Phase Field Simulation of Wetting Processes with OpenFOAM®

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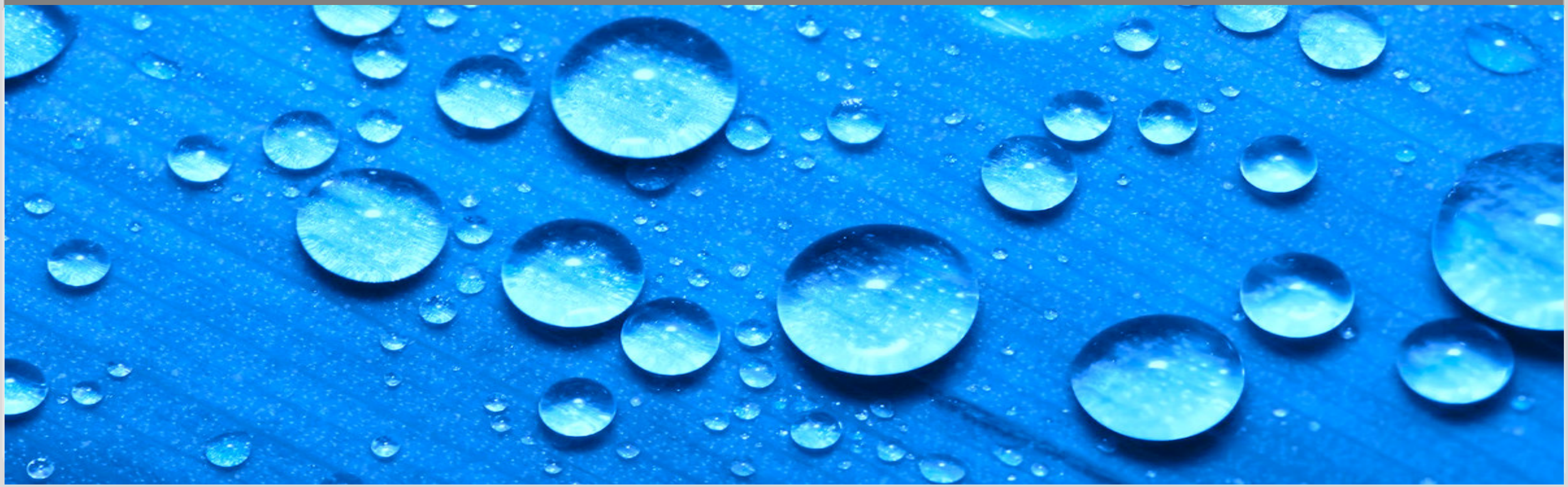

Outline

- Introduction
- Phase Field Method
- Validation for fundamental wetting phenomena
- Application for multiphase chemical reactors
- Conclusions and outlook

Motivation

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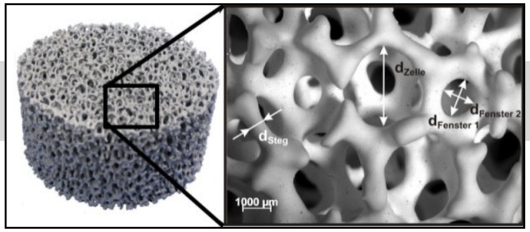
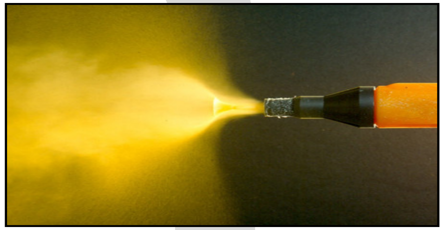
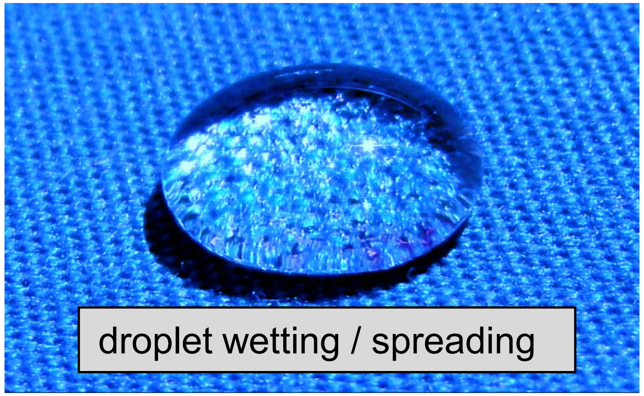
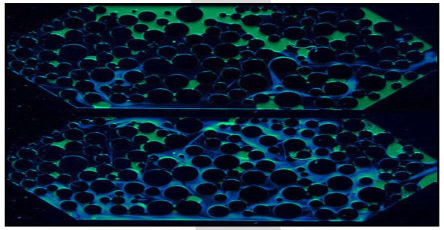


solid sponge chemical reactor


insecticides spray


coating


droplet wetting / spreading


oil recovery from porous structure

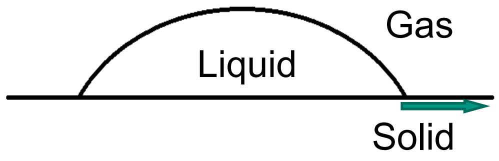
ink-jet printing



lubrication

- For numerical simulation of dynamic wetting processes accurate modeling of the **moving contact line** is necessary

Difficulty of numerical modeling



Paradox btw. motion of contact line & no-slip BC

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

F= liquid volume fraction

- This paradox can be resolved by

<u>Sharp</u> interface method

- ➢ e.g. VOF, Level-set method
- ➢ via Navier-slip BC

$$u_W = L_s \left.\frac{\partial u}{\partial n}\right|_W$$

- ➢ L_s is slip length (usually chosen empirically)

<u>Diffuse</u> interface method

- ➢ e.g. Phase Field Method
- ➢ via diffusion term

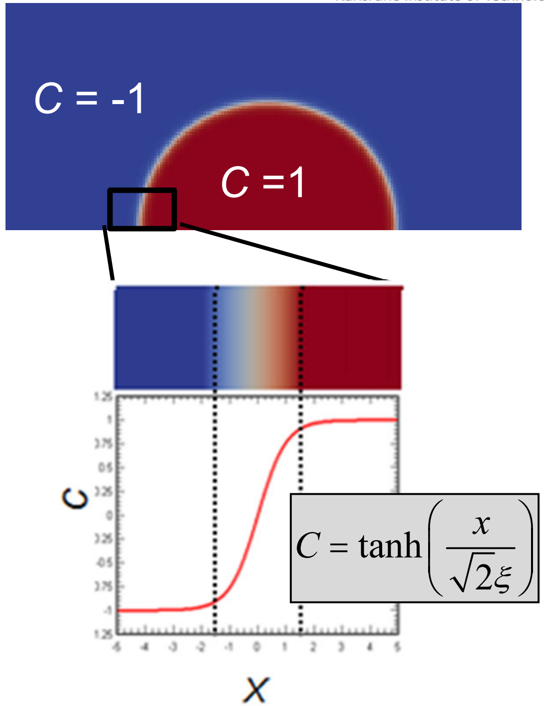
$$\frac{\partial C}{\partial t} + (\mathbf{u}\cdot\nabla)C = \kappa\nabla^2\phi$$

