Development of Phase Field Methods for Direct Numerical Simulation of Wetting Processes with OpenFOAM®

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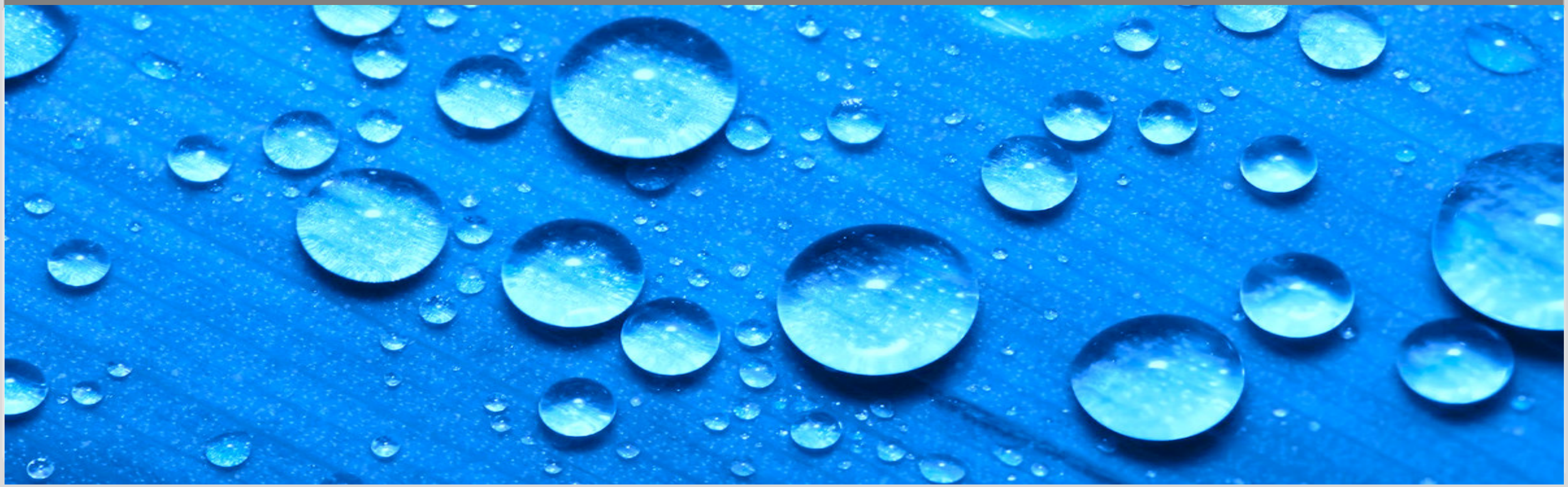
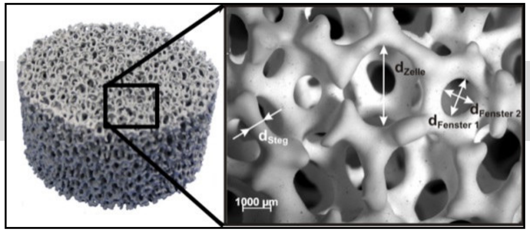


Outline

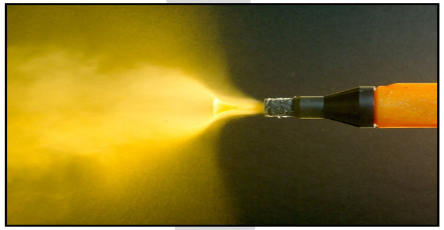
- Motivation
  - Wetting/spreading in industrial applications
  - Why phase field method?
- Numerical method
  - Governing equations
    Allen-Cahn and Cahn-Hilliard equations for phase field advection
  - Implementation in OpenFOAM®
- Verification
  - Mobility and surface tension term
  - Equilibrium contact angle boundary condition
- Droplet Wetting
  - 2D static mesh simulation
  - 3D adaptive-mesh-refinement simulation
- Conclusions, ongoing and next steps

