Karlsruhe Institute of Technology

TECHNISCHE UNIVERSITÄT DARMSTADT

Development of Phase Field Methods using OpenFOAM®
Part II: Application to Complex Wetting Physics

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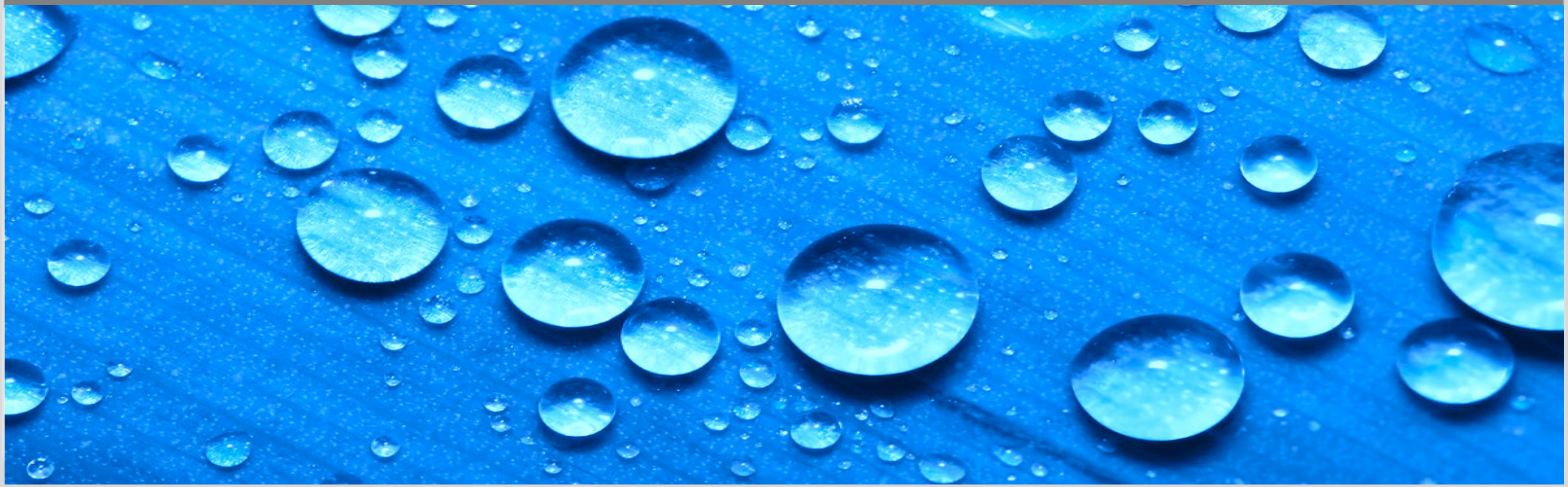
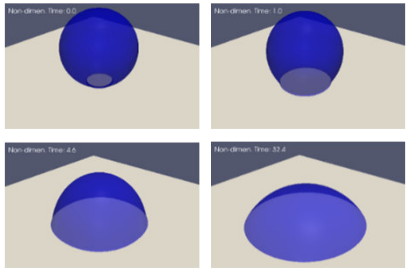
[2] **Technische Universität Darmstadt, Germany**

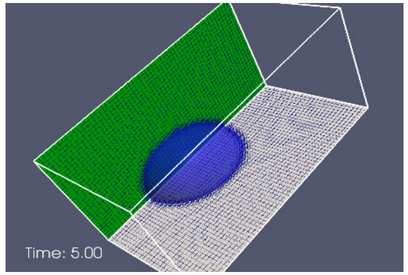
10th OpenFOAM® Workshop, June 29 – July 2, 2015 in Ann Arbor, Michigan, USA

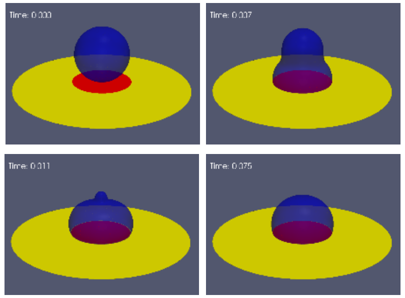


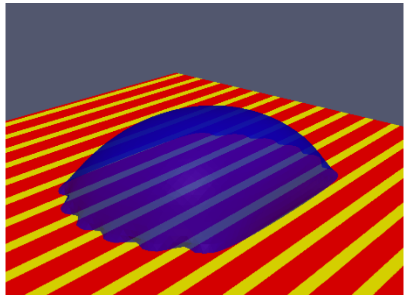
Outline

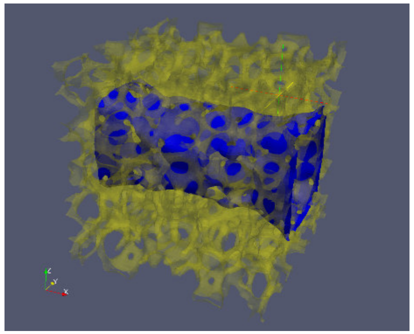
- Droplet spreading/sliding on flat/inclined surface
- Wetting on chemically heterogeneous surface
- Two-phase flows in sponge (foam) structure
- Rising bubble interacting with solid cell structure

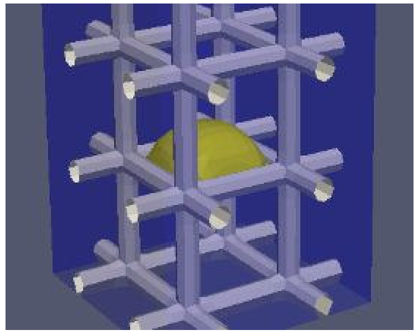






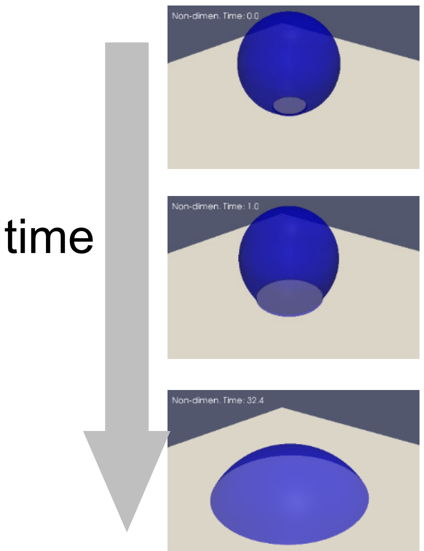


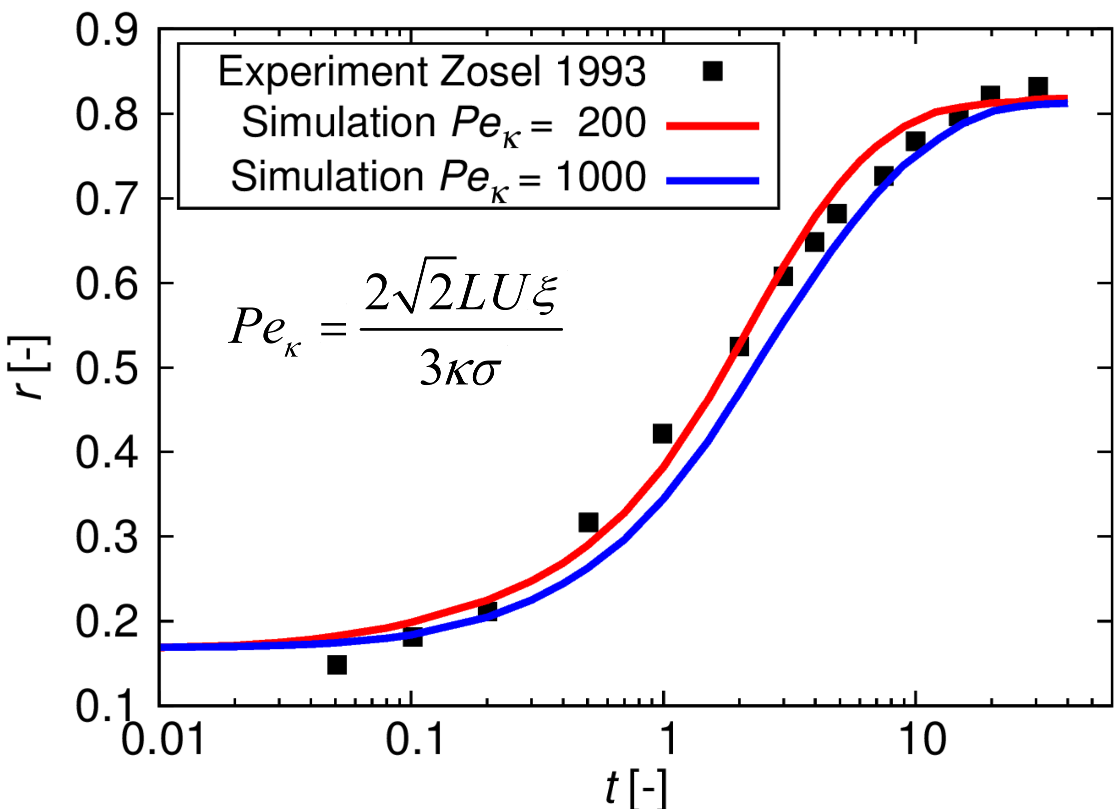




Droplet Spreading on Flat Surface

- **Experiment by Zosel 1993**
  - PIB solution μ = 25 pa·s
  - on smooth flat PTFE surface
  - contact angle θ_e = 58°
  - R_0 = 1.2 ~ 1.5 mm





Zosel, A., Studies of the Wetting Kinetics of Liquid-Drops on Solid-Surfaces. Colloid Polym Sci, 1993. 271(7): p. 680-687.

Rapid Wetting on Initial Spreading Stage

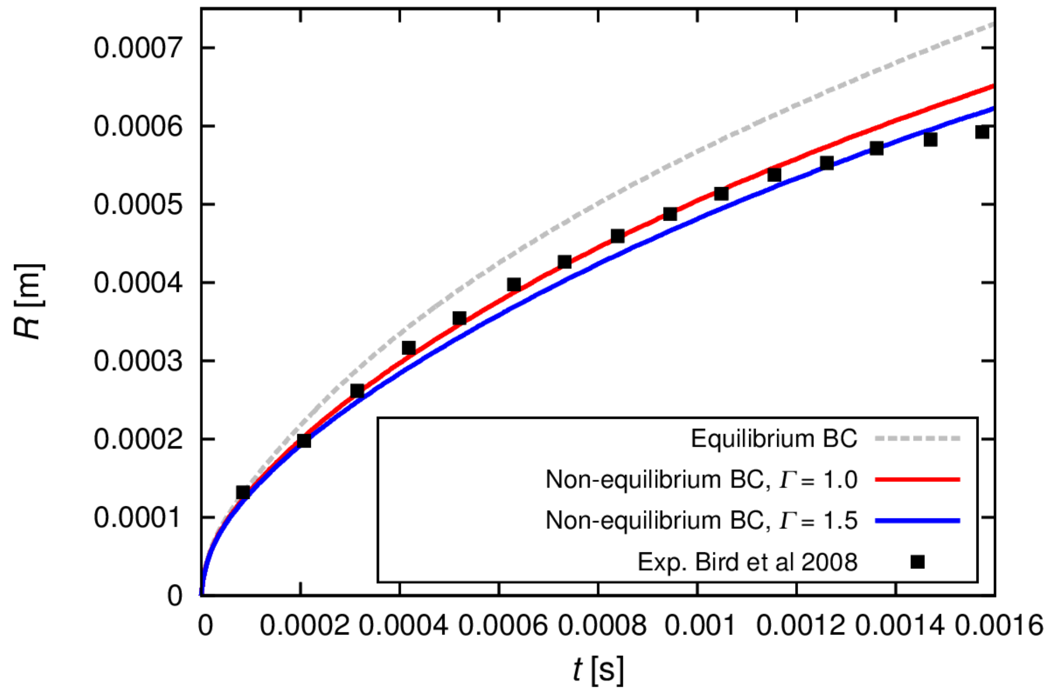
- Equilibrium contact angle BC

$$\mathbf{n}\cdot\nabla C+\frac{3}{4\lambda}\sigma cos\theta_e\left(C^2-1\right)=0$$

