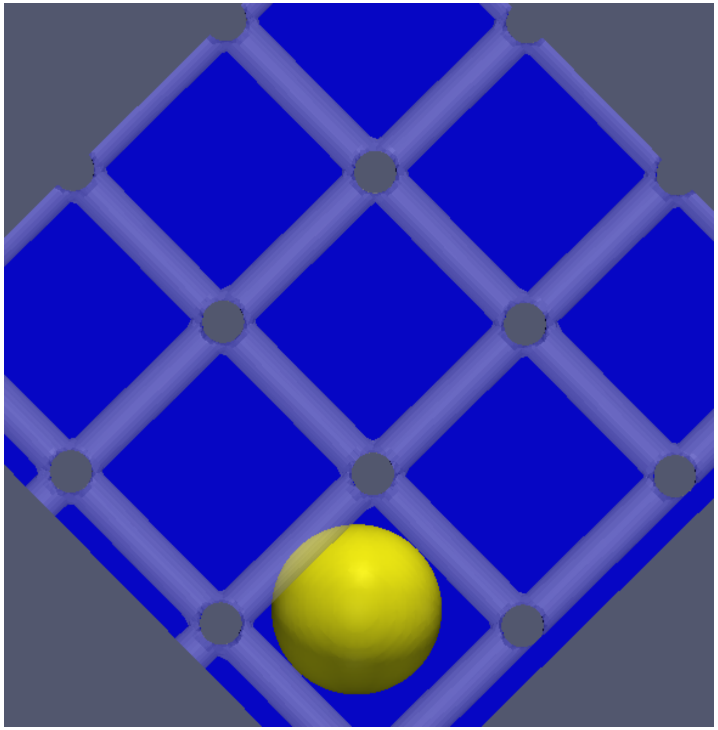
Bubble Rising in Periodic Open Cell Structure