Motivation

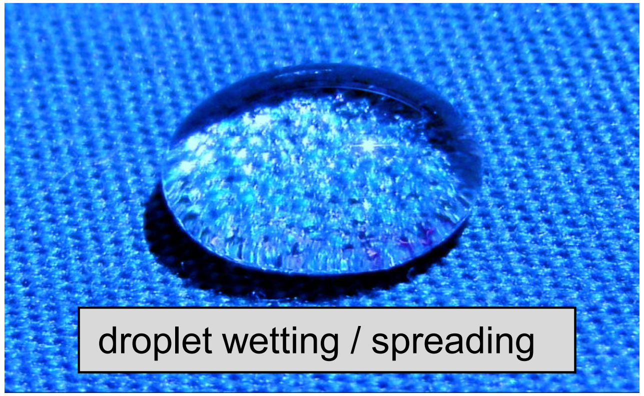


solid sponge chemical reactor

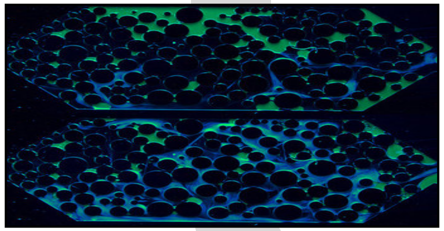
insecticides spray



coating



droplet wetting / spreading

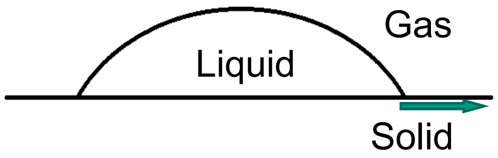


oil recovery from porous structure

lubrication

ink-jet printing

Focus & Difficulty of Numerical Modeling

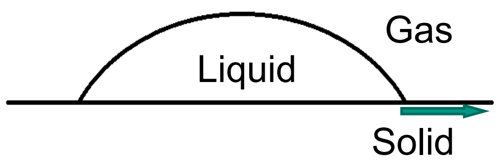


Paradox btw. motion of contact line & no-slip BC

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

α: volumetric phase fraction

Focus & Difficulty of Numerical Modeling



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

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

α: volumetric phase fraction

- This paradox can be resolved by:

Sharp interface method

- e.g. Volume-Of-Fluid method
- via Navier-slip BC

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

- L_s is slip length → difficult to choose in physical sense!

Diffuse interface method

- e.g. Cahn-Hilliard model
- via mobility term

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

- C is phase field (difference in volume fractions)
- Φ is chemical potential

$$\phi = \frac{\lambda}{\varepsilon^2}C(C-1)(C+1) - \lambda\nabla^2 C$$

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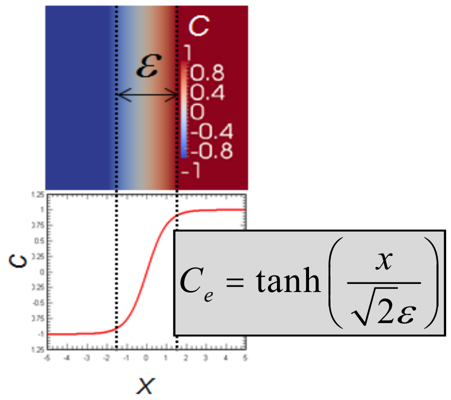
Phase Field Methods
(only Cahn-Hilliard model)

- Phase field (*C*) as phase indictor
  - difference of volumetric phase fractions
  - *C* = 1 for liquid, *C* = -1 for gas
- Cahn-Hilliard equation for phase field advection

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

$$\Phi = \frac{\lambda}{\varepsilon^2} C(C-1)(C+1) - \lambda \nabla^2 C$$

- Cahn-Hilliard equation is closely coupled to momentum equation through
  - Surface tension term
  - Linear momentum, viscous stress terms and buoyancy terms
    (mixture properties: density and viscosity)



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

Non-dimensional form:

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

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

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

Implementation in OpenFOAM®

- *interDyMFoam* as starting point
- Cahn-Hilliard (CH) and Allen-Cahn Equations (AC)
  - CH: mobility term is a 4th order derivative (for now treated in segregated manner with time-step sub-cycling)
  - AC: Lagrange multiplier to enforce phase volume conservation property
- Relative density flux term in momentum equation due to diffusion of components
  - Consistent use of conservative volumetric fluxes and central for volume conservation
- Surface tension term in energy formulation
  - Implemented 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 ρ, μ
4. Solve N-S eqs. for velocity

```
}
```

