A Phase Field Method with Adaptive Mesh Refinement for Numerical Simulation of 3D Wetting Processes with OpenFOAM®

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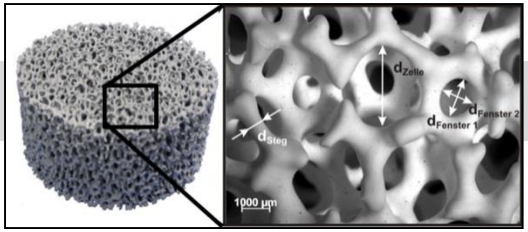
Agenda

- Motivation
- Numerical method
  - Phase field method coupled with Navier-Stokes
  - Implementation in OpenFOAM®
- Test-cases
  - Droplet spreading on flat surface
  - Droplet sliding on inclined surface
  - Anisotropic wetting on chemically-heterogeneous surface
  - Two phase flows in sponge structure
- Ongoing work and outlook

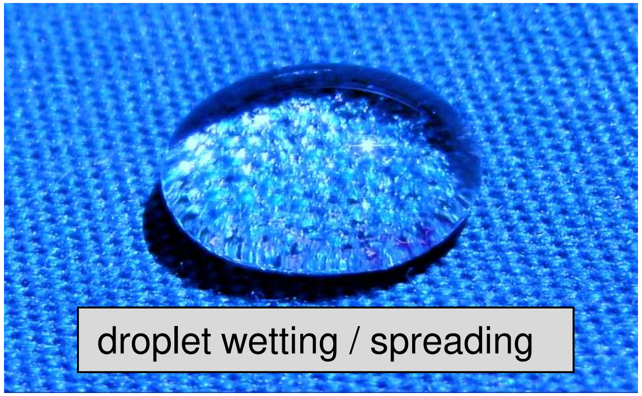
Motivation



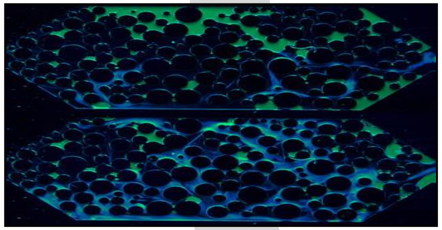
solid sponge chemical reactor

insecticides spray

coating



droplet wetting / spreading



oil recovery from porous structure

lubrication

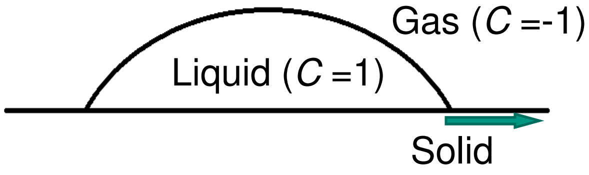
ink-jet printing

Phase Field Methods (only Cahn-Hilliard)

- Phase field (C) as phase indictor
  - difference of volumetric phase fractions
- Cahn-Hilliard eq. for phase field advection

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

  - resolve paradox at moving contact line
- Cahn-Hilliard eq. coupled to momentum eq.
  - surface tension term
  - linear momentum, viscous stress and buoyancy terms
  - mixture properties: density and viscosity



κ : mobility parameter
ε : mean-field thickness
λ : mixing energy parameter
L : reference length
U : reference velocity

- Non-dimensional form:

$$\frac{\partial C}{\partial t} + \mathbf{u}\cdot\nabla\ C = \frac{1}{Pe_\kappa}\nabla^2\phi$$

$$\phi = C^3 - C - Cn^2\nabla^2 C$$

$$Cn = \frac{\xi}{L}, \quad Pe_\kappa = \frac{2\sqrt{2}LU\xi}{3\kappa\sigma}$$

- Boundary condition:

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

Implementation in OpenFOAM®

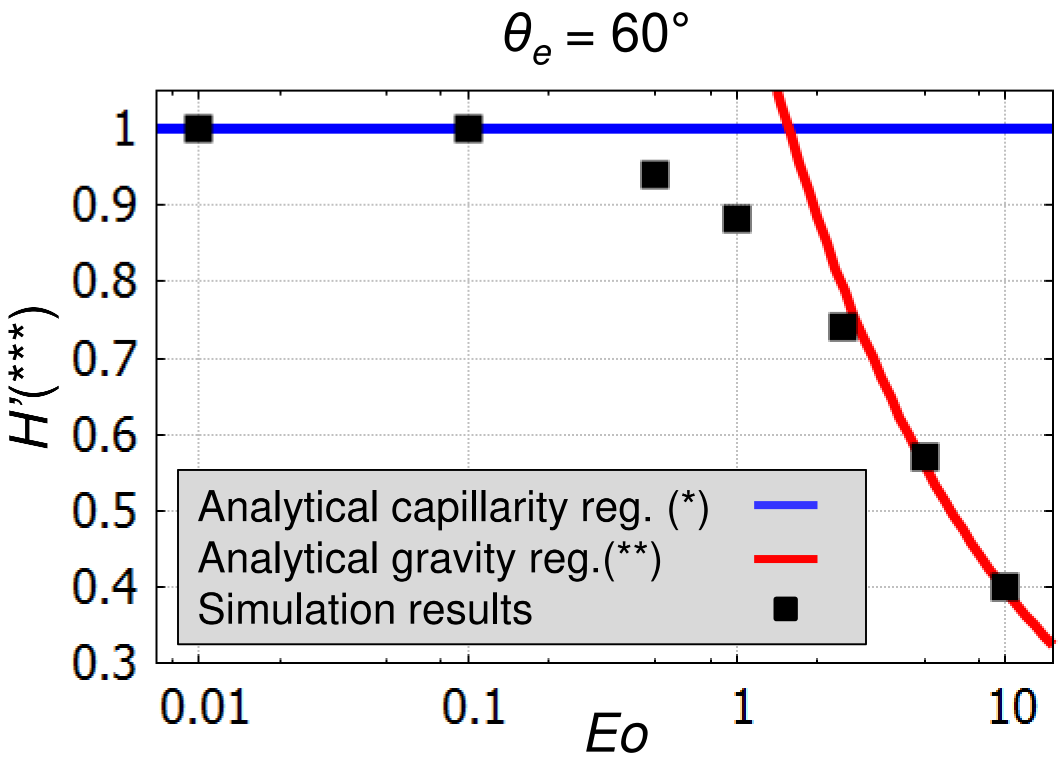
- *interDyMFoam* as starting point
- Phase field advection equation
    - **Cahn-Hilliard**: mobility term is a 4th order derivative (for now treated in segregated manner with time-step sub-cycling)
    - **Allen-Cahn**: Lagrange multiplier to enforce phase volume conservation
- Relative density flux term in momentum eq. due to diffusion of components

  (Ding et al. 2007, Abels et al. 2012)
    - Consistent use of conservative volumetric fluxes and central for volume conservation
- Surface tension in energy formulation
    - As surface tension energy density
    - Explicit source term transferred to pressure equation (Rhie-Chow interpolation practice)

Pseudo code:

```
while (runTime.run())
{
    1. Solve transport equation for phase field advection
    2. Update chemical potential
    3. Calculate surface tension, buoyancy & mixture $\rho$, $\mu$
    4. Solve N-S eqs. for velocity
}
```