- Dynamic contact angle model for energy relaxation (Jacqmin 2000)
  - Finite area method

$$\mathbf{n}\cdot\nabla C+\frac{3}{4\lambda}\sigma cos\theta_e\left(C^2-1\right)=-\Gamma(\frac{\partial C}{\partial t}+\mathbf{u_w}\cdot\nabla C)$$

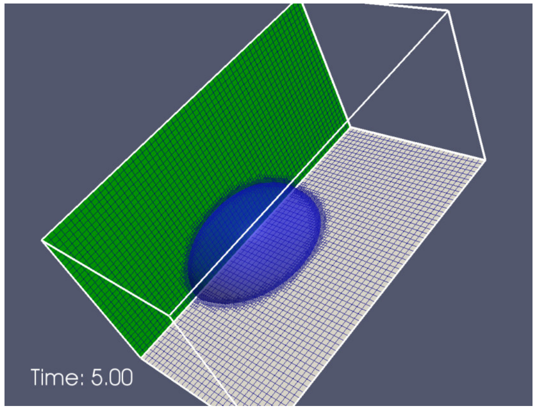
Sim.on 2D Axisymmetric Static Mesh

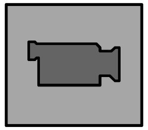


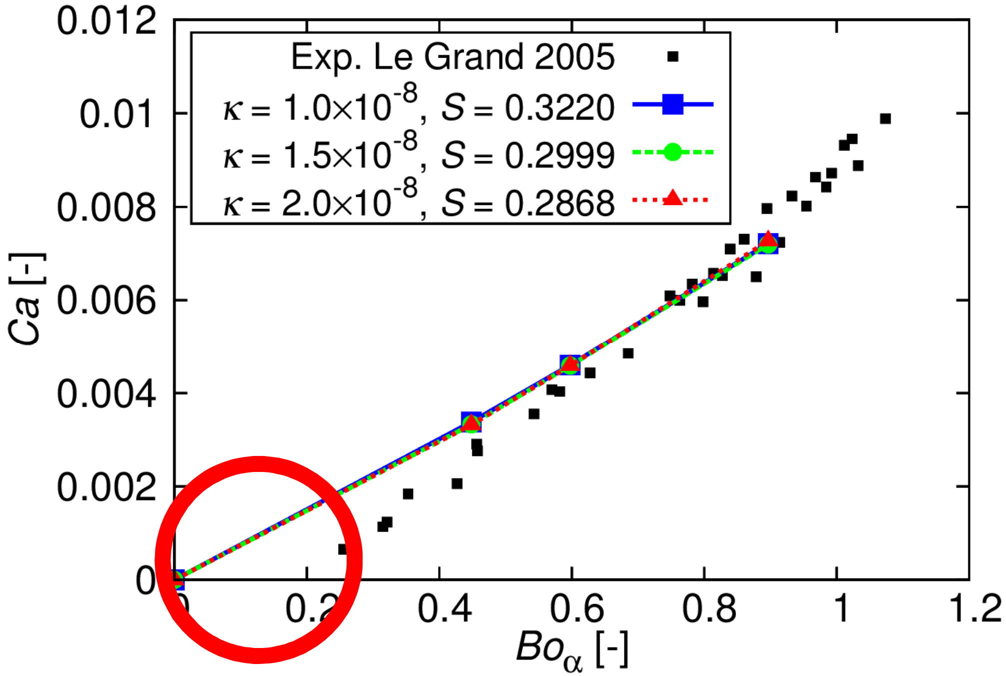
- Yue 2011 provides a guideline on how to choose Γ
  - Γ = 1 ~1.5 should produce best-fit with exp. data. → **Confirmed!**

Droplet Sliding on Inclined Surface

- **Experiment by Le Grand et al. 2005**
  - Droplet of silicon oil
  - Surface is inclined ($7° < \alpha < 52°$)
  - Contact angle θ_e = 52°
  - Droplet volume = 6 mm^3







$$Ca = \frac{\eta U}{\sigma} \qquad Bo_\alpha = V^{2/3}\left(\frac{\rho g}{\sigma}\right)\sin\alpha$$

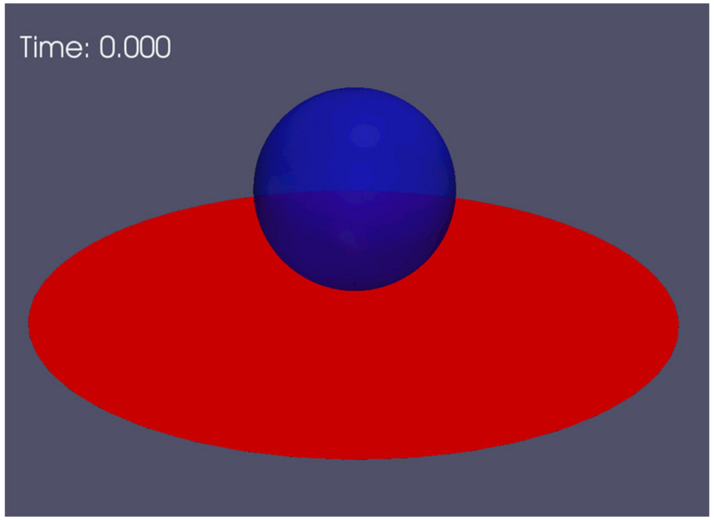
- Pinning effect (contact angle hysteresis)
- Our numerical modeling is under way

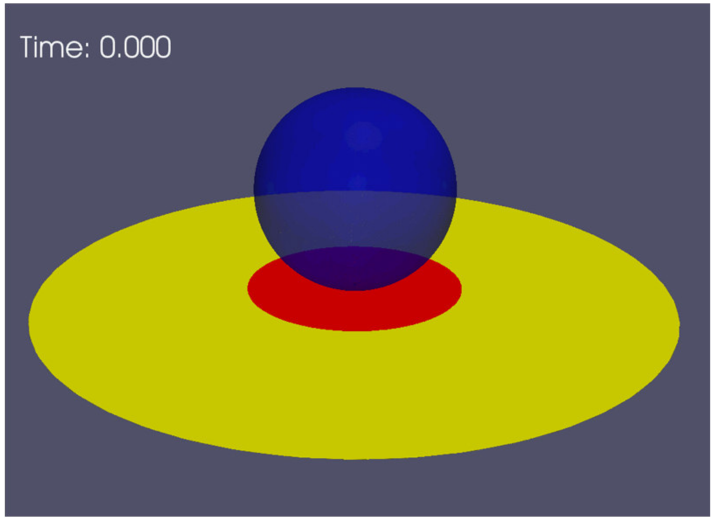
Spreading on Chemically Heterogeneous Surface

- Water droplets (initial radius: 1 mm) jetted onto circular chemically-patterned surface:

θ_e = 60° Hydrophilic	θ_e = 120° Hydrophobic

- Effect of surface pattern (impact velocity: 0 m/s)





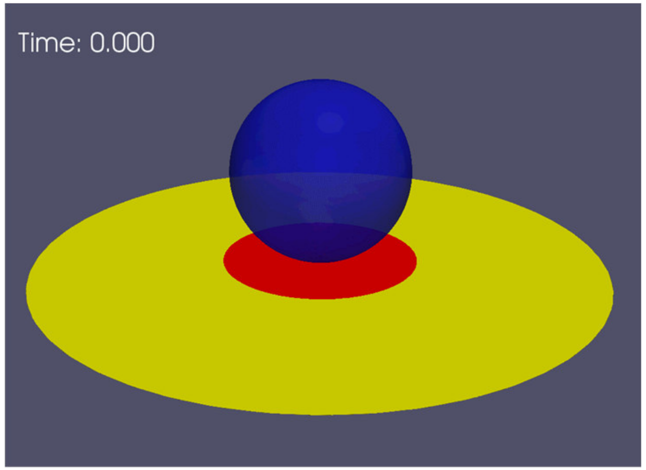
Spreading on Chemically Heterogeneous Surface

- Water droplets (initial radius: 1 mm) jetted onto circular chemically-patterned surface:

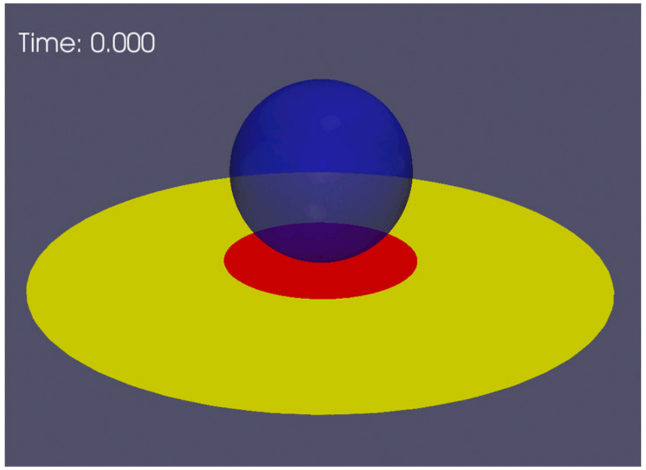
θ_e = 60° Hydrophilic	θ_e = 120° Hydrophobic

- Effect of droplet impact velocity (U_i)