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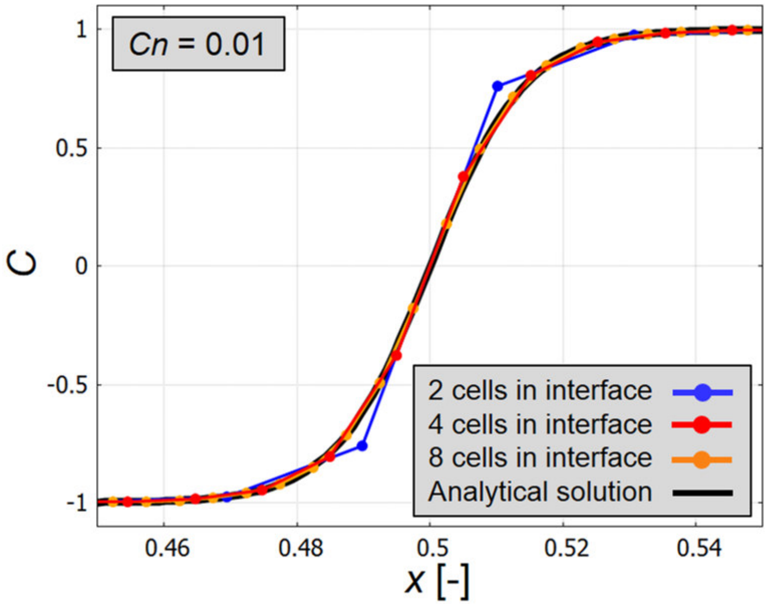
Verification of Mobility and Surface tension

- Mobility term: 4th order derivative

$$\frac{\partial C}{\partial t} = \nabla^2 (C^3 - C - Cn^2 \nabla^2 C)$$

➢ 8 cells for interface leads to very good agreement



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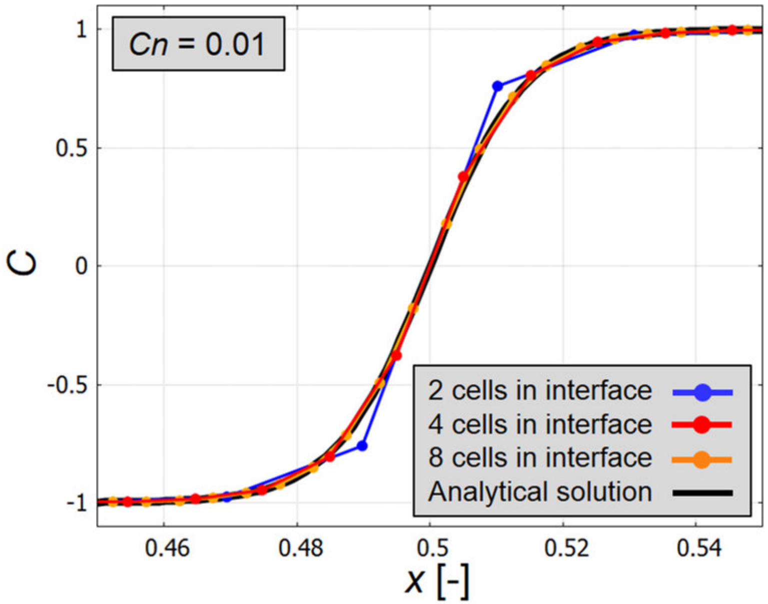
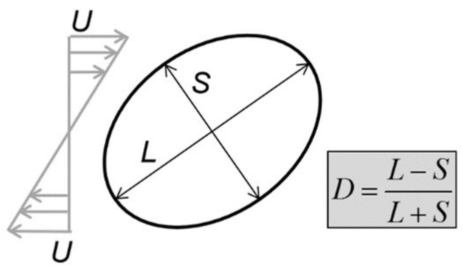
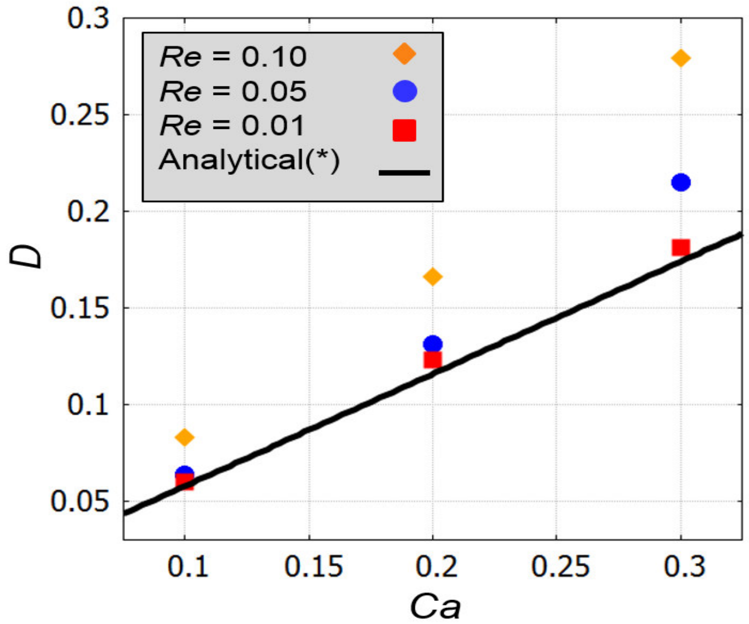