- ➢ *C* is phase field order parameter
- ➢ *Φ* is chemical potential

$$\Phi = \beta(C^3 - C) - \alpha\nabla^2 C$$

Phase field method

- Phase field (C) as phase indictor



- Cahn-Hilliard eq. for phase field evolution
  - Non-dimensional form

$$\frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla) C = \frac{1}{Pe_\kappa} \nabla^2 \phi \qquad \Phi = C^3 - C - Cn^2 \nabla^2 C$$

- Coupled with Navier-Stokes equation

$$\rho(C) Re\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u}\right) = -\nabla p + \mu(C)\nabla^2 \mathbf{u} - \frac{1}{Ca \cdot Cn} C \nabla \Phi(C) - \frac{1}{2}\frac{Eo}{Ca}(C+1)\mathbf{e_z}$$

- Boundary condition for equilibrium contact angle θ_e

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

θ_e is an input parameter for the simulation!

Implementation in OpenFOAM®

- Top-level solver **phaseFieldFoam**
  - Cooperation with Dr. Holger Marschall from TU Darmstadt
- Phase field Cahn-Hilliard equation
  - Diffusion term is a 4th order derivative (for now treated in segregated manner with time-step sub-cycling)
- Relative density flux term in momentum eq. due to diffusion of components (Ding et al. 2007, Abels et al. 2012)
  - Consistent use of conservative volumetric fluxes
- Surface tension in energy formulation
  - As surface tension energy density

Pseudo code:

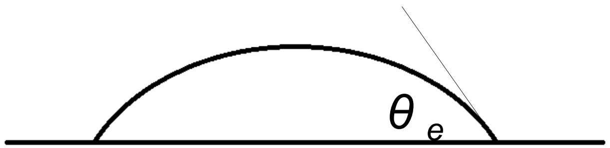
```
while (runTime.run())
{
```

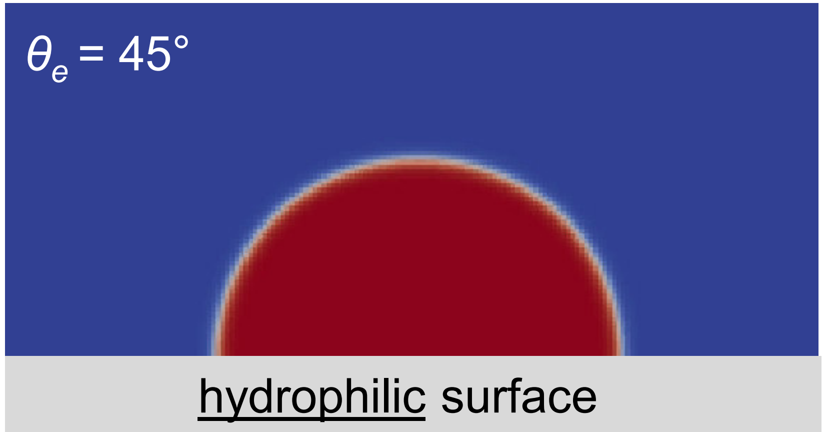
1. Solve transport equation for phase field advection
2. Update chemical potential
3. Calculate surface tension, buoyancy & mixture ρ, μ
4. Solve N-S eqs. for velocity

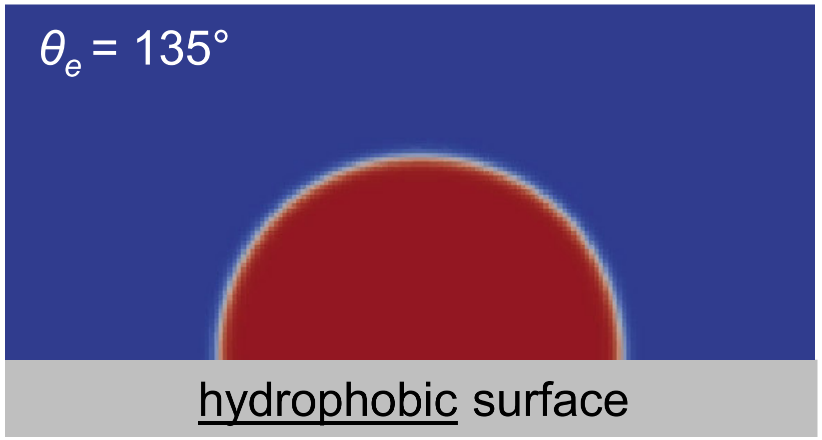
```
}
```

Capillarity-driven droplet spreading / dewetting

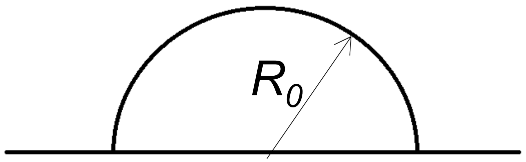
- Wettability of surface
  - Equilibrium contact angle θ_e
    θ_e <= 45° : hydrophilic
    θ_e = 135° : hydrophobic