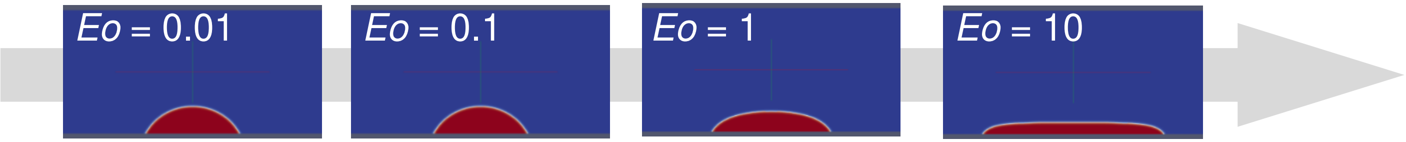
2D Simulation of Droplet Spreading



- Eötvös number (*Eo*):

$$Eo = \frac{(\rho_a - \rho_b) g D^2}{\sigma}$$

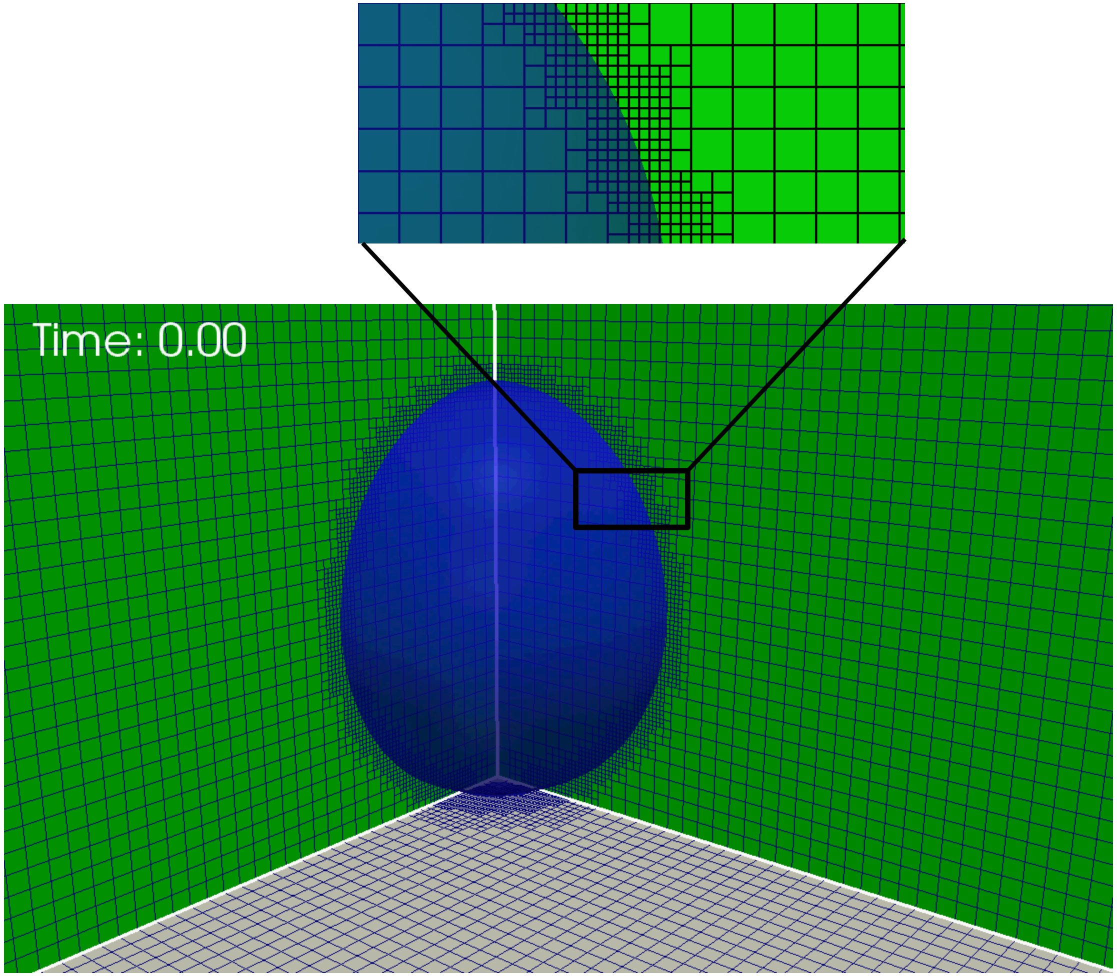
- $Eo \ll 1$
  capillarity-driven regime
- $Eo \gg 1$
  gravity-driven regime
- $Eo \approx 1$
  transitional regime



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

Droplet Spreading on Flat Surface

- **Experiment by Zosel 1993**
  - droplet of PIB solution
  - on smooth flat PTFE surface
  - Static contact angle θ_e = 58°
  - R_0 = 1.2 ~ 1.5 mm
- **Simulation setup**
  - Eötvös no. = 0
  - density ratio = 1
  - viscosity ratio = 0.05
- **Quarter symmetry**
- **Adaptive Mesh Refinement**
  - two level refinement
  - at each time-step