- Surface tension term



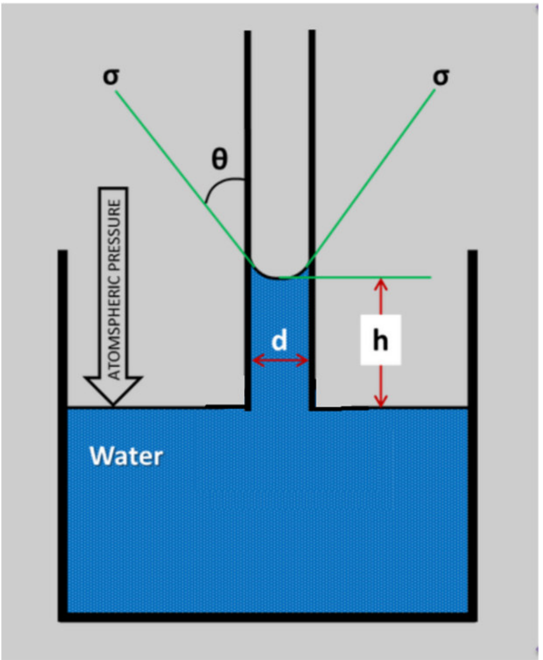


(*) Tayler 1932

Capillary Rise Between Parallel Plates

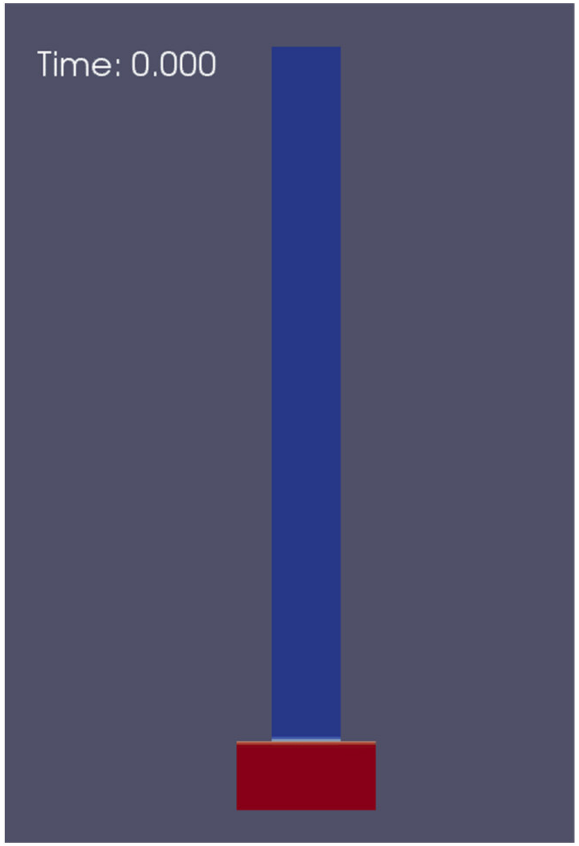
- Neumann boundary condition for equilibrium contact angle θ