U_i = 0.5 m/s

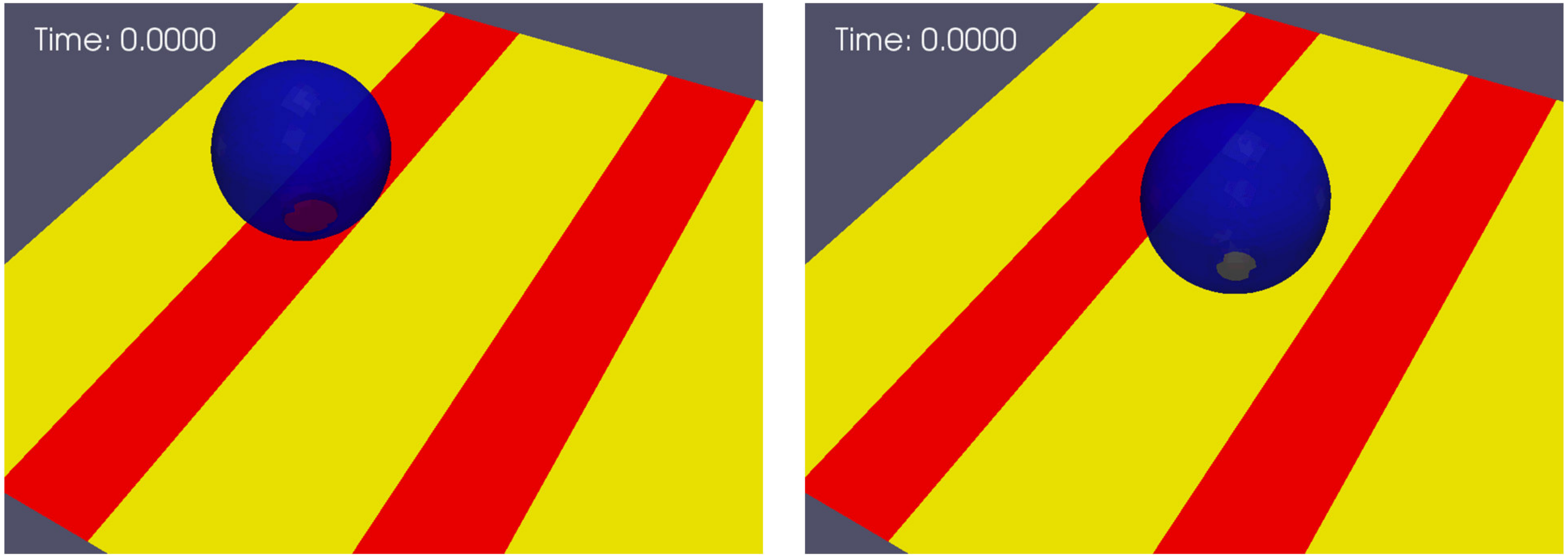


U_i = 1.0 m/s

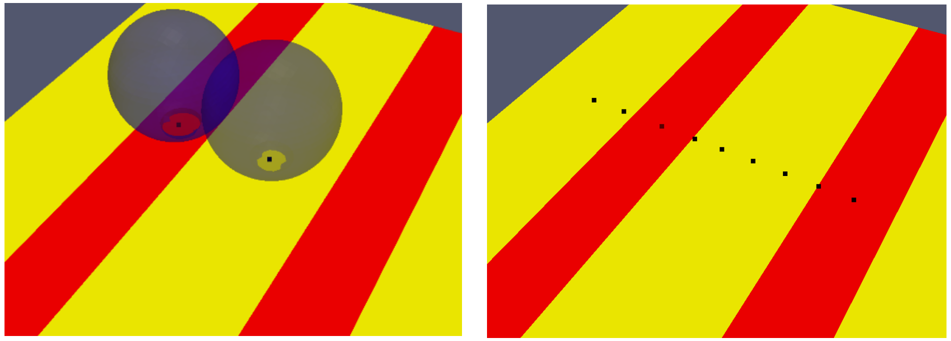


Spreading on Chemically Heterogeneous Surface

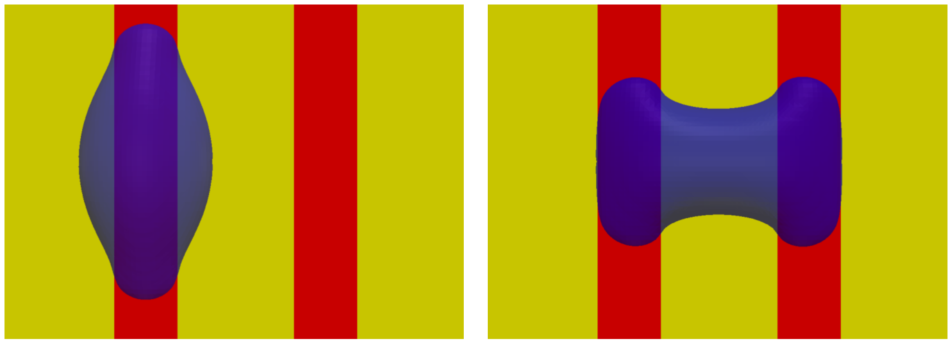
- Experiment by Léopoldès at al. 2003
  - Inkjet droplets (initial radius = 11 μm)
  - released onto rectangular patterned surface: $\theta_e = 20°$ $\theta_e = 64°$



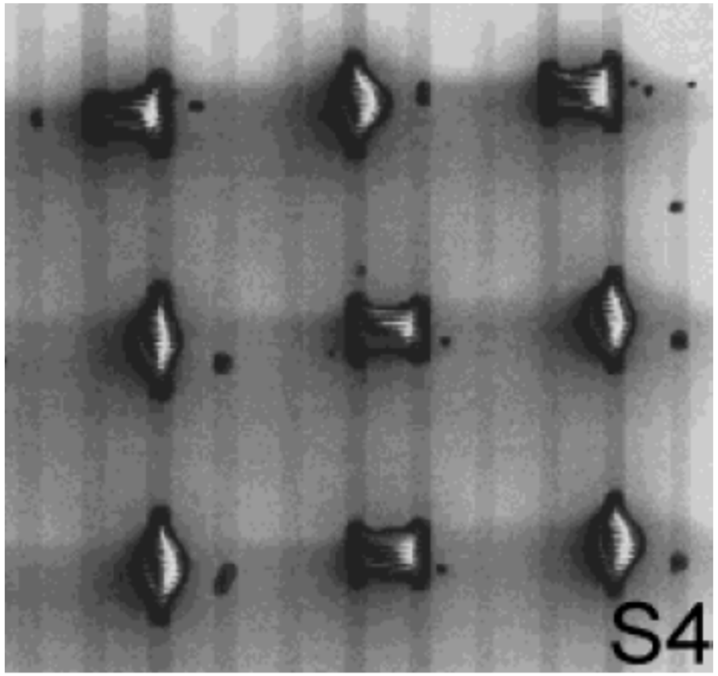
Spreading on Chemically Heterogeneous Surface



Different initial impact points



Final droplet shapes

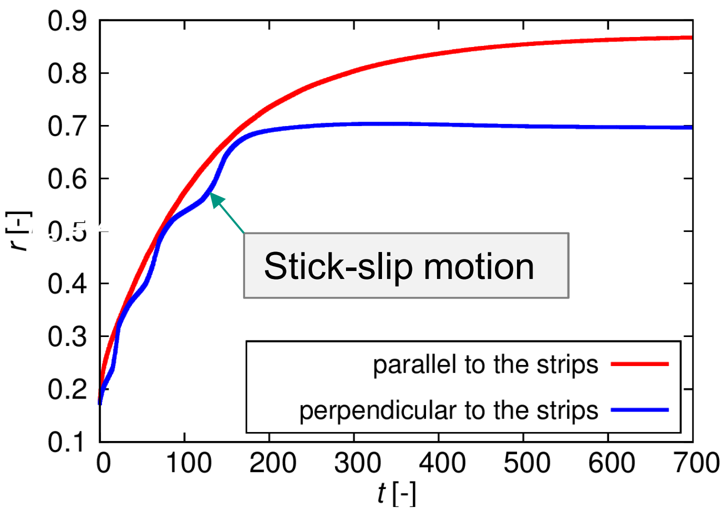


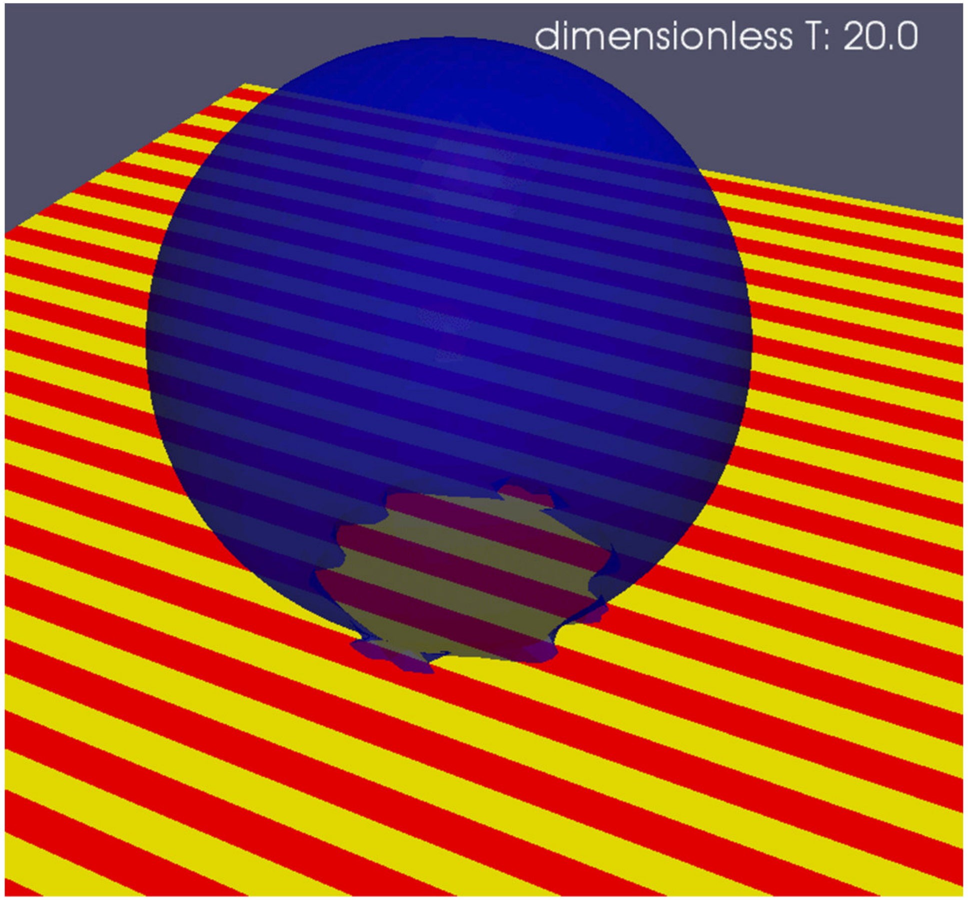
Experimental observation on final droplet shapes using scanning electron microscope (source: Léopoldès at al. 2003)

Spreading on Chemically Heterogeneous Surface

- Experiment by Jansen et al. 2013
- Alternating stripes made of:

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





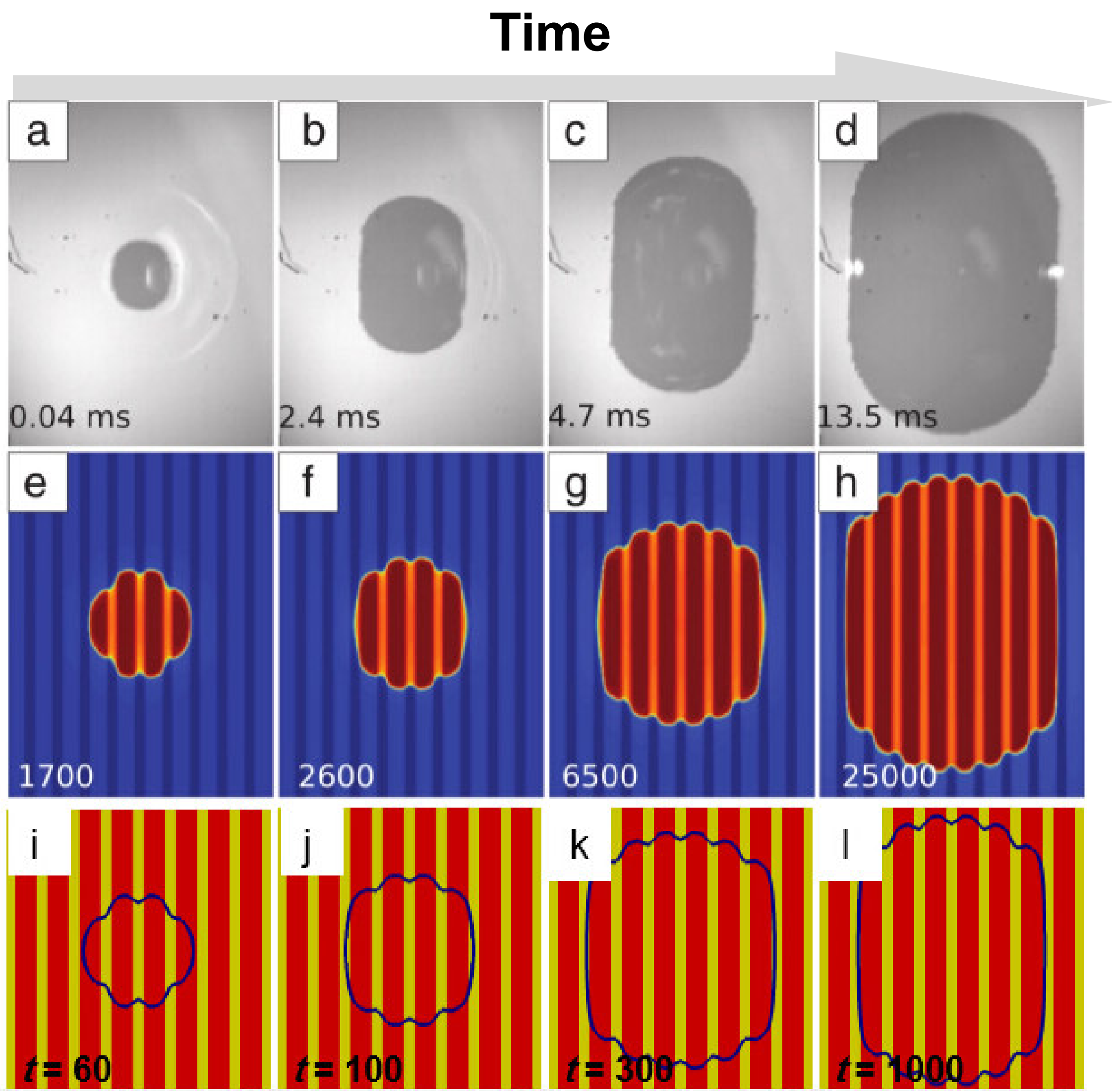
H.P. Jansen et al., Lattice Boltzmann modeling of directional wetting: comparing simulations to experiments, Phys. Rev. E 88 (2013) 013008–013017.

Bottom View

Experiment
Jansen et al. 2013

Lattice-Boltzmann simulation
Jansen et al. 2013

Our simulation
(four cells per stripe)

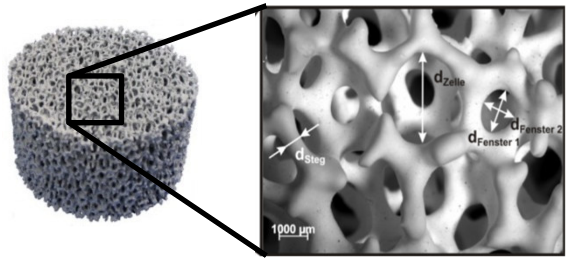


Two Phase Flow in Sponge (Foam) Structure

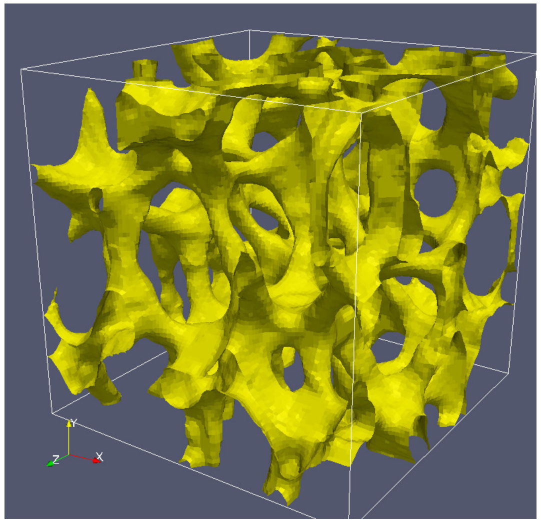
- Institute of Thermal Process, KIT provides the sponge geometry
  - (µ)CT scannings
  - reconstruction of sponge structure in MATLAB produces STL file
- calculations on exemplary sponge sample type:
  - Al_2O_3
  - porosity = 80%
  - 20 pores per inch (ppi)

→ investigations on SiSiC sponge ongoing

- *blockMesh* + *snappyHexMesh*



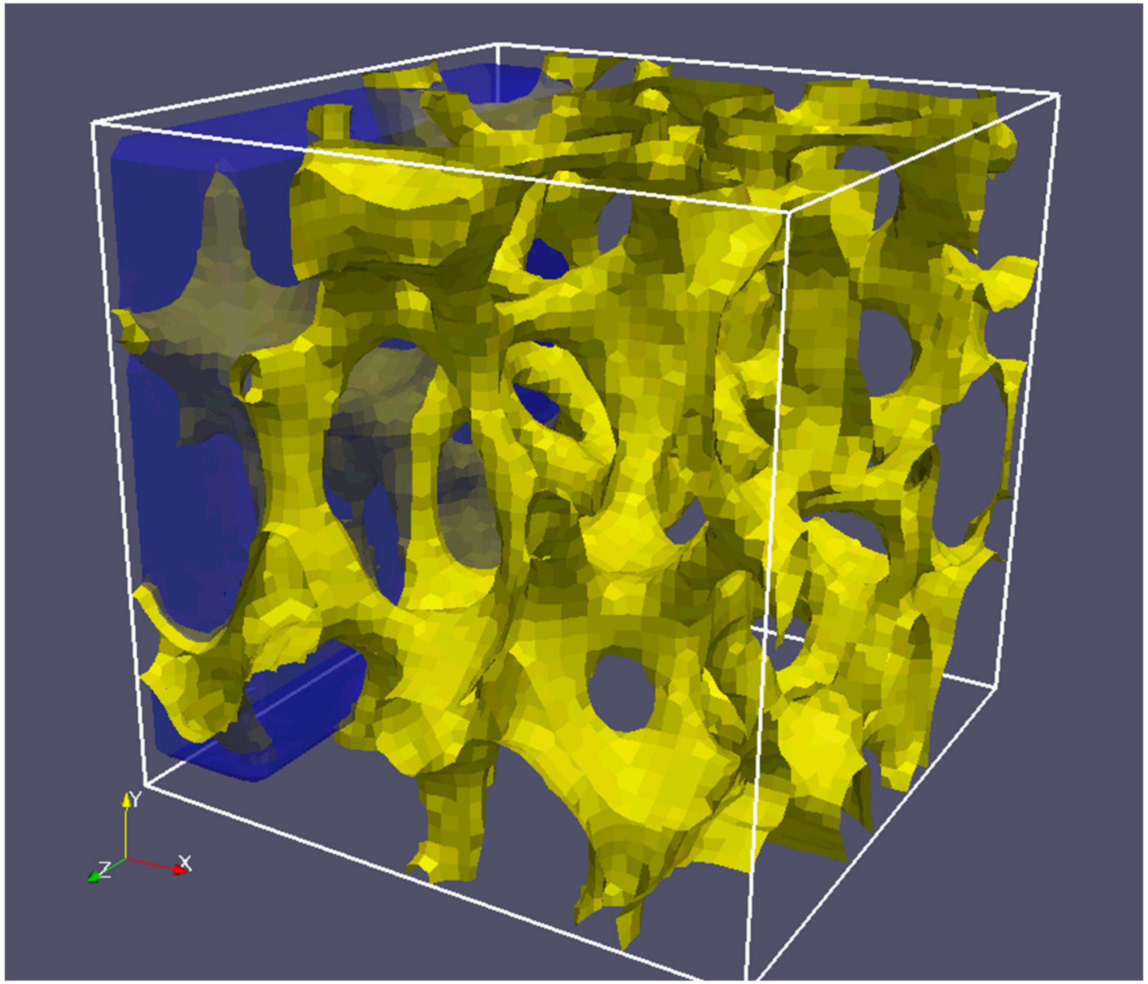
solid sponge chemical reactor



Representative Elementary Volume (REV) for CFD

Two Phase Flow in Sponge (Foam) Structure

- Blue iso-surface → interface btw. liquid and gas
- Pressure-driven (from left to right)



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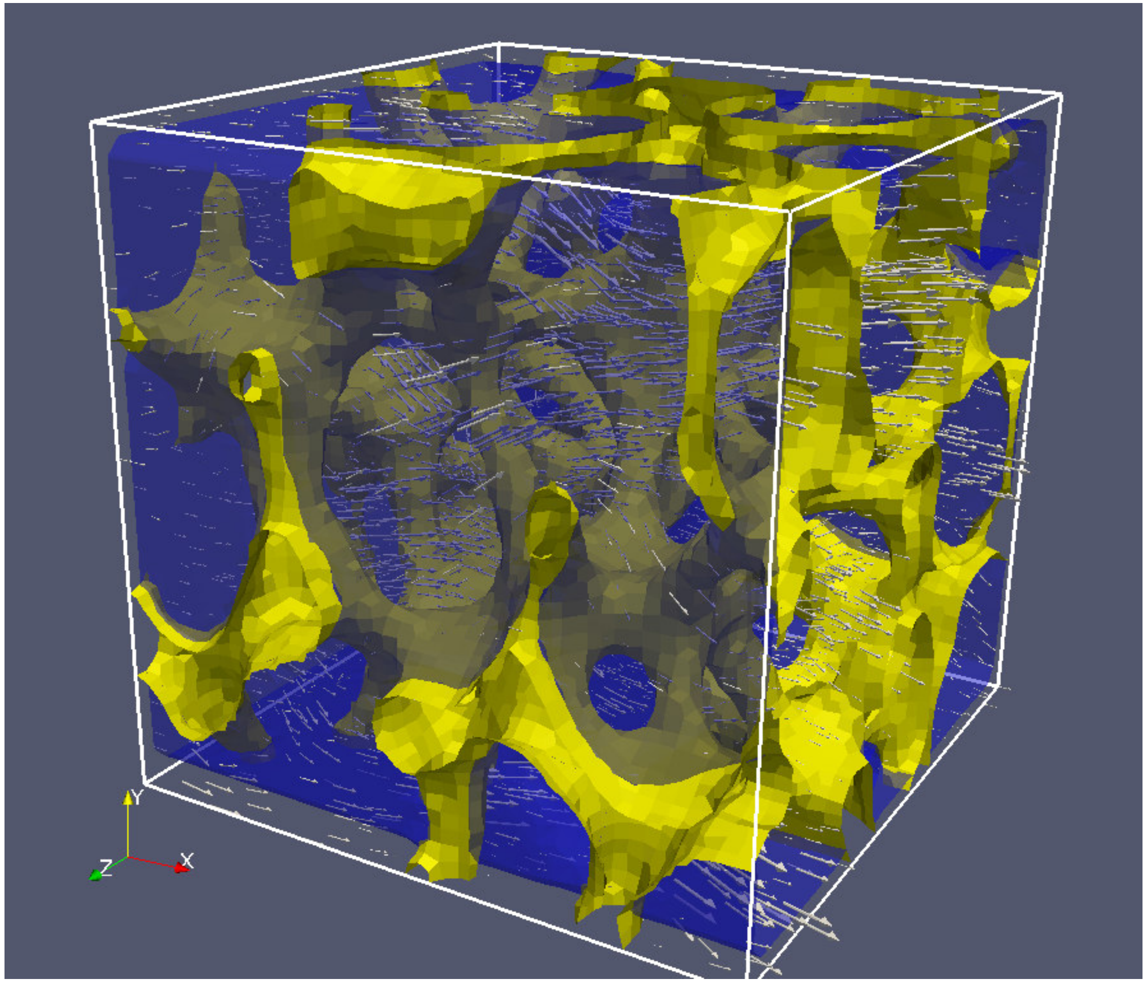
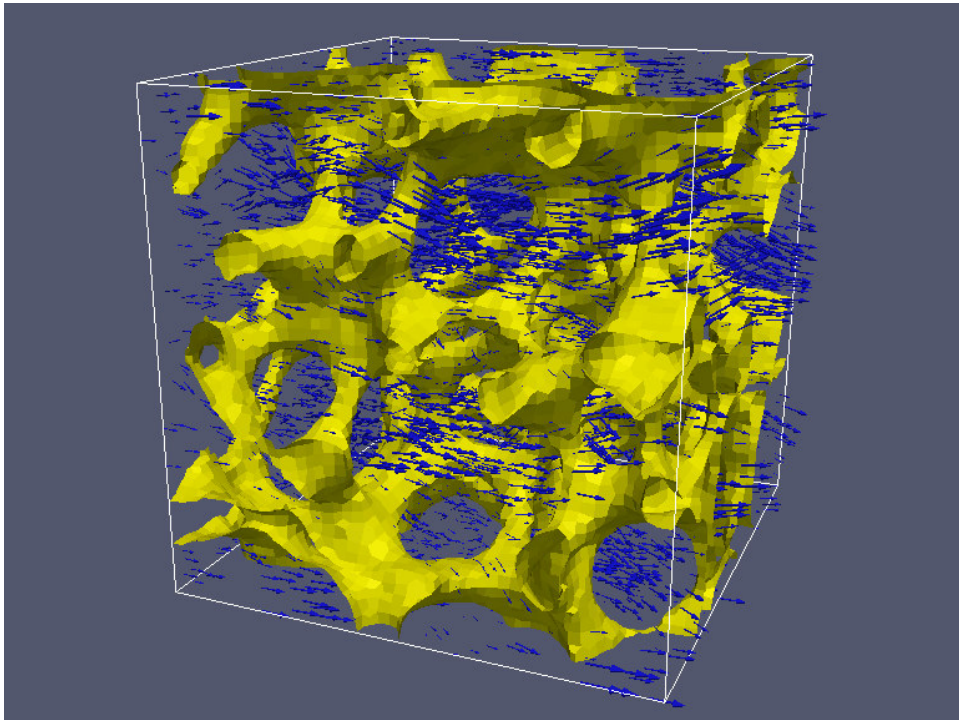