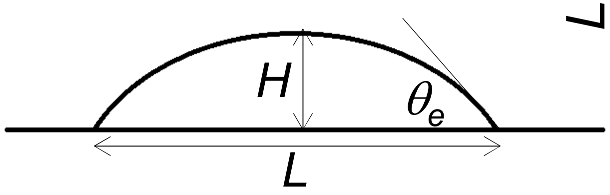




Capillarity-driven Droplet Spreading / Dewetting

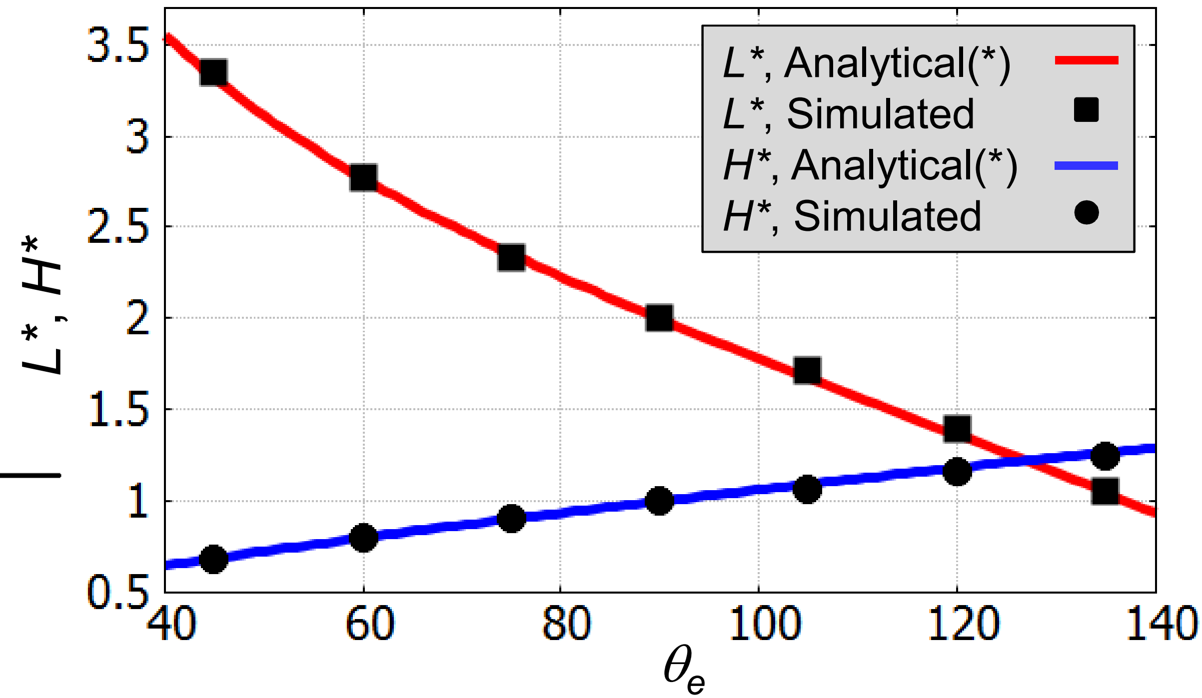


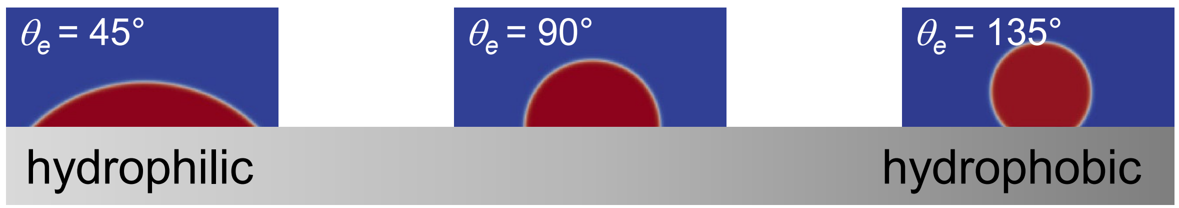
Initial shape



Final shape

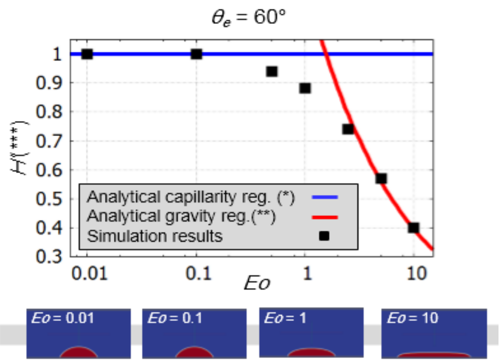
$L^* = L / R_0$
$H^* = H / R_0$



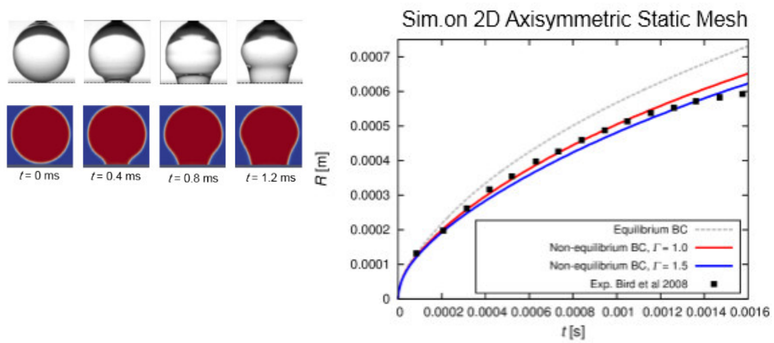


(*) Chen et al. 2009

Further test cases for fundamental wetting



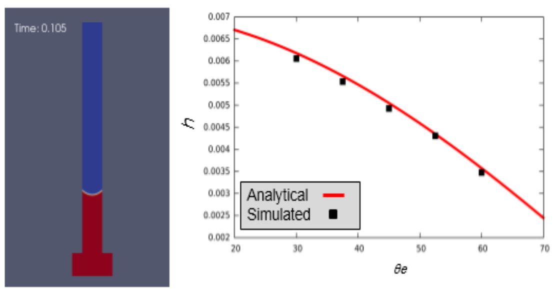
Gravitational effect on droplet shape



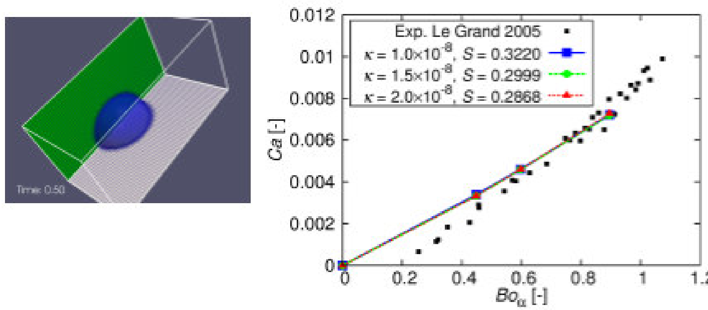
Rapid Wetting in Initial Stage