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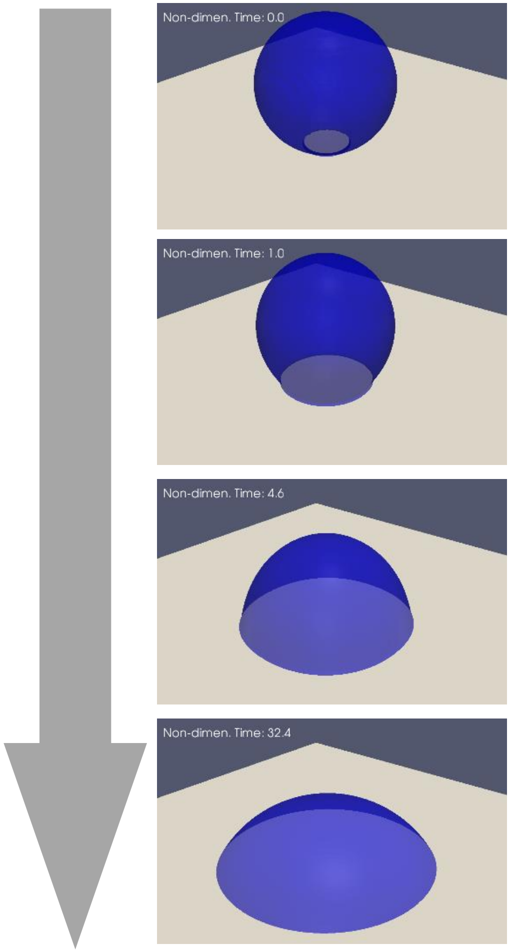
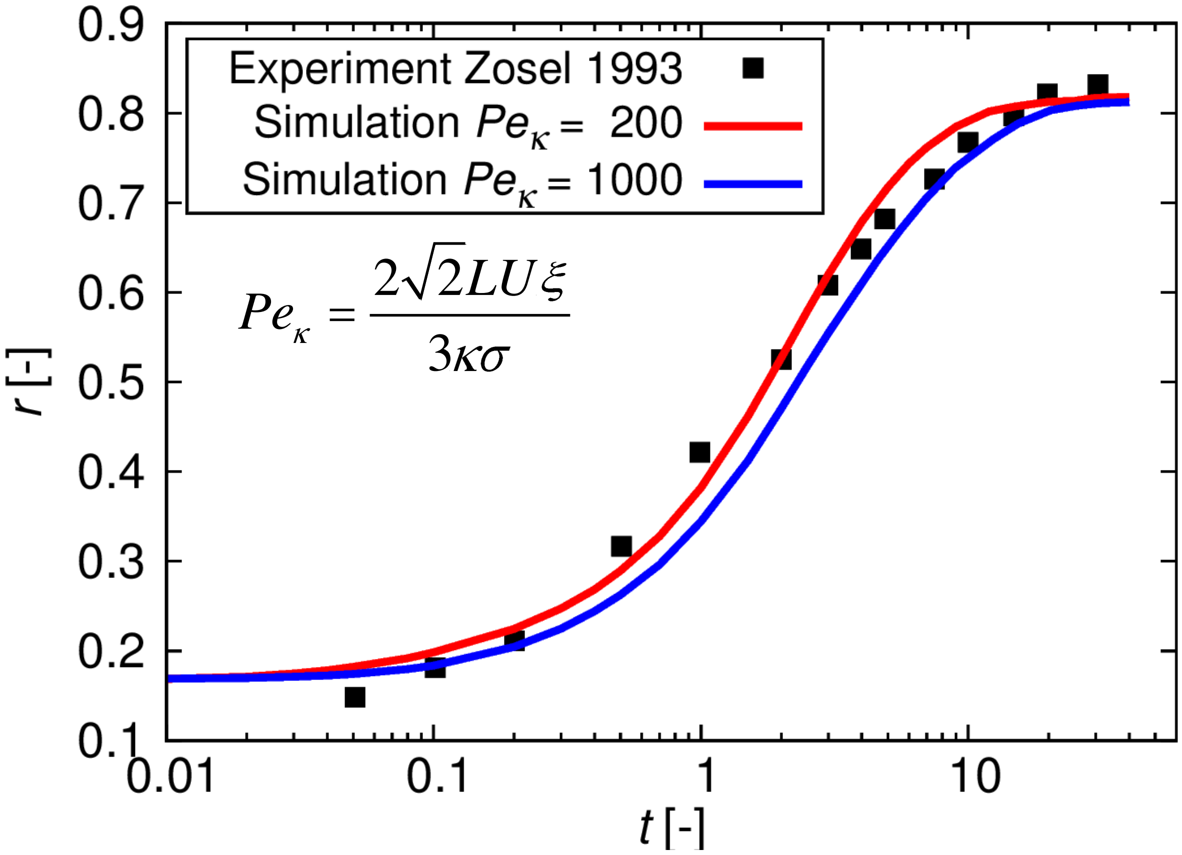
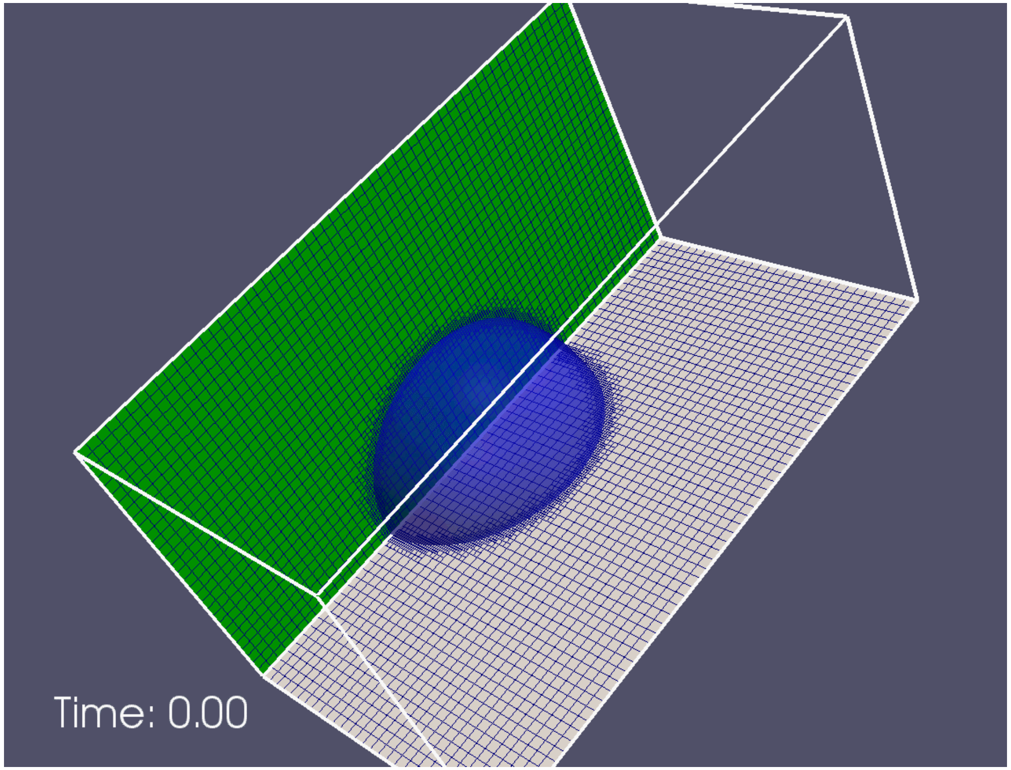




Zosel, A., Studies of the Wetting Kinetics of Liquid-Drops on Solid-Surfaces. Colloid Polym Sci, 1993. 271(7): p. 680-687.

Droplet Sliding on Inclined Surface

- **Experiment by Le Grand et al. 2005**
  - droplet of silicon oil
  - inclined surface (7° < α < 52°)
  - $\theta_e = 52°$
  - Droplet volume = 6 mm^3
- **Half symmetry**
- **Adaptive Mesh Refinement**
  - two level refinement
  - at each time-step



N. Le Grand, A. Daerr, L. Limat, Shape and motion of drops sliding down an inclined plane, J. Fluid Mech. 541 (1) (2005) 293.