Validation for Hydrodynamics of Gas Flow

- Apply the solver for gas flow through sponge structure
- Compare simulated pressure drop versus superficial velocity against:
  - experimental results (Dietrich et al. 2009 [1])
  - CFD results using "simpleFoam" (Meinicke et al. 2014 [2])



sample sponge type: Al_2O_3, 80% porosity, 20 ppi

[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, B. Dietrich, Th. Wetzel. CFD-Simulation der einphasigen Durchströmung fester Schwammstrukturen ProcessNet Fachausschuss CFD, Mischvorgänge u. Rheologie,Würzburg, 2014

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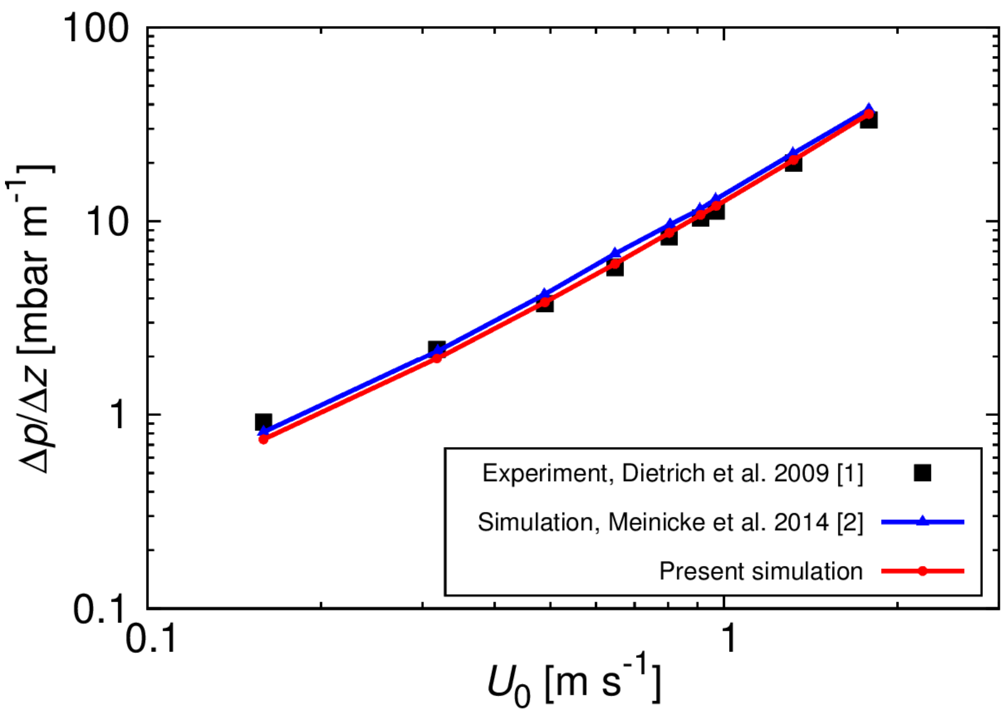

- U_0: superficial gas velocity
- $\Delta p / \Delta z$: pressure drop per unit length

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Hydrodynamics of Two Phase Flows

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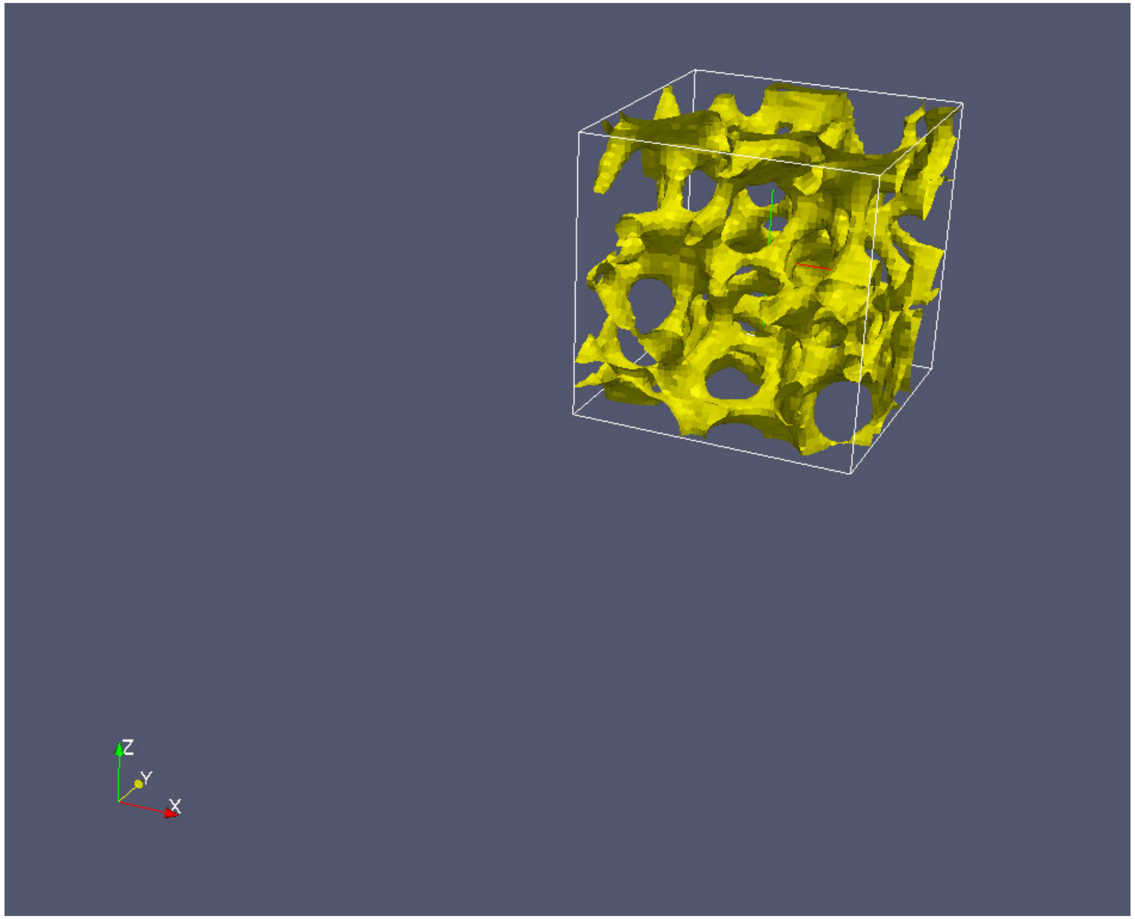
- Exp. data will be provided by our project partner
- Representative domain → difficult to get inlet liquid distribution from exp.



Hydrodynamics of Two Phase Flows

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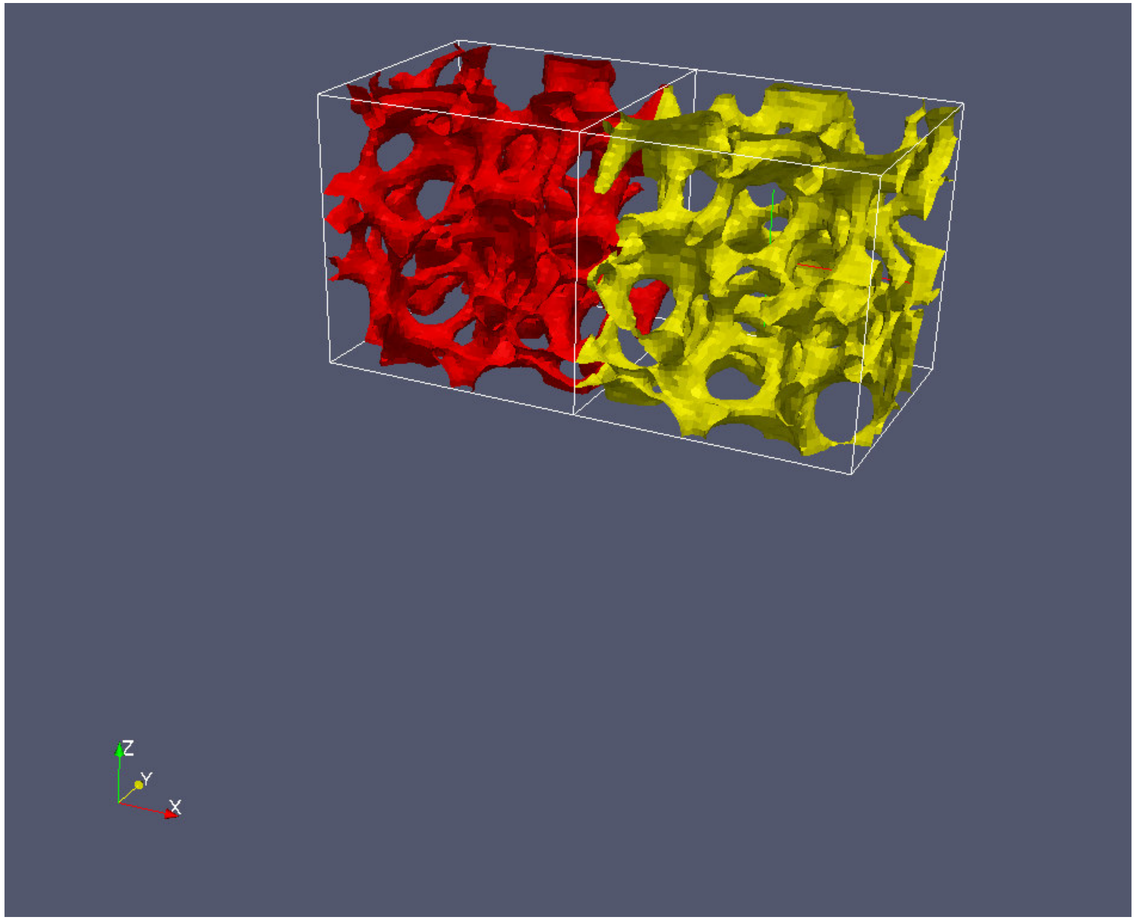
- Mirroring original geometry and applying periodic boundary conditions