Comparison with analytical solutions

Comparison with experiments



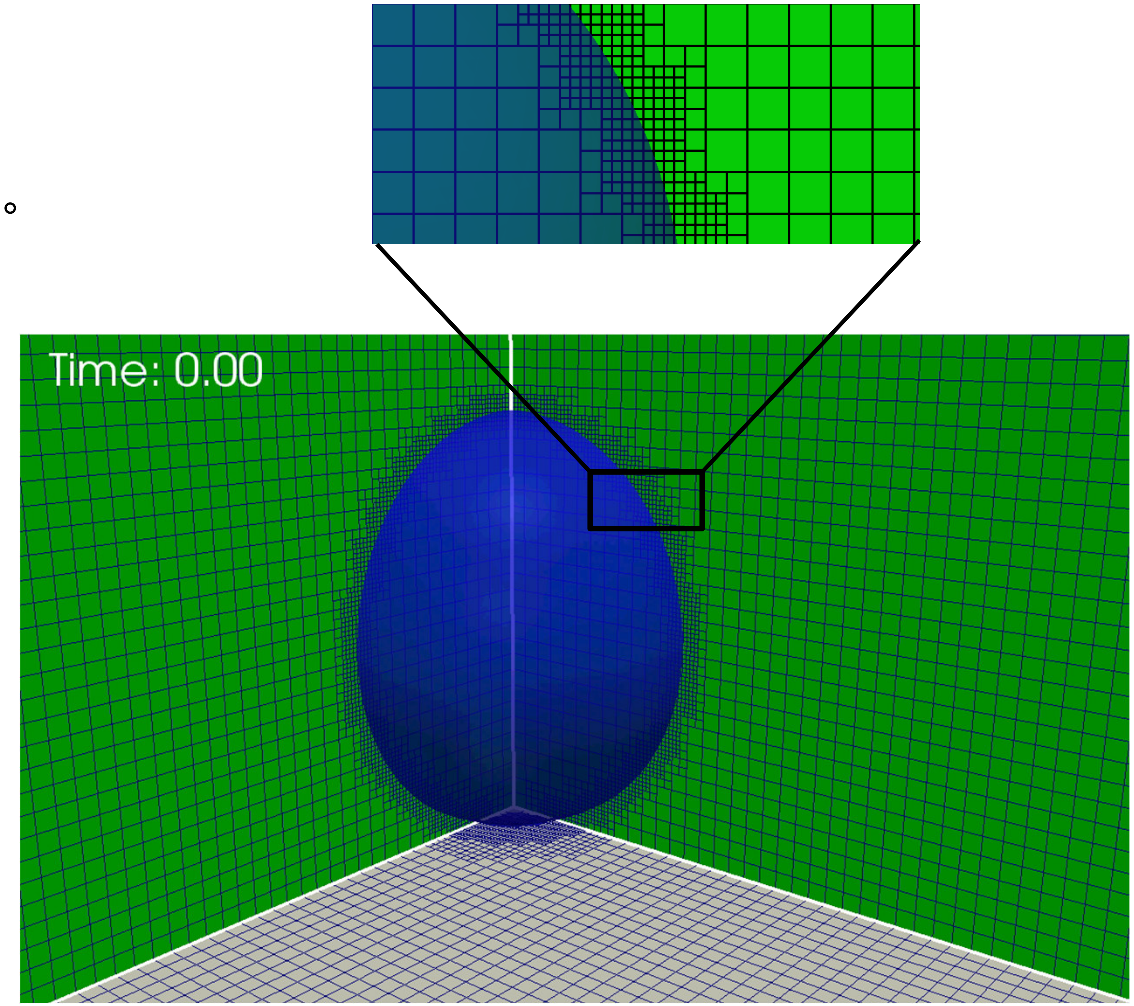
Capillary rise on narrow tube



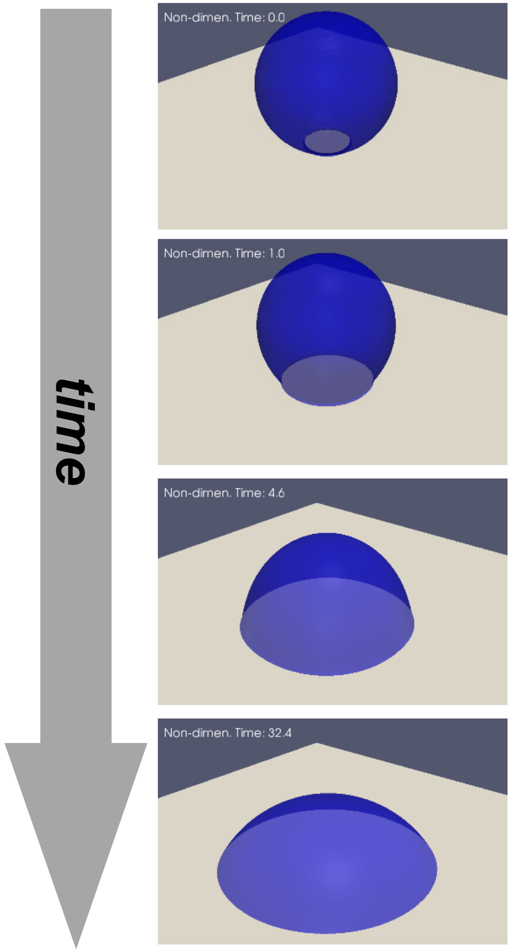
Sliding dynamics on inclined surface surface

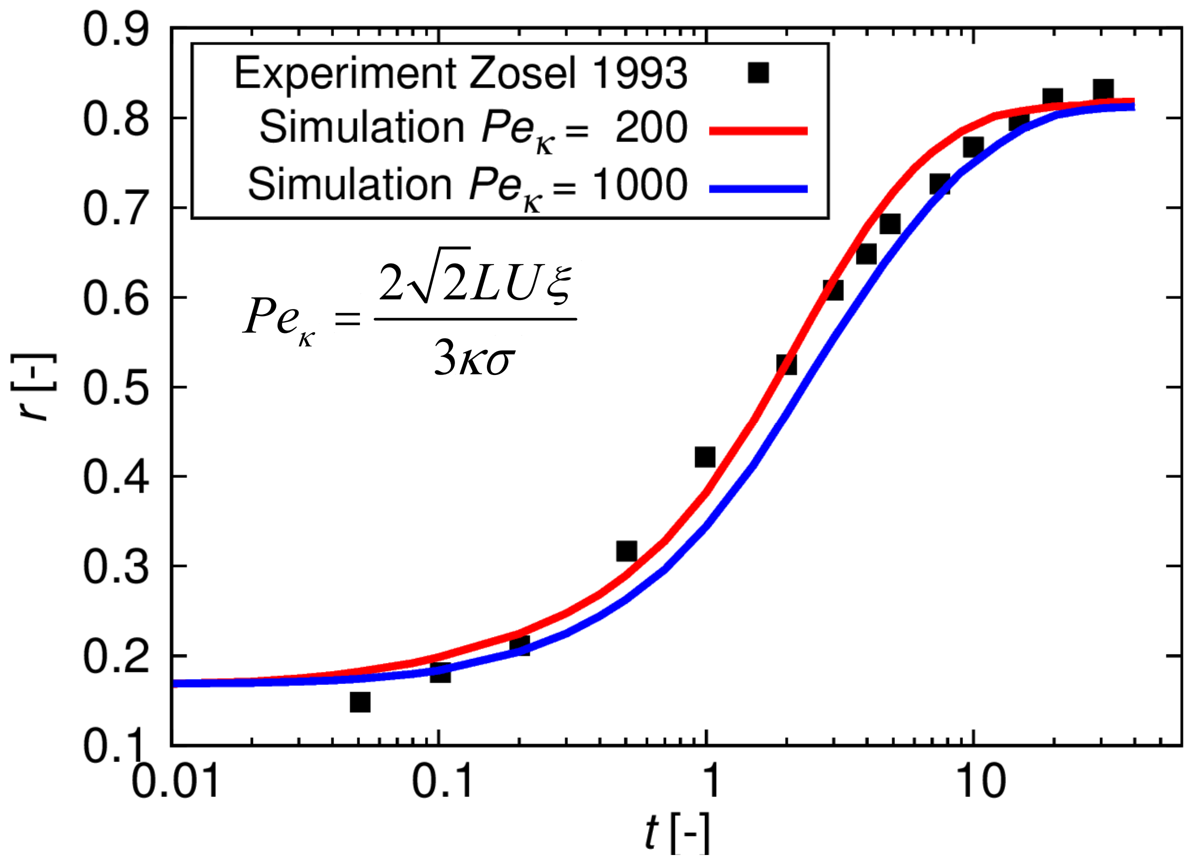
Droplet Spreading on Flat Surface

- **Experiment by Zosel 1993**
  - Droplet of PIB solution
  - Smooth flat PTFE surface
  - Static contact angle θ_e = 58°
  - R_0 = 1.2 ~ 1.5 mm
- **Quarter symmetry**
- **Adaptive Mesh Refinement**
  - Two level refinement
  - For each time-step