Droplet Sliding on Inclined Surface

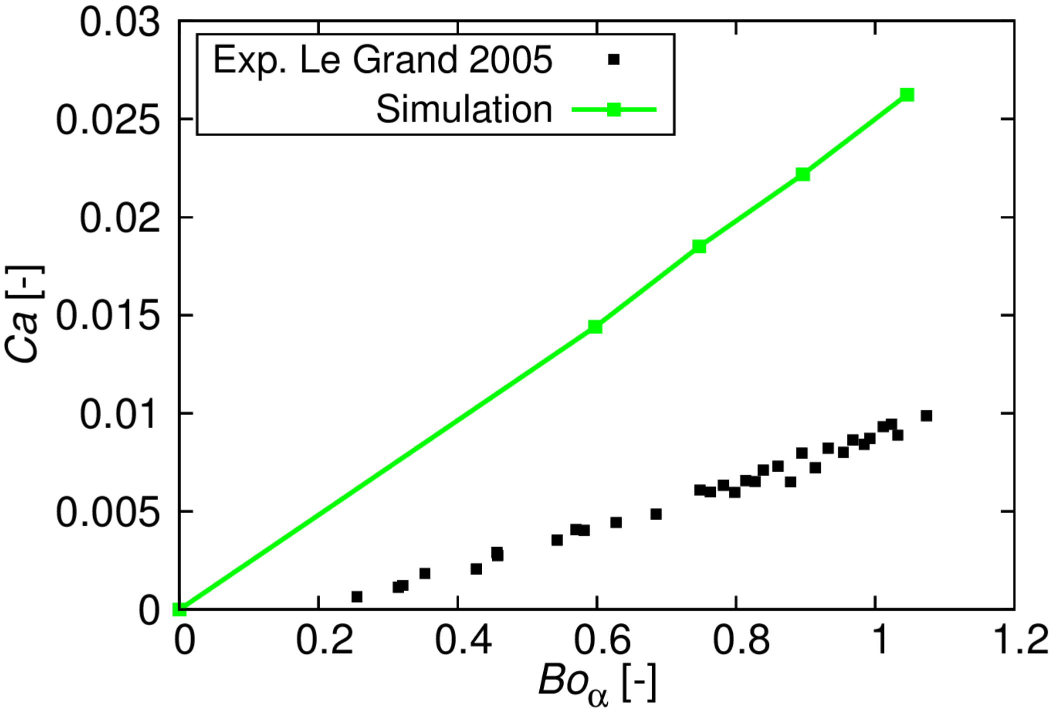
- Dimensionless parameters

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

  - U : sliding velocity
  - α : inclination angle

- Mismatch btw. physical interface thickness and one used in simulation

  → **simulated *U** >> exp. *U***



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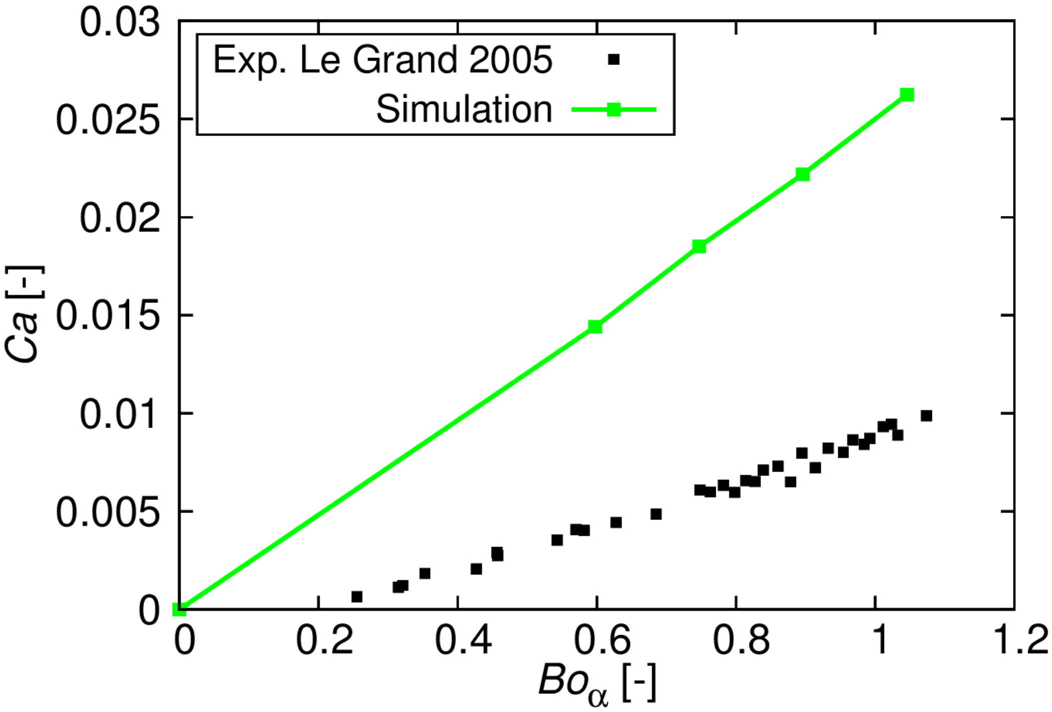
→ **simulated U^* >> exp. U**

- Combining Kim et al. 2002 and Yue et al. 2010, we derive:

$$S = \frac{U}{U^*} = \frac{\ln(R_b/\lambda^*)}{\ln(R_b/\lambda)} \in (0.3, 0.4)$$

  - R_b : droplet radius
  - λ : physical slip length
  - λ^* : numerical slip length



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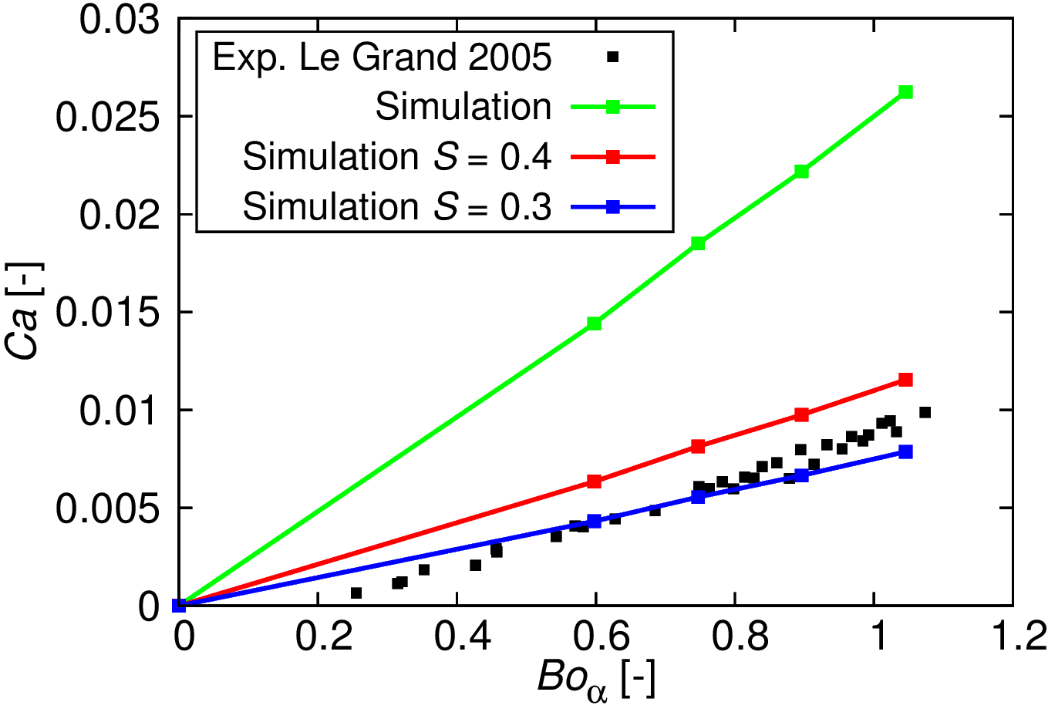