- 2D lateral view



$\theta_e = 0°$



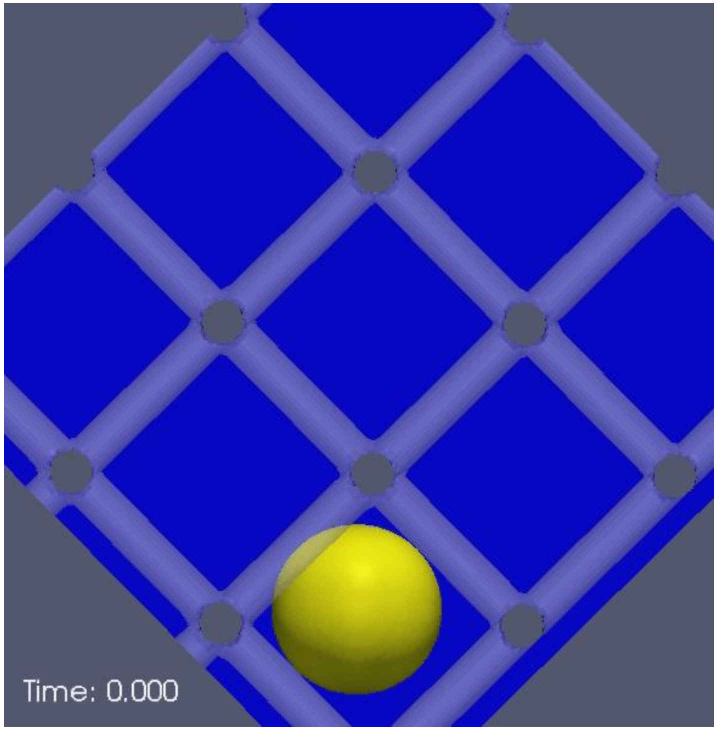
$\theta_e = 90°$

Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2015**, submitted

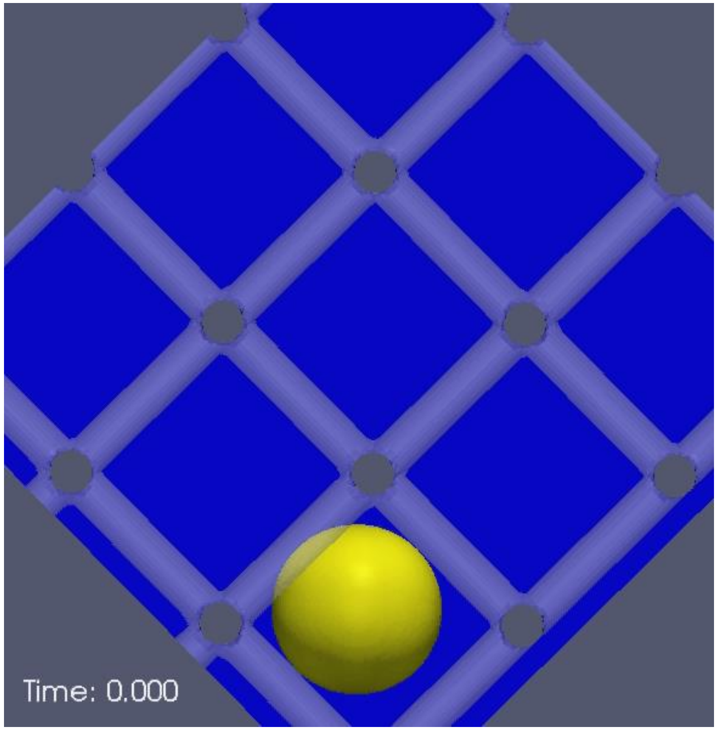
Bubble Rising in Periodic Open Cell Structure

- 2D lateral view

$\theta_e = 0°$



$\theta_e = 90°$



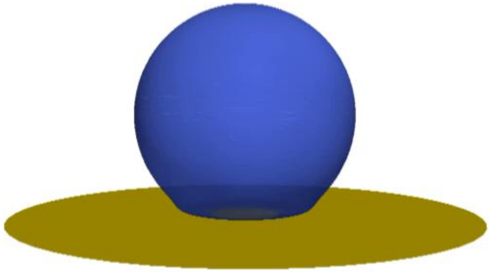
Reference: X. Cai, M. Wörner, H. Marschall and O. Deutschmann, *Catalysis Today*, **2015**, submitted

Summary and Outlook

- Phase Field Method and *phaseFieldFoam* in OpenFOAM
  - Outlook: release the code to foam-extend
- A series of test cases for elementary and complex wetting phenomena
  - Outllook: include models for contact angle hysteresis and surface roughness
- Interface-resolving for two-phase flows in sponge structure
  - Outlook: further DNS for deriving closure relation for Euler-Euler model
- Rising bubble in periodic open-cell structure
  - Outlook: combination of present numerical studies with experiment

Ongoing works

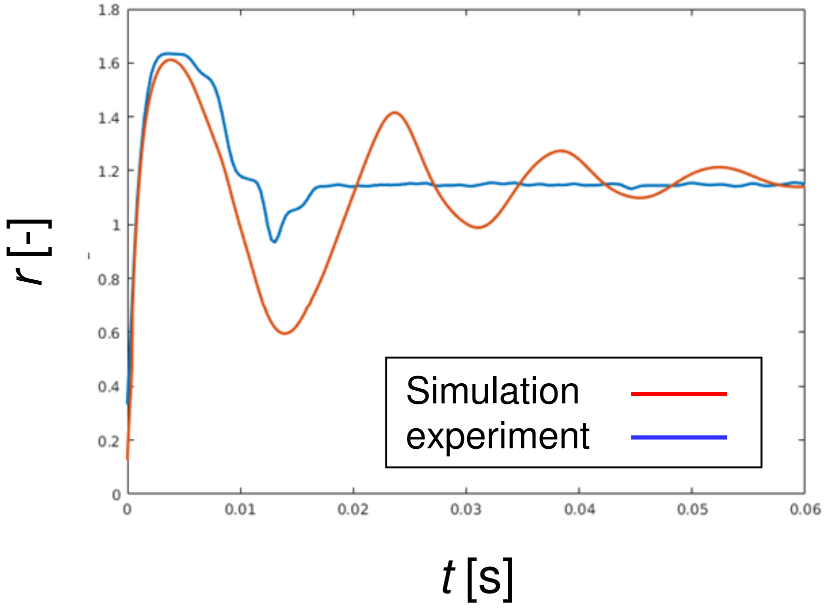
- Droplet impact onto solid surface
  - Cooperation with Institute of Fluid Mechanics (Prof. Frohnapfel), KIT