Droplet Spreading on Flat Surface

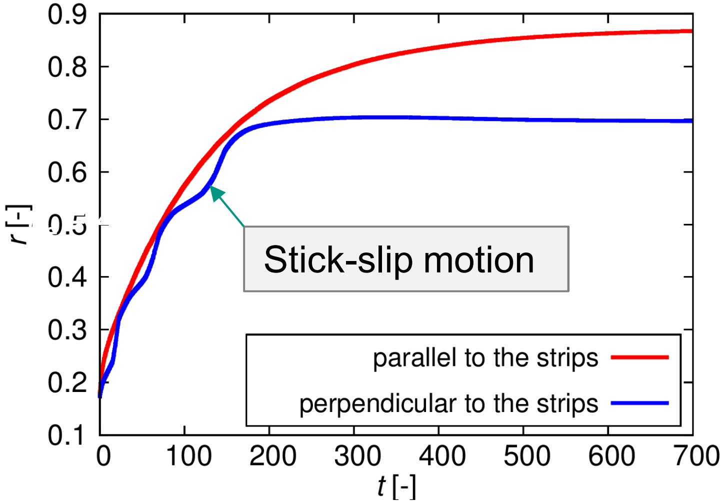




Zosel, A., Studies of the Wetting Kinetics of Liquid-Drops on Solid-Surfaces. Colloid Polym Sci, 1993. 271(7): p. 680-687.

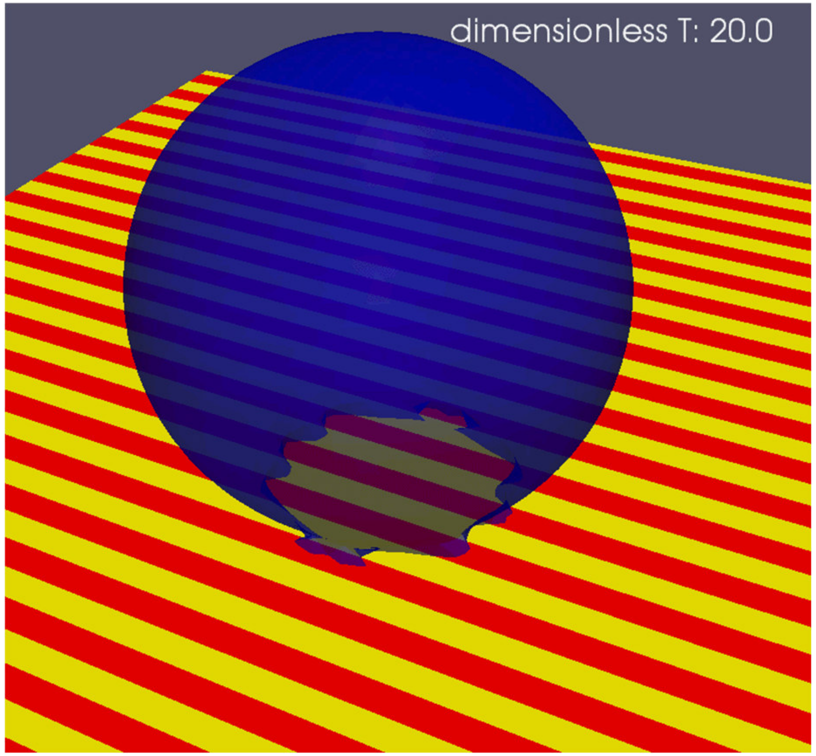
Spreading on chemically heterogeneous surface

- Spreading on a chemically patterned surface
- Alternating stripes made of
  - SiO_2, hydrophilic θ_e = 40°
  - PFDTS, hydrophobic θ_e = 110°
- Anisotropic wetting
  - Droplet is elongated in direction parallel to stripes