- Validation of our derived *S*
- Currently the code has not considered the pinning effect (i.e. contact angle hysteresis)

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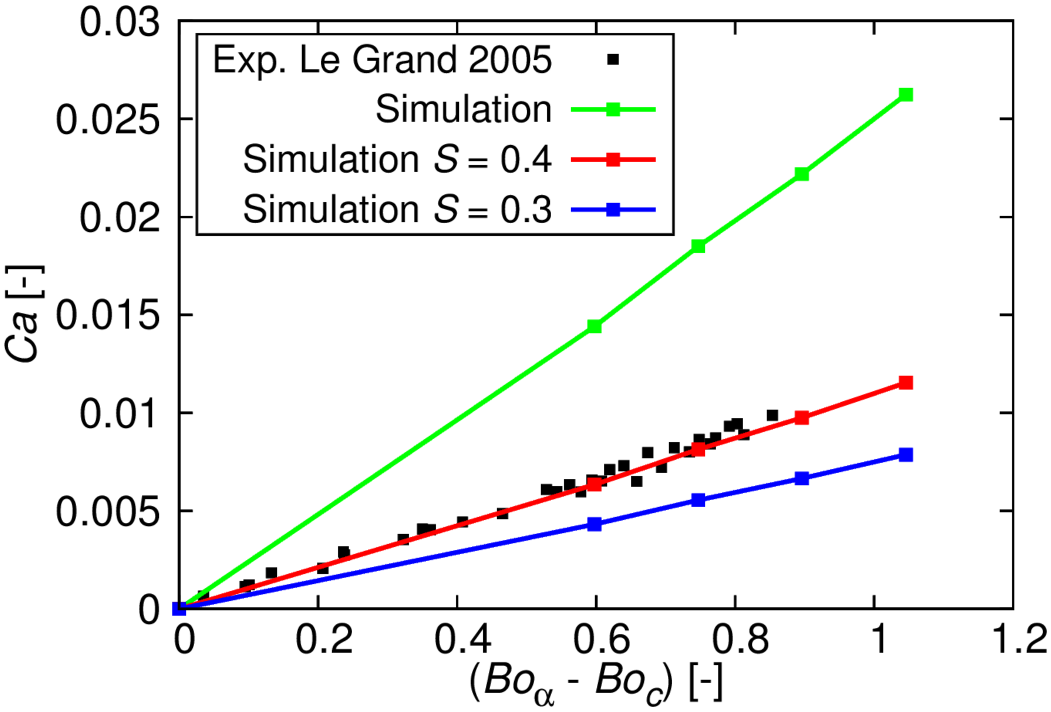


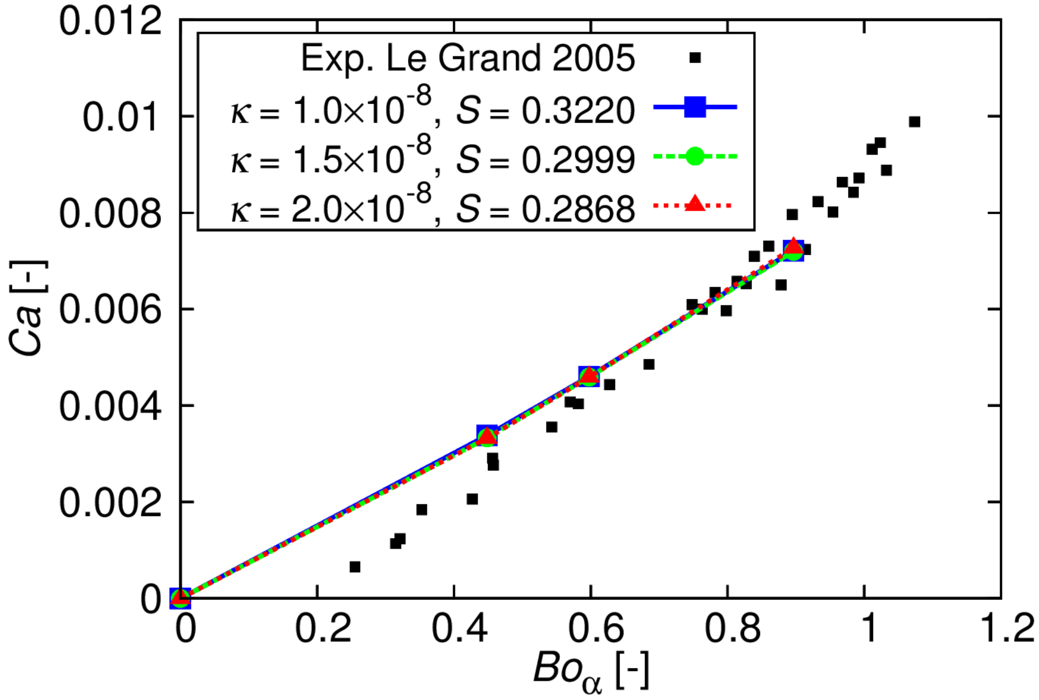
- Bo_c is constant for pining effect

$$Bo_c = V^{2/3}(\frac{\rho g}{\sigma})\sin\alpha_c$$

  - α_c is critical inclination angle

Droplet Sliding on Inclined Surface

- Scaling factor *S* is related to mobility factor *κ*
- Simulation results using different *S* (resp. different *κ*) collapse into a single curve
- Via *S*, numerical results are independent of *κ*