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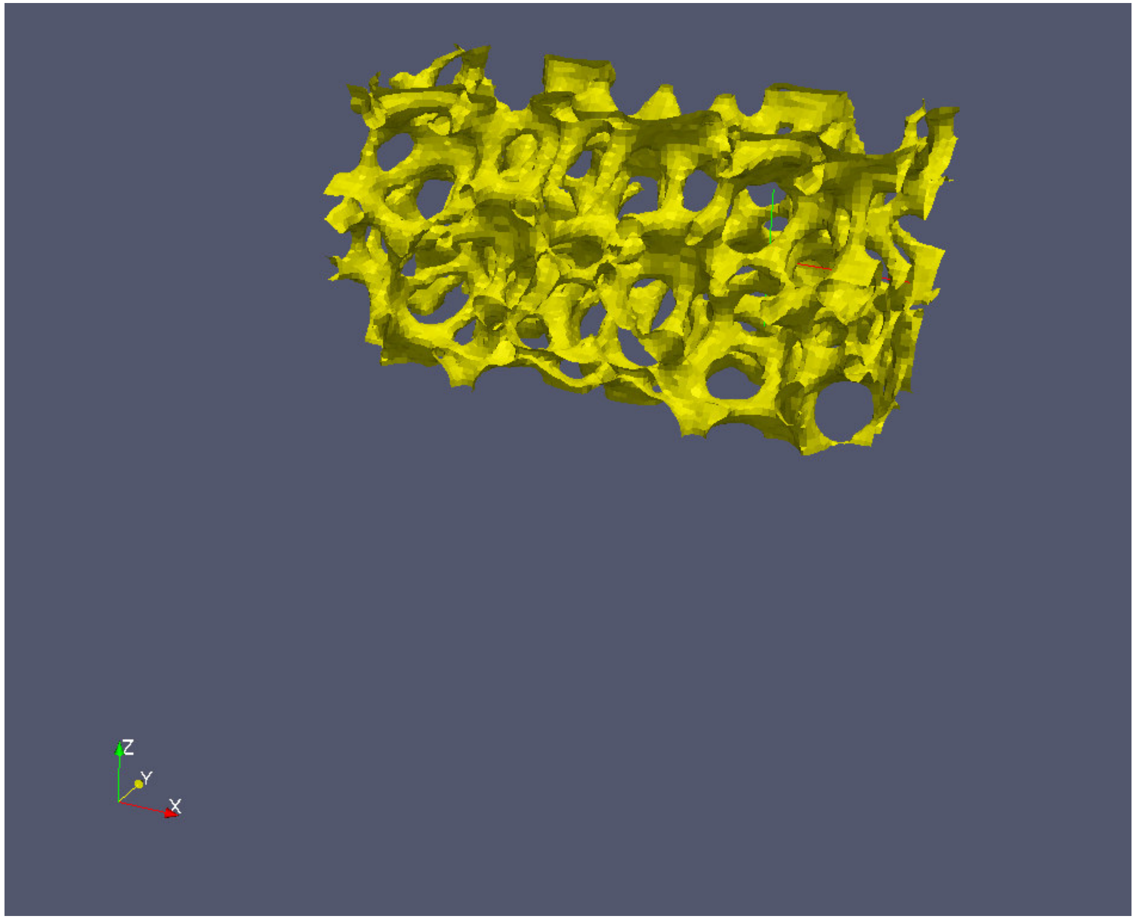

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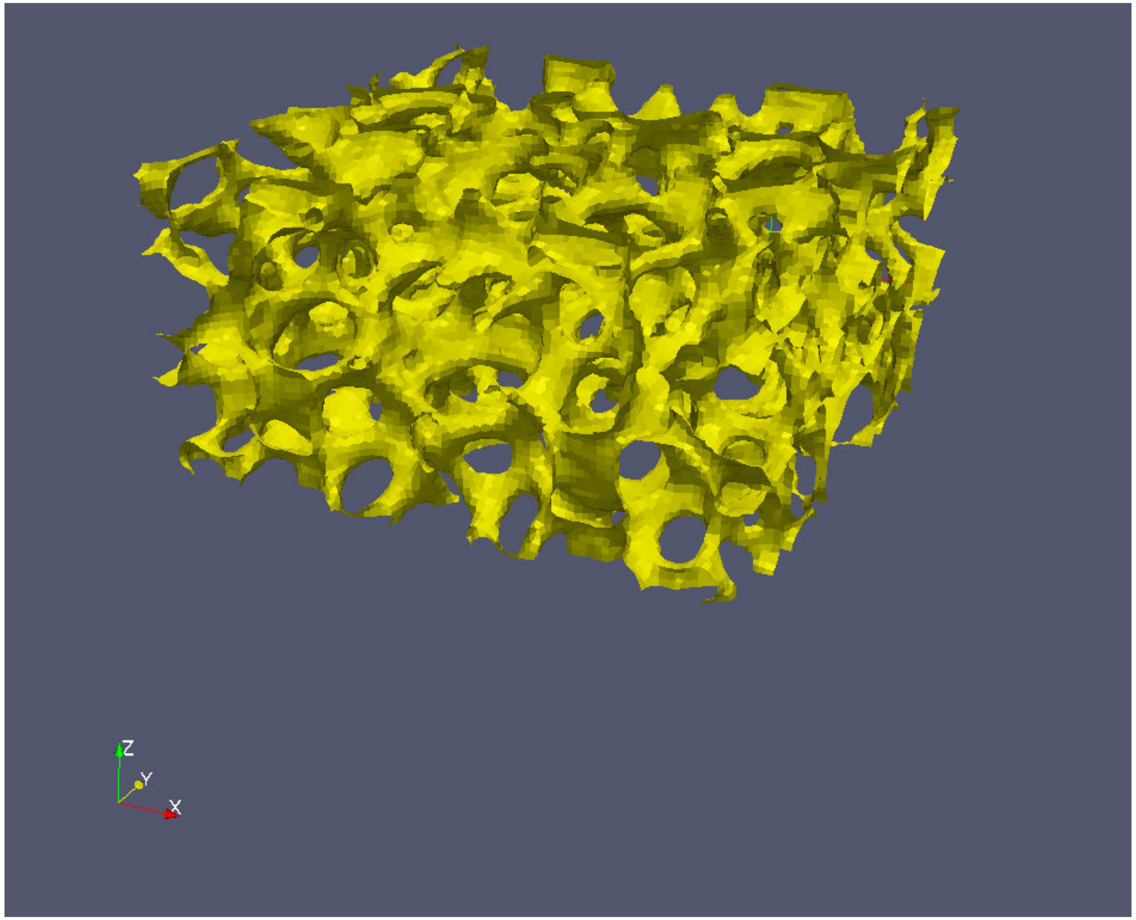

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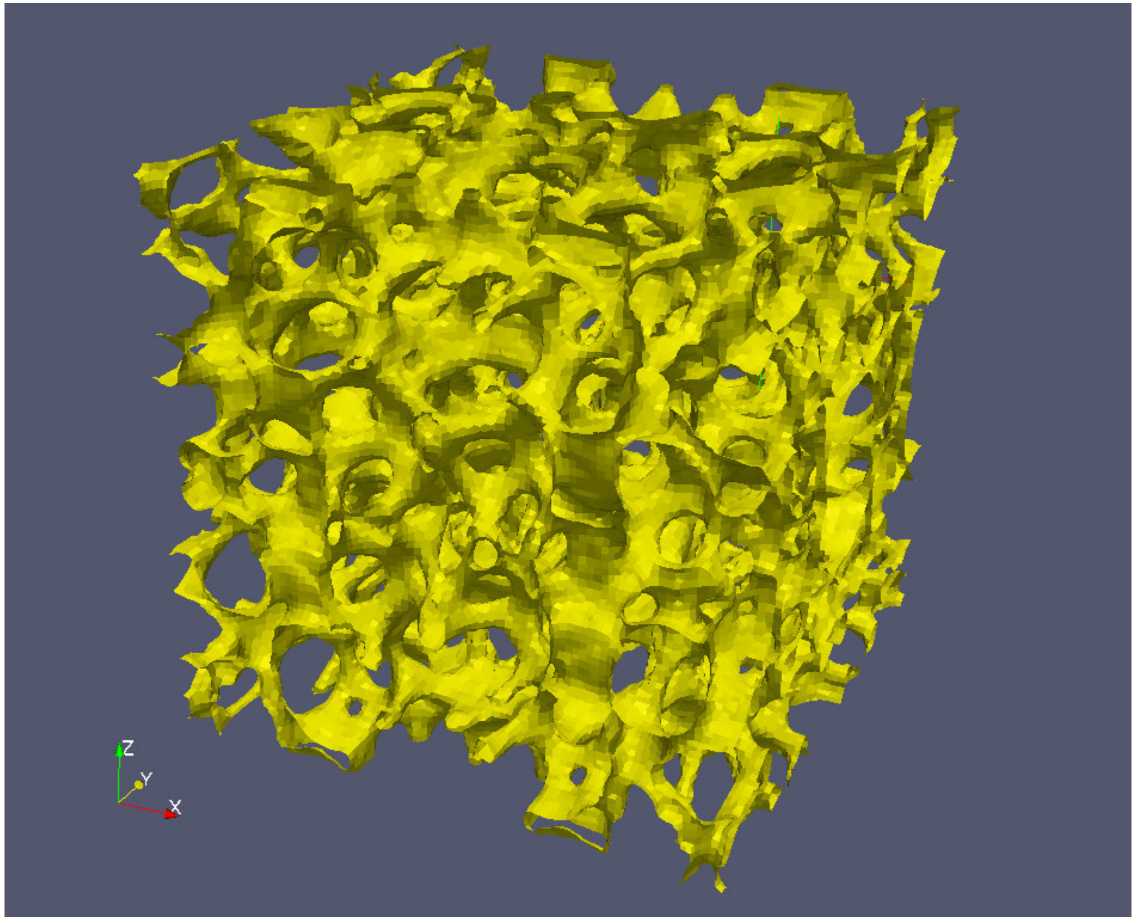
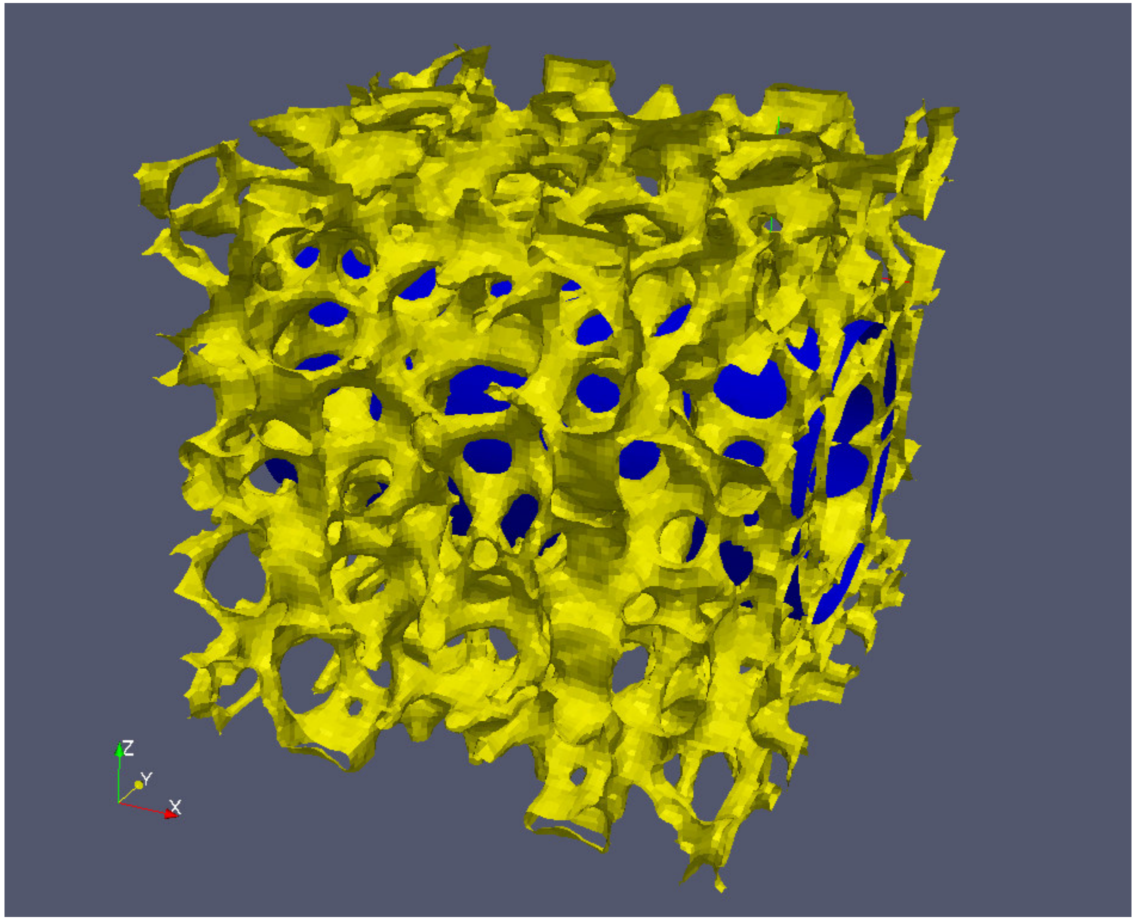