θ_e = 40°

θ_e = 110°

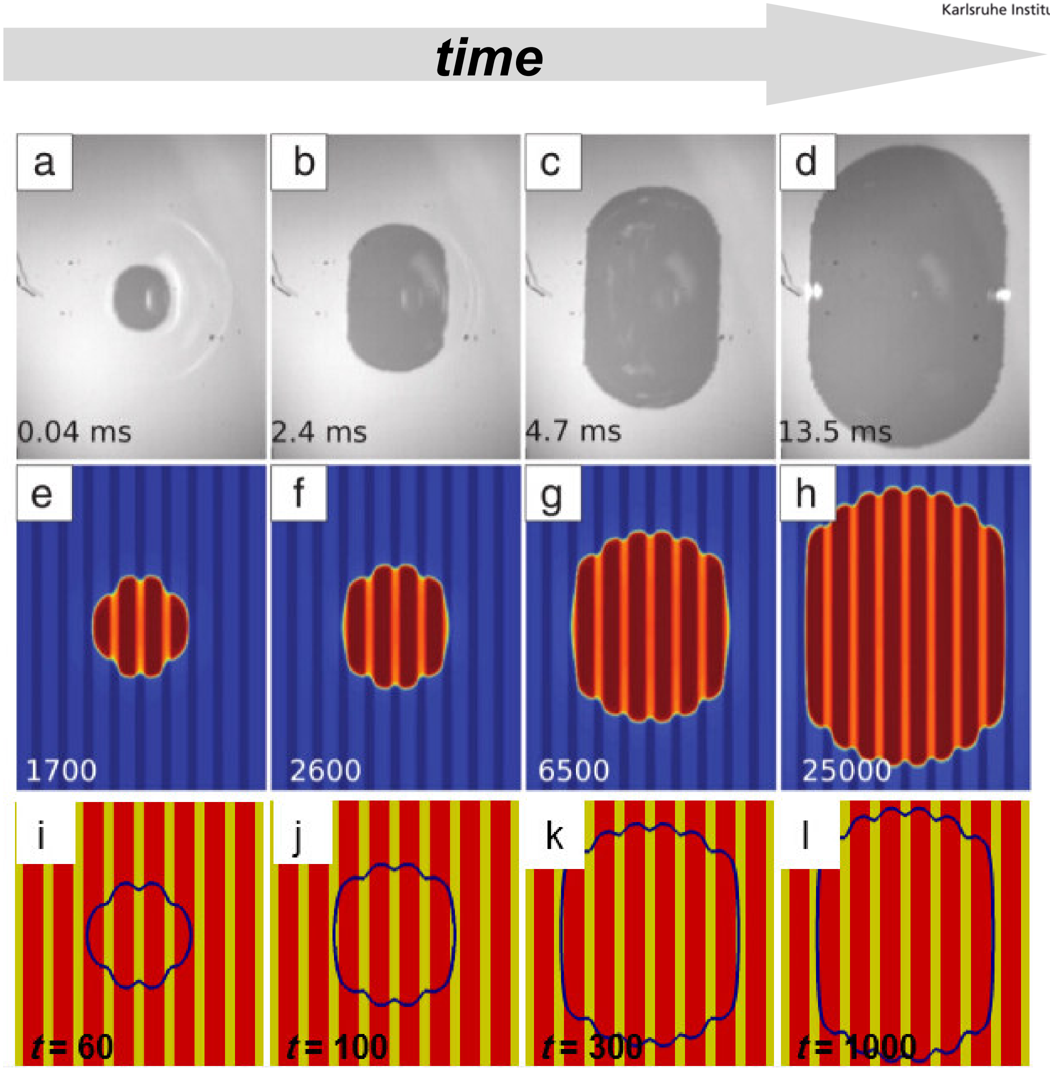


Bottom View

Experiment
Jansen et al. 2013

Lattice-Boltzmann simulation
Jansen et al. 2013

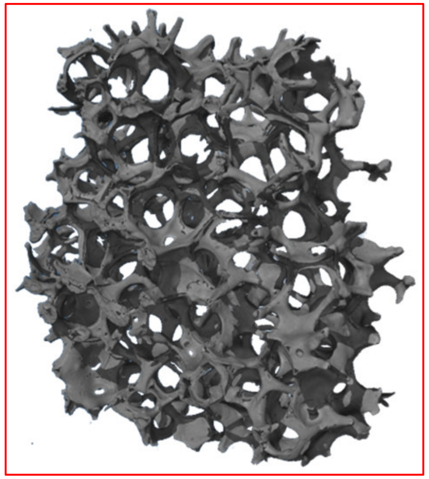
Present simulation
(four cells per stripe)

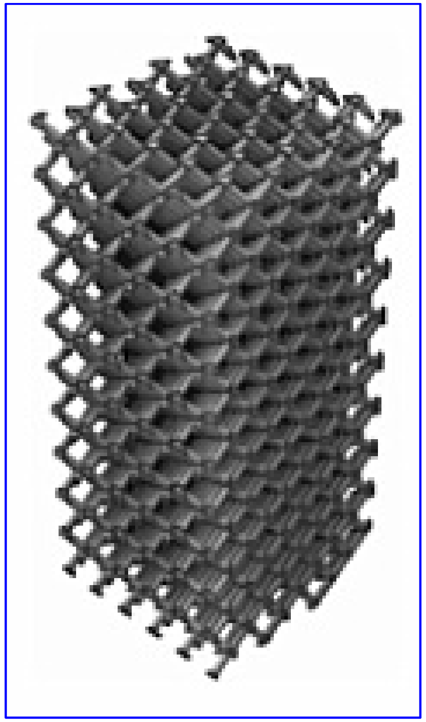


H.P. Jansen et al., Phys. Rev. E 88 (2013) 013008–013017

Solid sponges and POCS

Open-cell foams (sponges) and periodic open cell structures (POCS) combine advantageous properties

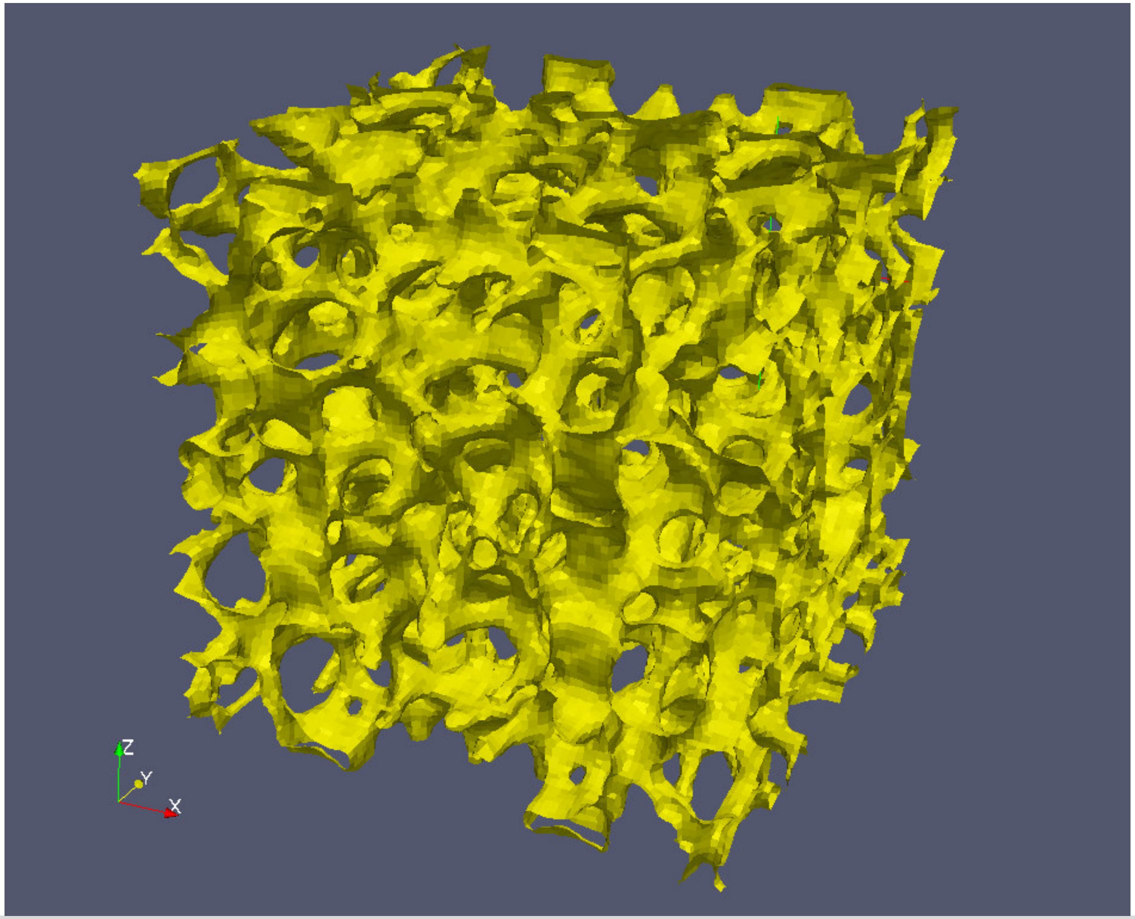




- High porosity
  - Low pressure drop
  - Low weightiness
- High specific surface area
  - Advantageous for heterogeneous reactions and fluid-solid heat/mass transfer
- Continuous solid phase
  - Advantageous for heat transport
  - Possibility for utilizing heat of highly exothermic reactions in a separate process (→ *energy efficiency*)