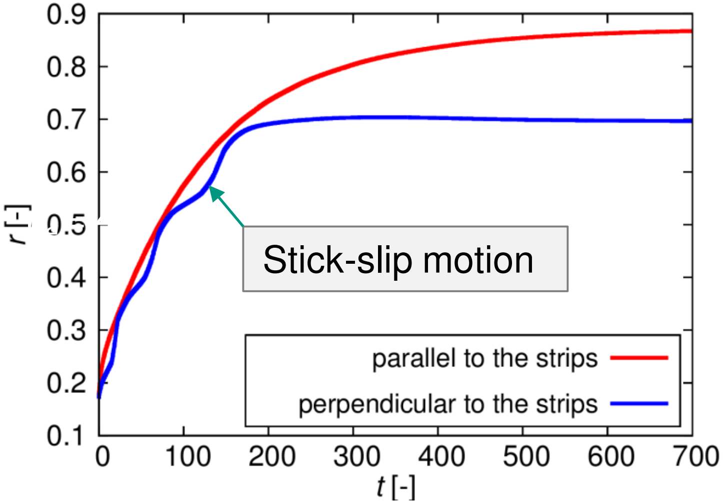


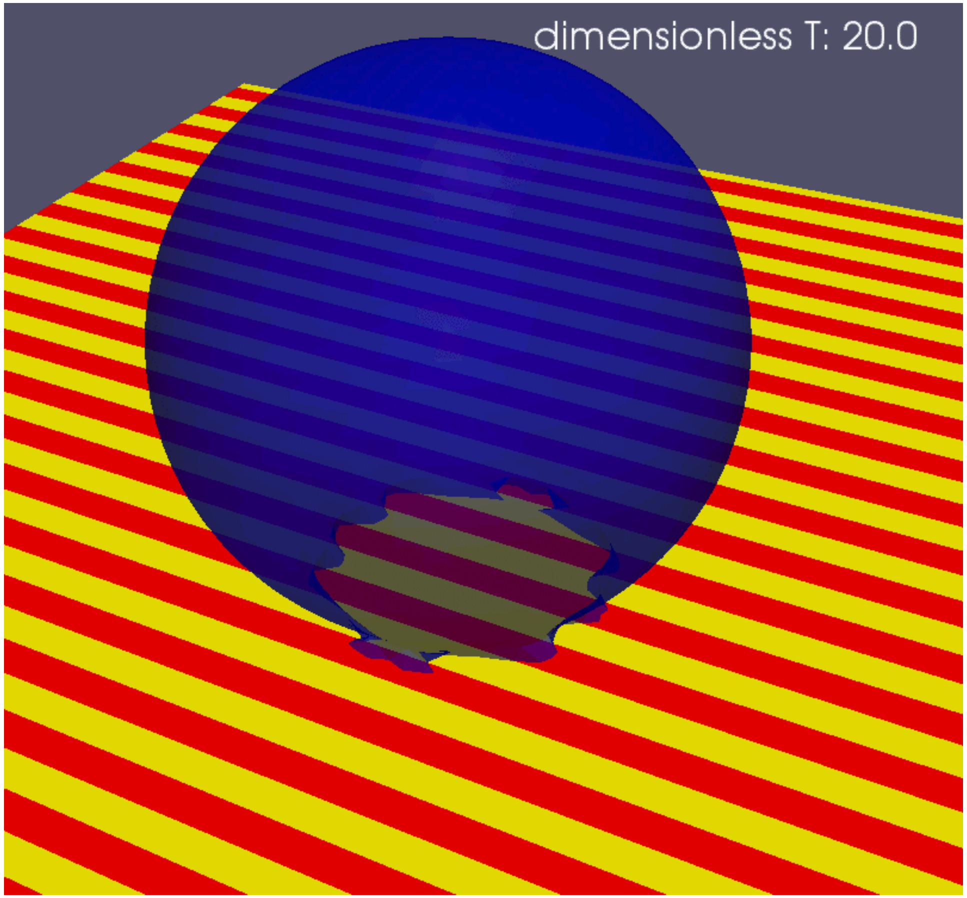
- **Provided physical slip length is known, phase field simulation is a predictive tool!**

Spreading on Chemically Heterogeneous Surface

- Experiment by Jansen et al. 2013

- Alternating strips made of:
  - SiO_2, hydrophilic, $\theta_e = 40°$ (red)
  - PFDTS, hydrophobic, $\theta_e = 106°$ (yellow)
- Anisotropic wetting
  - droplet elongated in direction parallel to strips





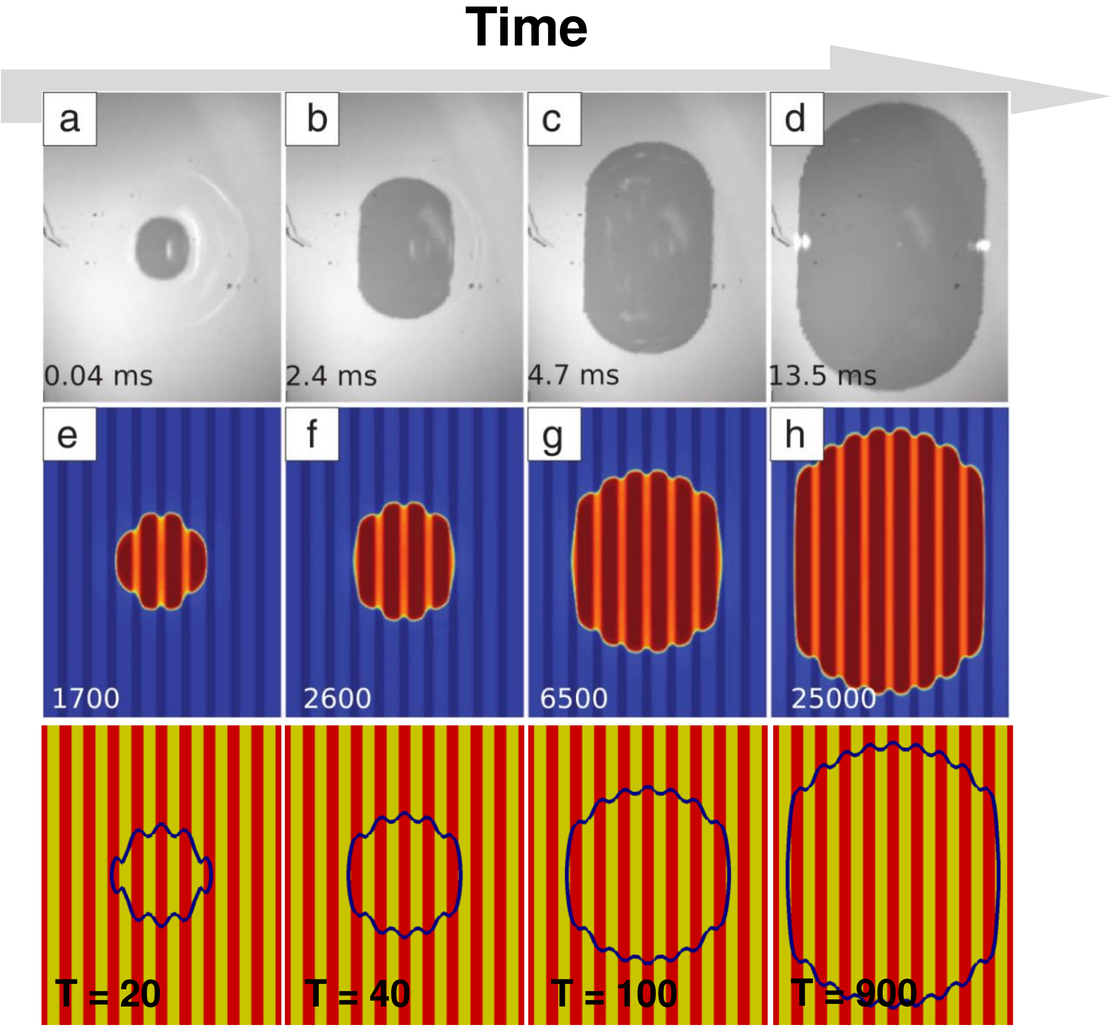
H.P. Jansen et al., Lattice Boltzmann modeling of directional wetting: comparing simulations to experiments, Phys. Rev. E 88 (2013) 013008–013017.