Simulation

Experiment

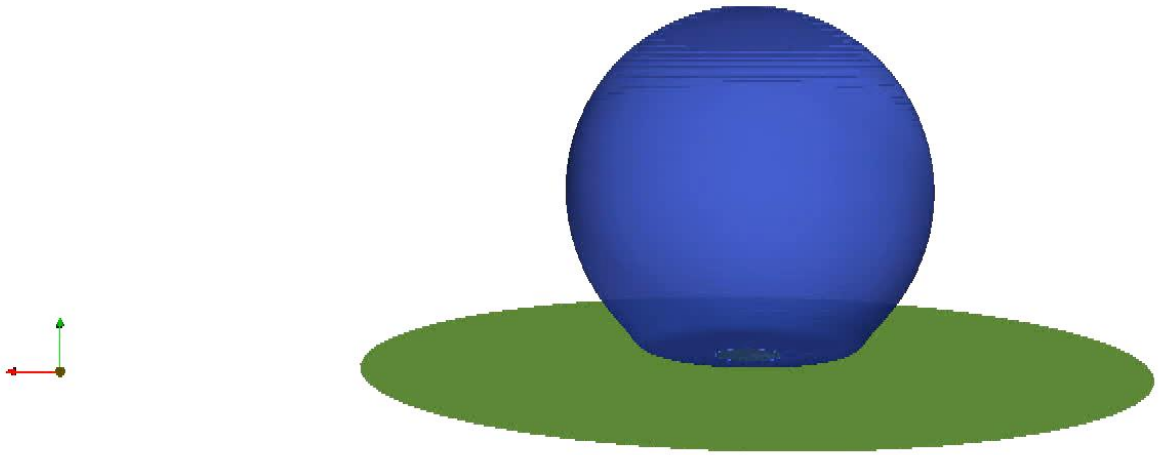
Droplet base radius over time



- Water droplet: Diameter = 2 mm; initial impact velocity = 0.62 m/s
- PDMS surface: **static contact angle = 100° (Hydrophobic)**

Ongoing works

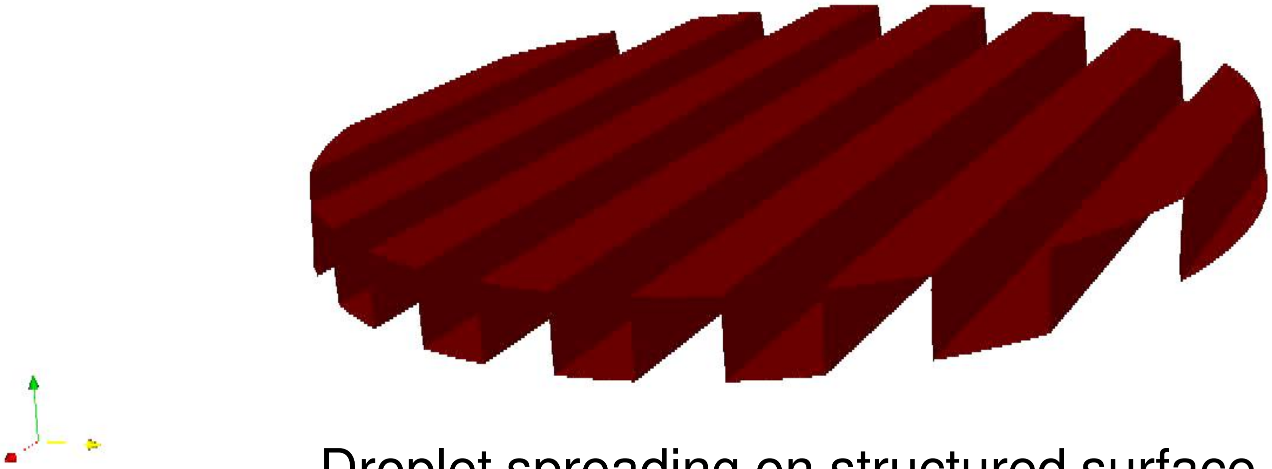
- Droplet impact onto solid surface
  - Cooperation with Institute of Fluid Mechanics (Prof. Frohnapfel), KIT



- Water droplet: Diameter = 2 mm; initial impact velocity = 0.62 m/s
- PDMS surface: **static contact angle = 140° (superhydrophobic)**

Single droplet wetting dynamics

- Droplet spreading on topologically-heterogeneous surface (ongoing)



Droplet spreading on structured surface

Reference: R. Bernard. Master-thesis, **2016**

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  - Prof. P. Yue (Virginia Tech, USA)
  - Prof. H. Alla (USTO, Oran, Algeria)