Two-phase flow in sponge – approach

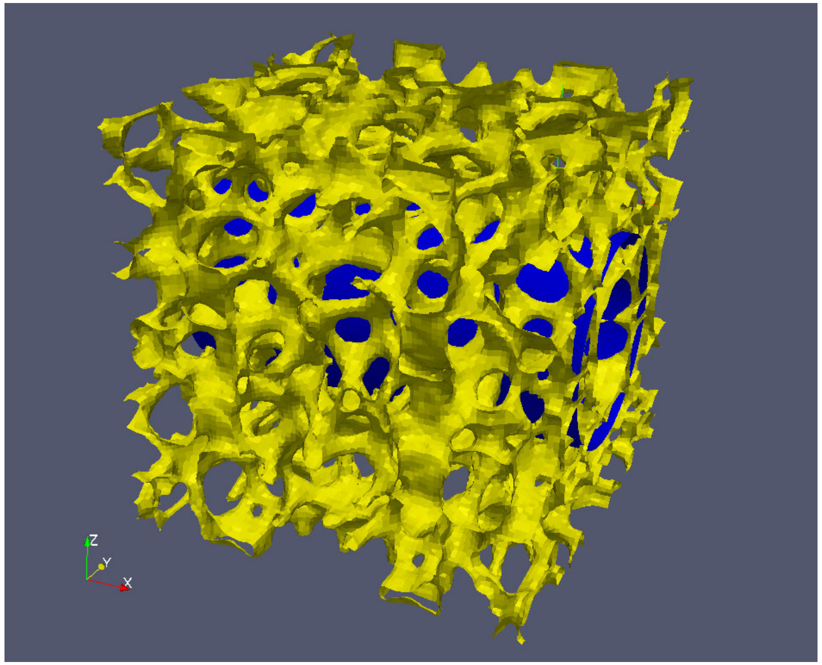
- Problem: realistic inlet conditions for phase distribution
- Solution: mirror domain and use periodic boundary conditions



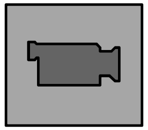
- Sponge geometry reconstructed from micro-CT by KIT-TVT
- Al_2O_3 sponge, 80% porosity, 20 ppi

Two-phase flow in solid sponge

- Specify initial phase distribution in domain and axial pressure drop which drives the flow (source term in N-S equation)
- Simulations for different parameters are under way
- Goal: derive closure relations for use in Euler-Euler model
  - Specific wetted surface area
  - Specific gas-liquid interfacial area
  - …
  - as function of superficial velocities
  - …
  - under variation of materials, porosity and pore size



(about one million mesh cells, $\theta_e = 90°$)



Validation for single phase gas flow

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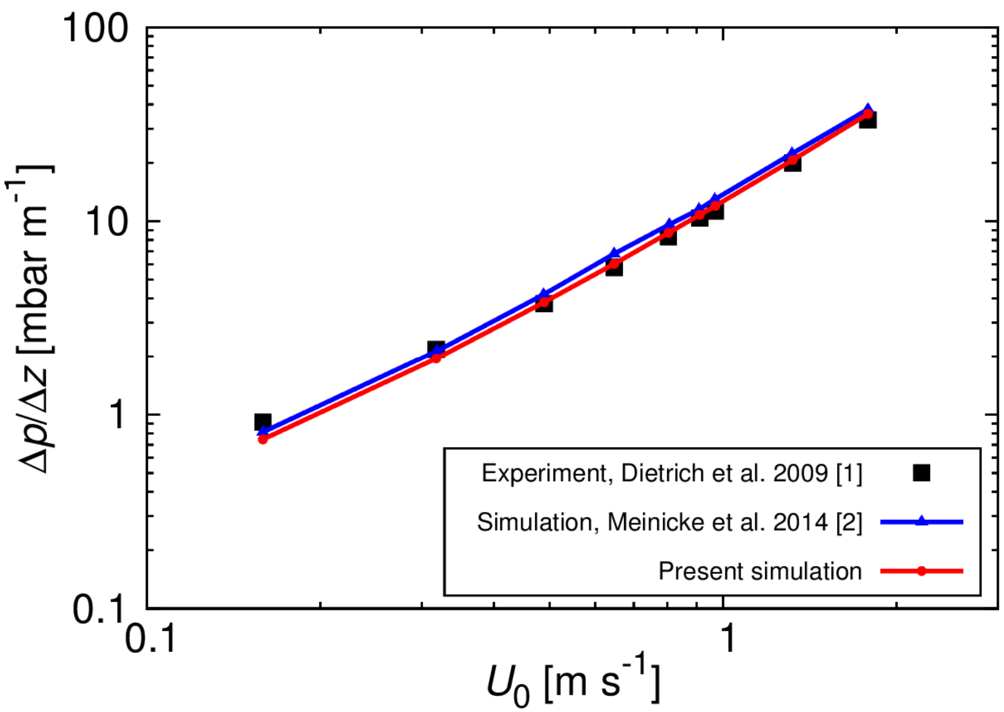
- Apply the solver for gas flow through sponge structure
- Compare simulated pressure drop versus superficial velocity against:
  - Experimental results Dietrich et al. 2009 [1]
  - CFD results using "simpleFoam" Meinicke et al. 2014 [2]



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

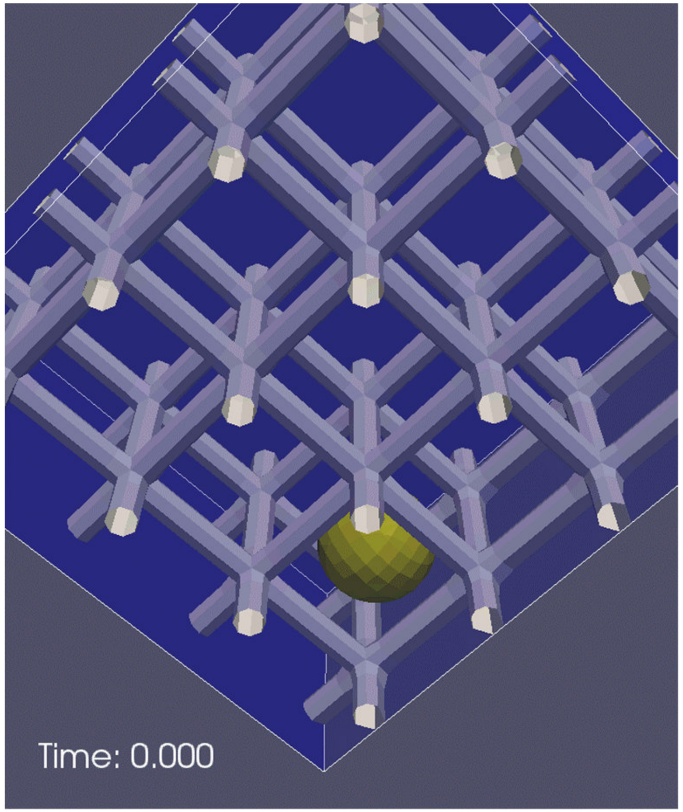
[1] B. Dietrich, W. Schabel, M. Kind, H. Martin. Pressure Drop Measurements of Ceramic Sponges - Determining the Hydraulic Diameter. Chem. Eng. Sci. 64 (16), 3633-3640. 2009

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

Bubble rise in POCS

POCS as internals in bubble column reactors can **enhance gas-liquid mass transfer** (by disturbing/renewing the liquid concentration boundary layer) while only slightly increasing the pressure drop (→ *energy efficiency*)