Bottom View

Experiment
Jansen et al. 2013

Lattice-Boltzmann
simulation
Jansen et al. 2013

Our simulation
(four cells per strip)



Wetting in Solid Sponge Structure

- **S. Meinicke (Institut für Thermische Verfahrenstechnik, KIT)** provides the sponge geometry

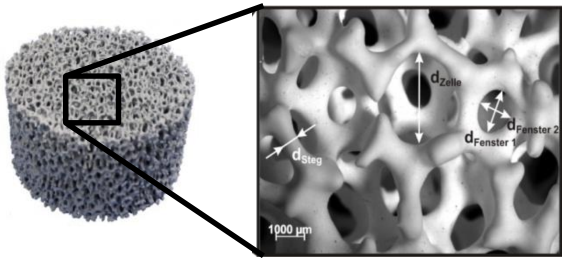
- calculations on exemplary sponge sample type:
  - Al_2O_3
  - porosity = 80%
  - 20 pores per inch (ppi)

→ investigations on further sponge types planned/projected/ongoing

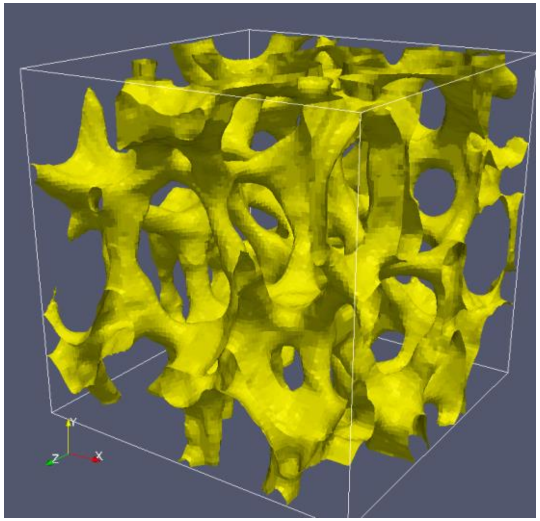
- based on MRI and (µ)CT scannings

- reconstruction of sponge structure in MATLAB produces STL file

- *blockMesh* + *snappyHexMesh*



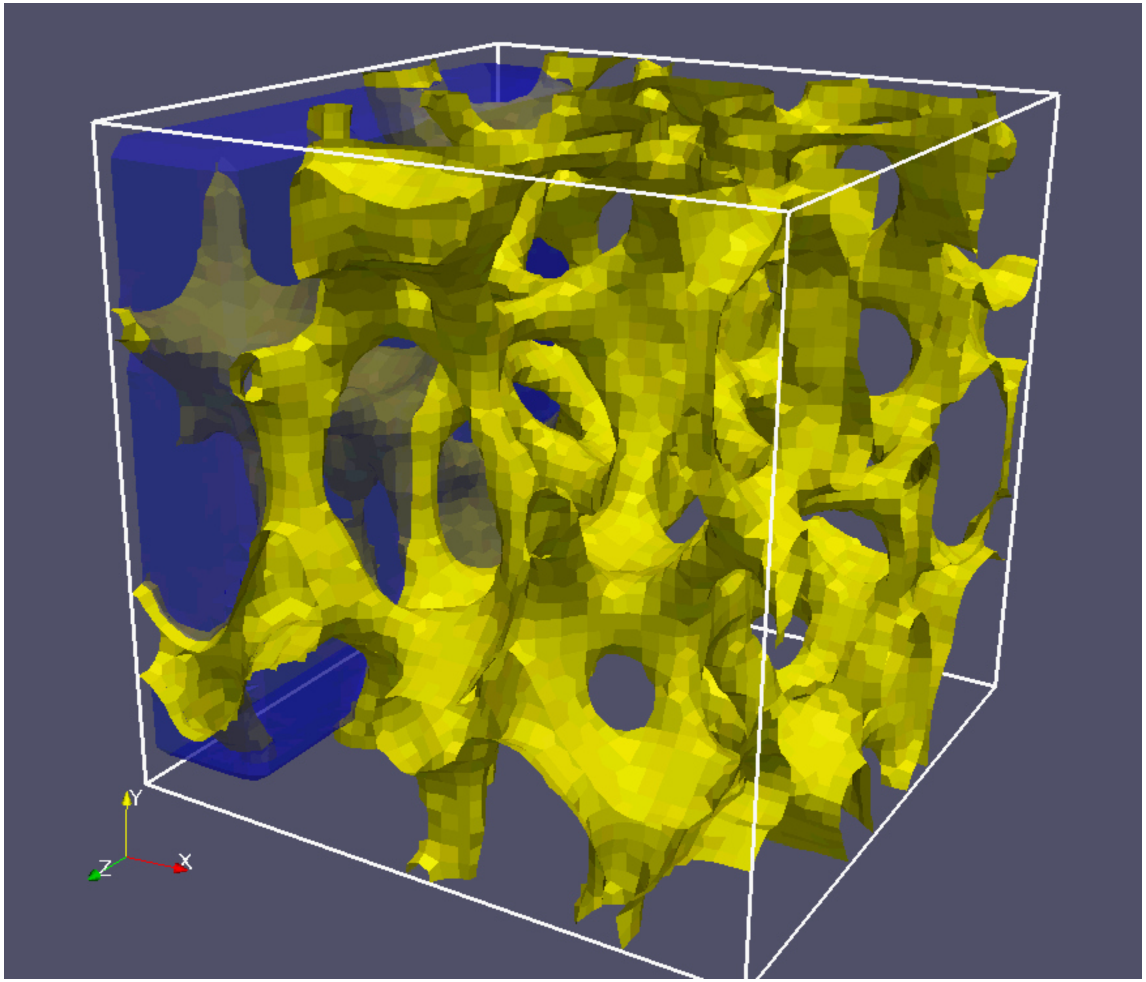
solid sponge chemical reactor



geometry for CFD simulation

First Results

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



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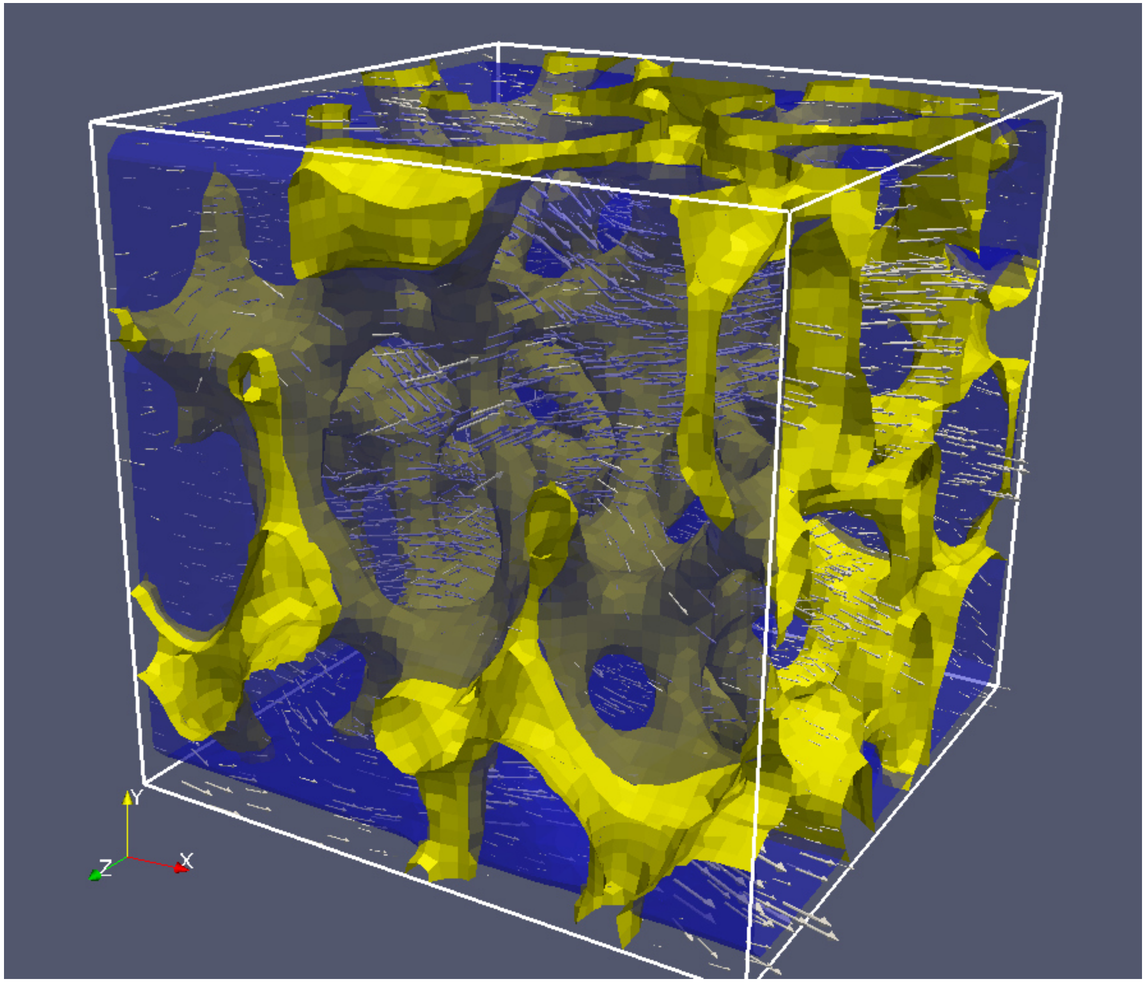


Ongoing work – Numerical Method Development

- Current state:
  - **Novel top-level solver**: `phaseFieldFoam`, supporting foam-typical algorithmic flexibility, e.g.

    ```
    rhoPhi = phaseField.correct(C, Phi);
    ```

  - **3 new model libraries**
    (following common strategy design pattern; run-time selection via factory method)
    - `diffuseInterfaceModels`

      Abstract base class for diffuse interface models.
    - `diffuseInterfaceProperties`

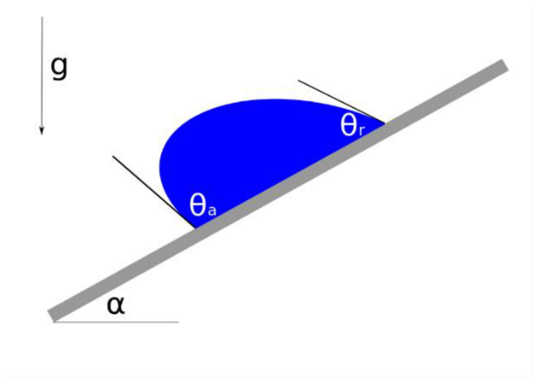
      Diffuse interface mixture properties from phase transport properties.
    - `phaseContactAngle` (generalization of `alphaContactAngle`)

      Abstract base class for phaseContactAngle boundary conditions **for both the volume-of-fluid and the phase-field approach.**