Hydrodynamics of Two Phase Flows

- Specify initial liquid distribution along x
- Mesh Info
  - Background: 80*80*80
  - Two-level mesh refinement near solid surface



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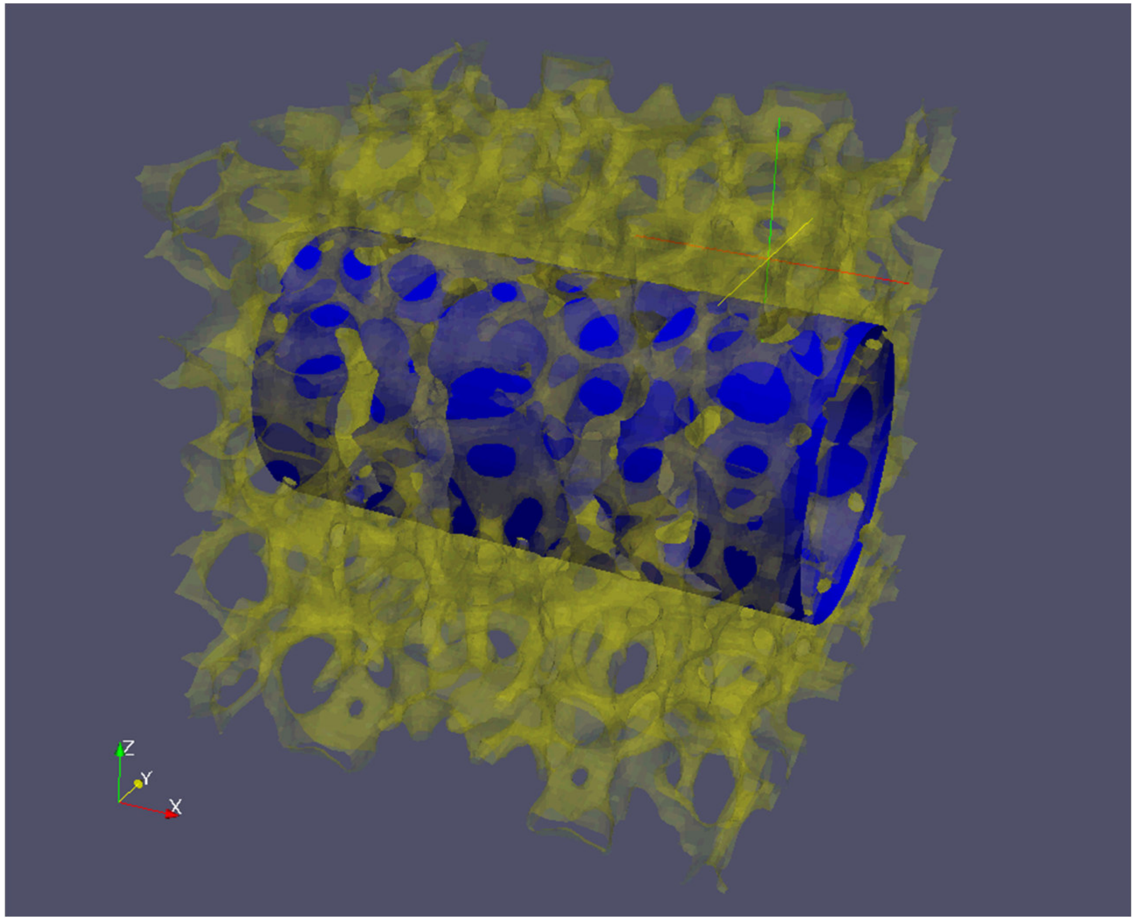
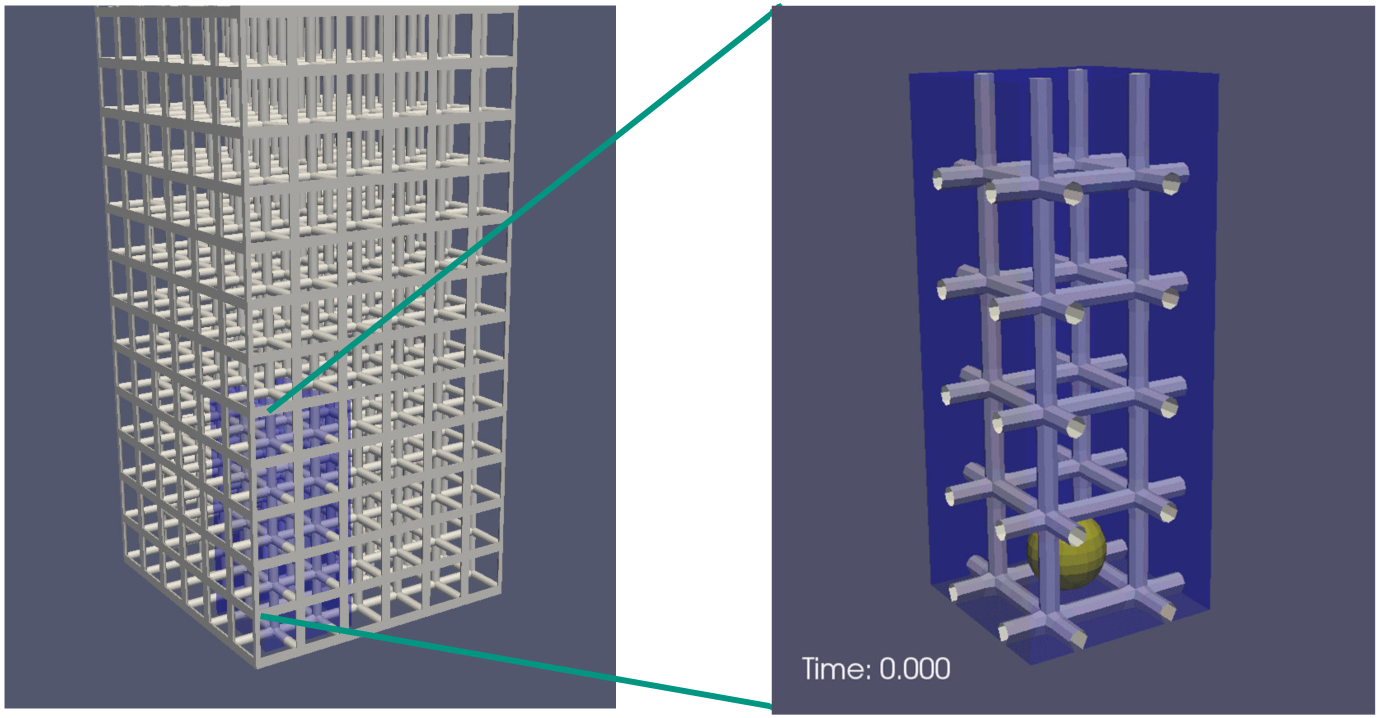


Bubble Rise in Periodic Open Cell Structure (POCS)

- POCS as internals in bubble column reactor can enhance gas-liquid mass transfer (by disturbing/renewing the liquid concentration boundary layer)
  - Cooperation with Institute of Multiphase Flows, TU Hamburg-Harburg, Germany



Windows size: 4mm; Grid Angle: 90°
Manufactured at FAU Erlangen, Germany
Geometry provided by TUHH, Germany

Subdomain for CFD simulation
A gas bubble (D = 4mm) in stagnant water
Surface Wettability: $\theta_e = 90°$

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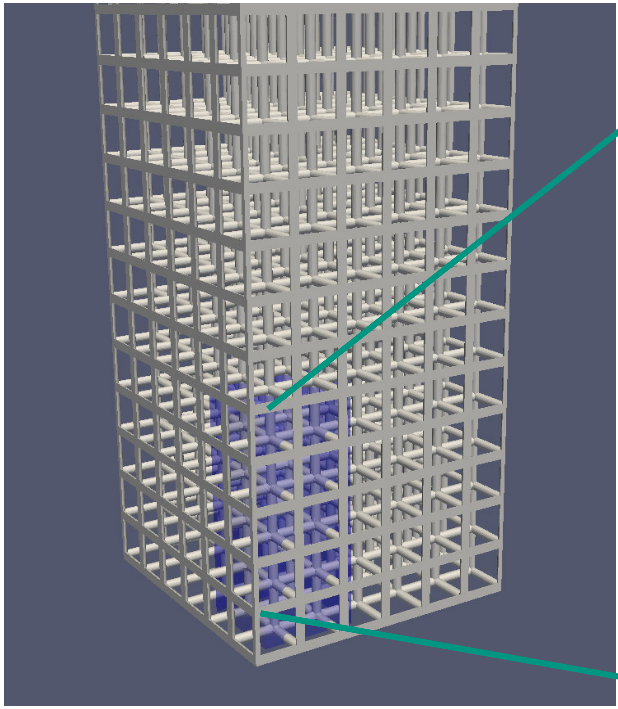