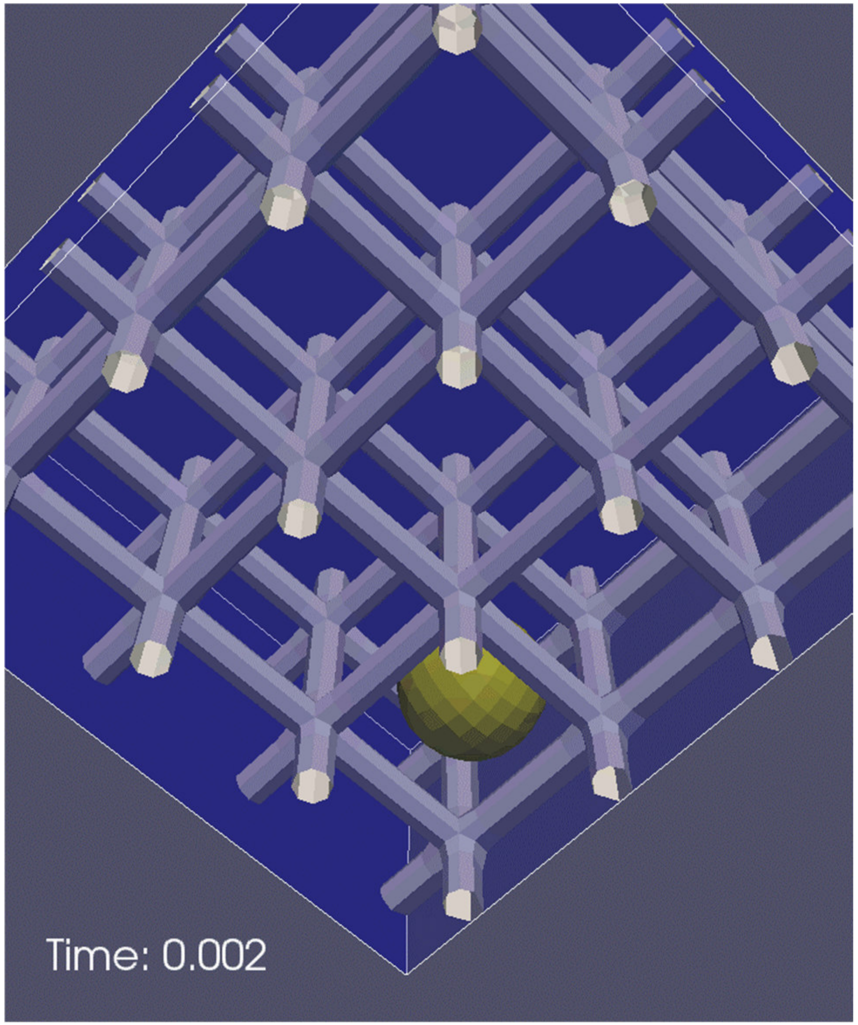
- POCS with window size 4 mm tilted by 45°
- Water and air are initially at rest
- Spherical bubble (diameter 4 mm) is placed so that it will hit the strut during its rise
- Structure is partially wetting (contact angle $\theta_e = 90°$)



POCS from FAU Erlangen

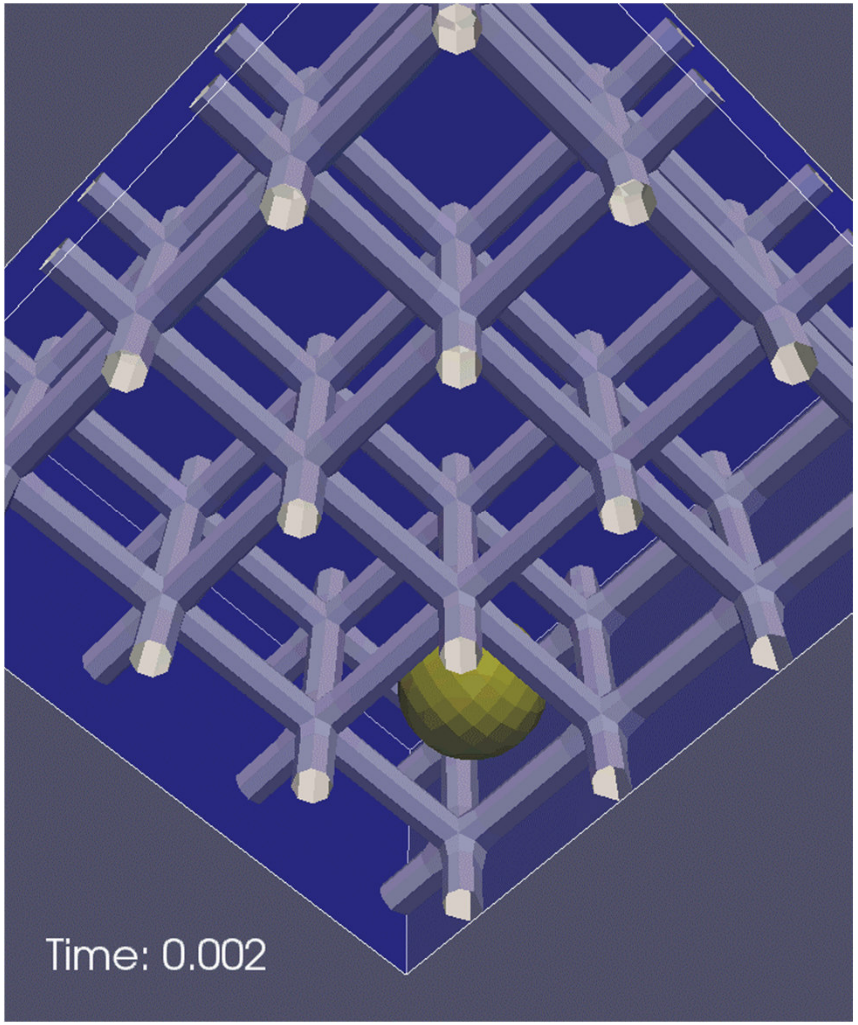
Bubble rise in POCS

- Structure is hydrophilic (contact angle $\theta_e = 0°$)



Bubble rise in POCS

- Structure is hydrophobic (contact angle θ_e =135°)
- Though at this stage, our simulations are qualitative, they show that the bubble interaction with the structure depends on wettability
- Validation is ongoing



Summary and outlook

- Phase Field Method has been successfully implemented in OpenFOAM®
  - Method can handle real density and viscosity ratios
- Successful validation for various fundamental wetting phenomena
- Applications for innovative chemical multiphase reactors
  - Further validation by experimental data required
- In Future: release of **phaseFieldFoam** to OpenFOAM-extend under GNU General Public License

Acknowledgement

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- **Partners**
  - Dr. B. Dietrich, S. Meinicke (KIT-TVT)
  - Dr. H. Marschall (TU Darmstadt)
  - Prof. H. Alla (USTO, Oran, Algeria)
  - Prof. P. Yue (Virginia Tech, USA)