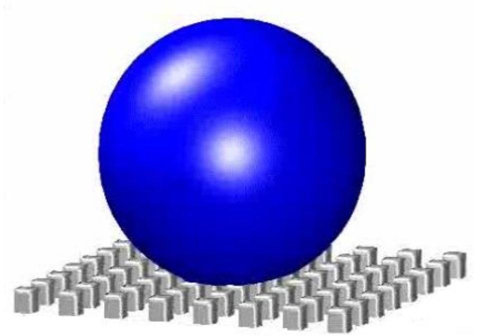
      Static and dynamic contact angle models, e.g. **FAM-based impl. of wall energy relaxation.**
  - **Bunch of utilities** for pre- and post processing, e.g. generic `smoothField` utility.
- Further steps:
  - Implementation of so-called **compensation scheme** for wall energy relaxation model.
  - Implementation of **block-coupled solution approach to phase field transport** (simultaneous solution of decomposed Cahn-Hilliard equation).

Next Steps towards Application

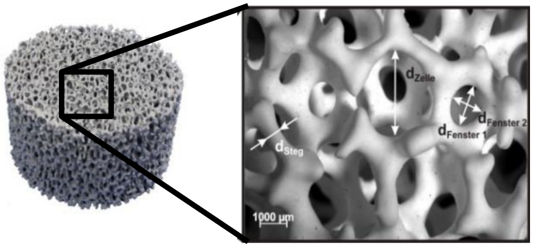
- Pinning effect of droplet on inclined surface



- Droplet wetting on topologically heterogeneous (rough) surface



- Two-phase flows in sponge structure
  - Provide closure for macroscopic model
  - Coupling hydrodynamics with mass transfer and chemical kinetics



Further Outlooks

- Release of the solver **phaseFieldFoam** to OpenFOAM-extend under GNU General Public License

- **phaseFieldFoam** advantageously applied for a wide range of multi-scale multi-phase flows:
  - Droplet/bubble breakup/coalescence
  - Viscoelastic two-phase flow
  - … …

- Phase field simulation in sponge structure can also be applied in:
  - Fuel cells
  - Oil recovery
  - Heat exchanger
  - … …

Acknowledgement

- Funded by Helmholtz Energy Alliance "Energy-efficient chemical multiphase processes" (HA-E-0004)(*)
  - Partners:

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HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

KIT Karlsruher Institut für Technologie

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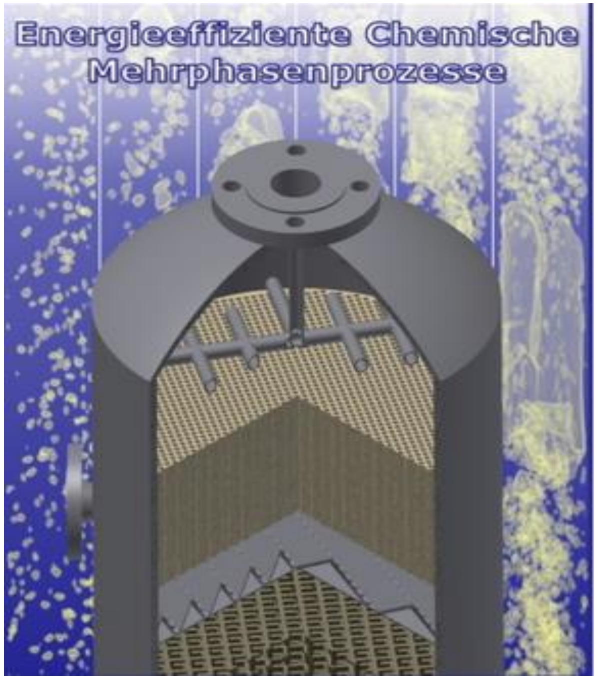

(*) Website: https://www.hzdr.de/db/Cms?pNid=2972