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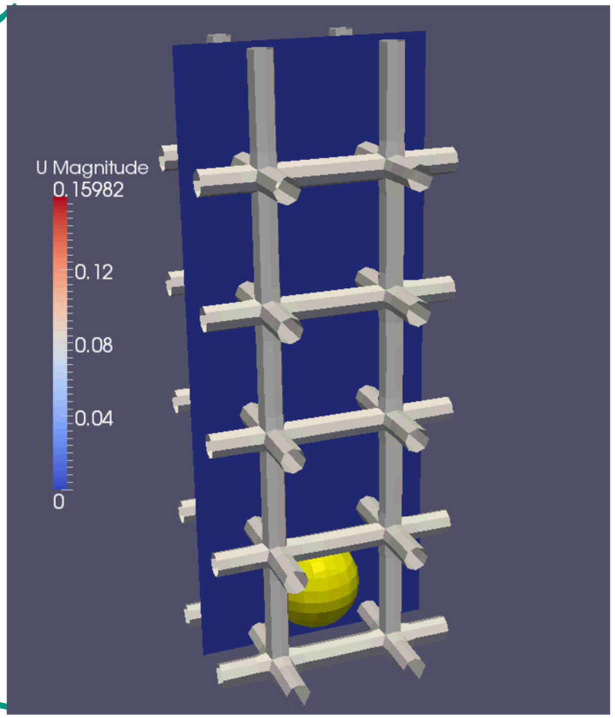
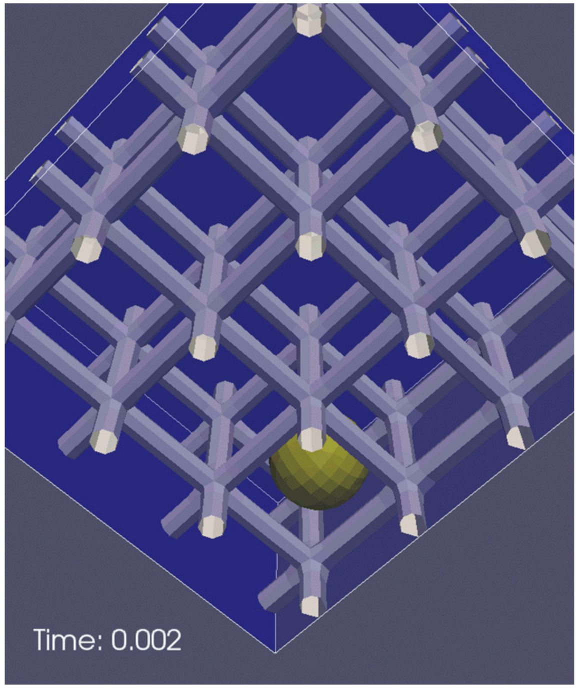


Subdomain for CFD simulation
A gas bubble (*D* = 4mm) in stagnant water
Surface Wettability: $\theta_e = 90°$

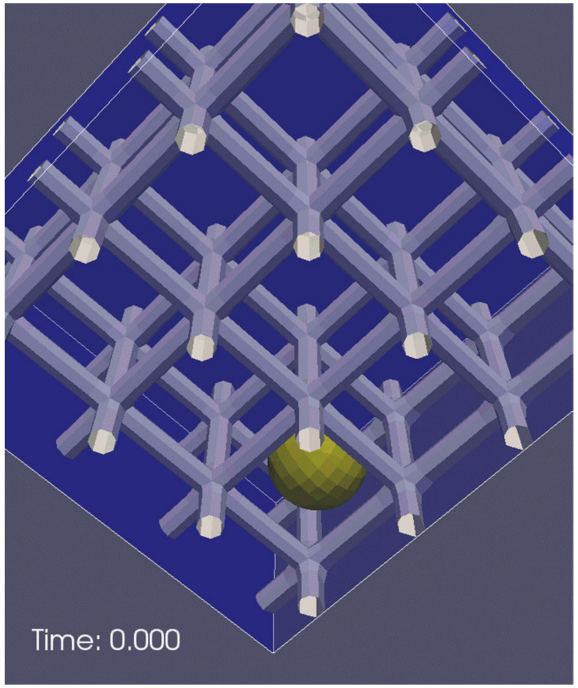
Bubble Rising in Periodic Open Cell Structure

- Wettability effect on interaction of rising bubble with cell structure

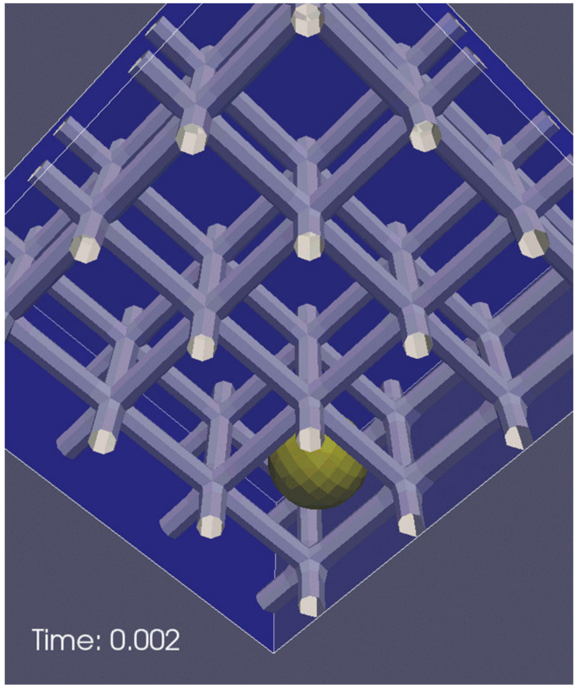
$\theta_e = 0°$



$\theta_e = 90°$



$\theta_e = 135°$



Summary

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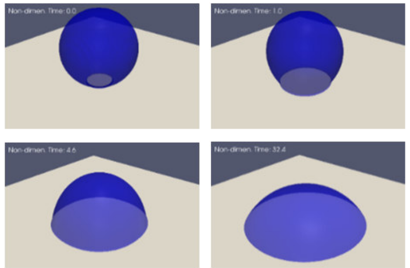
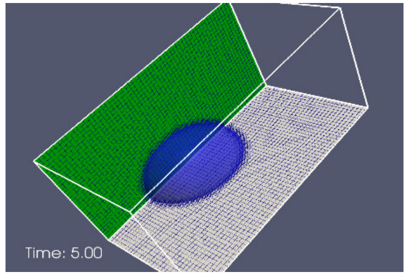
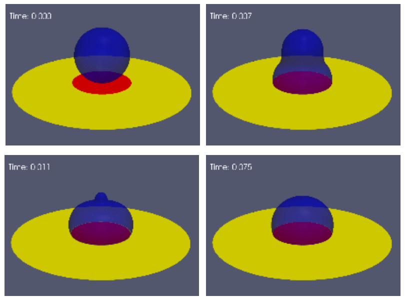
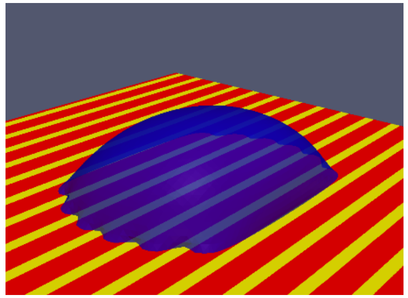
- Droplet spreading/sliding on flat/inclined surface



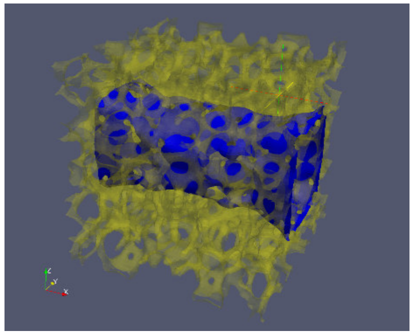


- Wetting on chemically heterogeneous surface

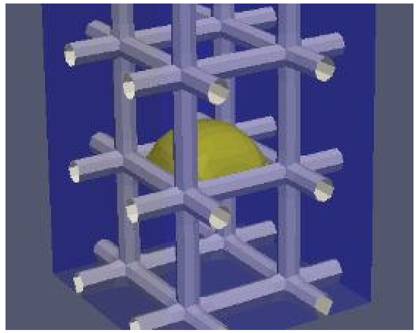




- Two-phase flows in sponge (foam) structure

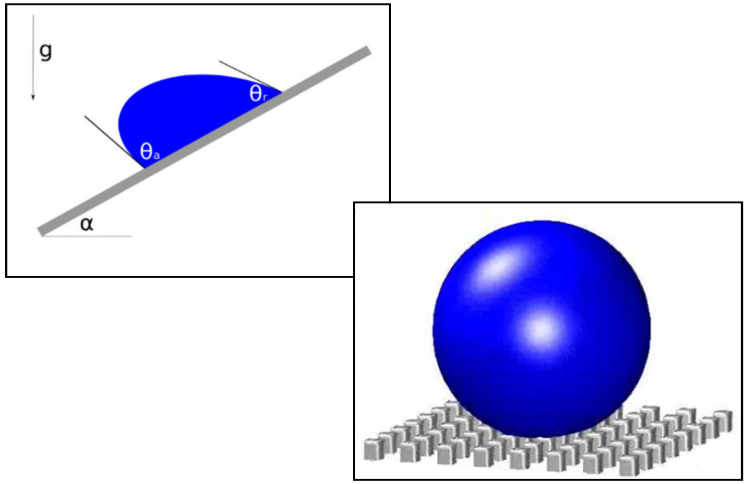


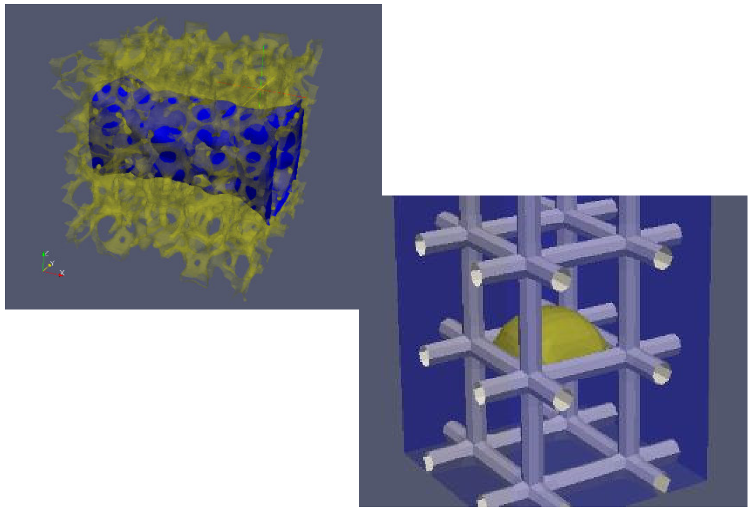
- Rising bubble interacting with solid cell structure



Outlooks

- Pinning effect of droplet on inclined surface (contact angle hysteresis)
- Droplet wetting on topologically heterogeneous surface
- Provide closure relation (e.g. interfacial area) for Euler-Euler simulation for sponge structure
- Coupling hydrodynamics with heat transfer, mass transfer and chemical reactions …





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- **Partners:**
  - Dr. B. Dietrich, S. Meinicke (KIT-TVT, Germany)
  - Prof. M. Schlüter, C. Möller (TU Hamburg-Harburg, Germany)
  - Prof. M. Grünewald, C. Hecht (Ruhr Uni. Bochum, Germany)
  - Prof. P. Yue (Virginia Tech, USA)
  - Prof. H. Alla (USTO, Oran, Algeria)