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



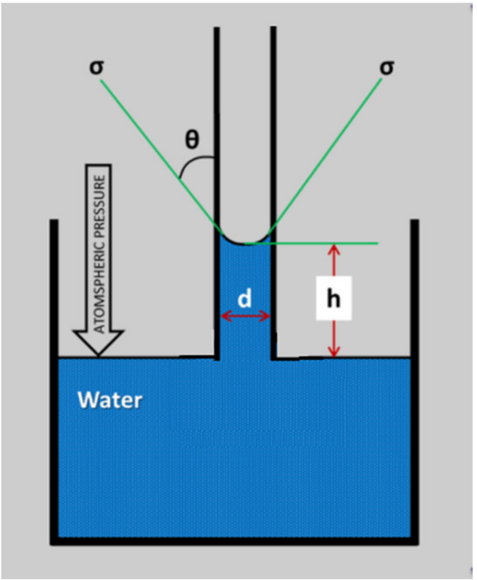
➢ wall adhesion force

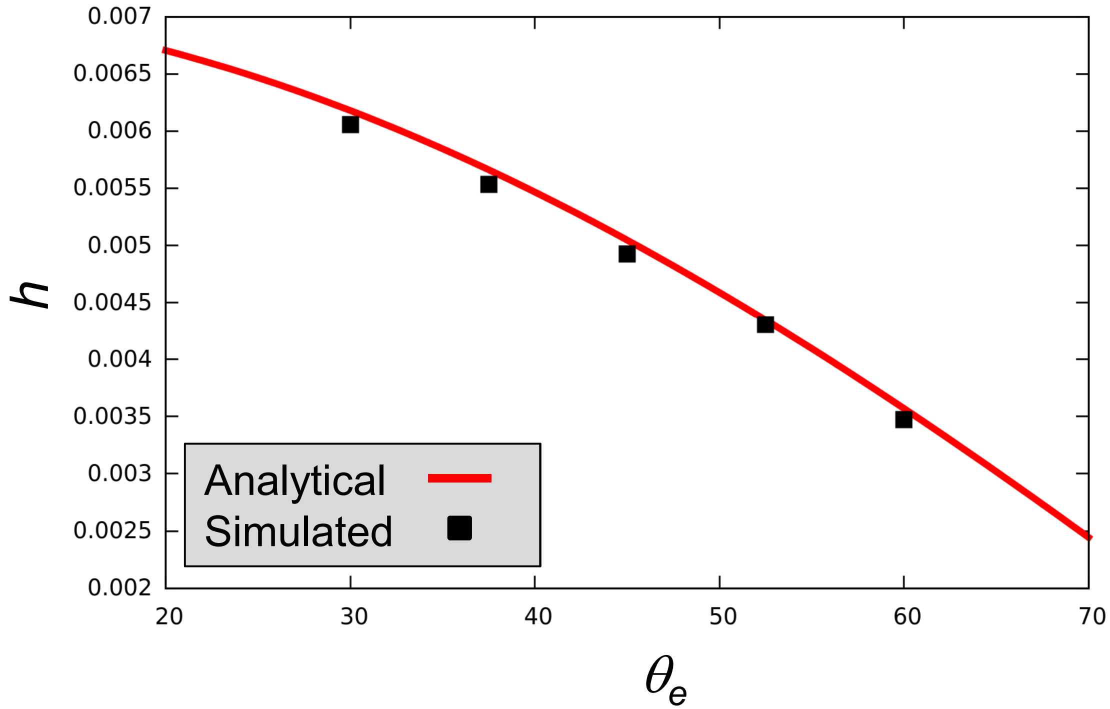
$\theta = 45°$



Capillary Rise Between Parallel Plates

- At equilibrium, capillary force is balanced by gravity





$$h = \frac{2\gamma \cos(\theta)}{\rho g d}$$

- Good agreement between analytical solution and simulation results

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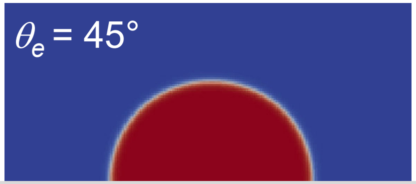
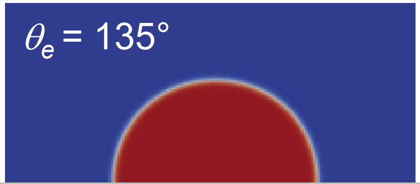
Capillarity-driven Droplet Spreading / Dewetting

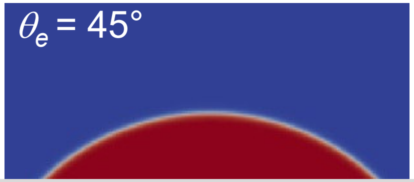


Hydrophilic surface

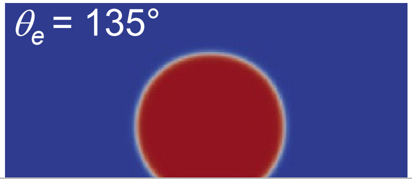


hydrophobic surface

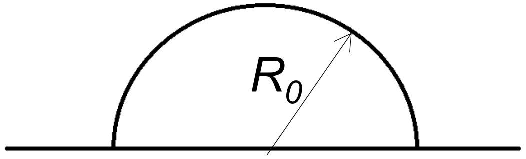
Capillarity-driven Droplet Spreading / Dewetting



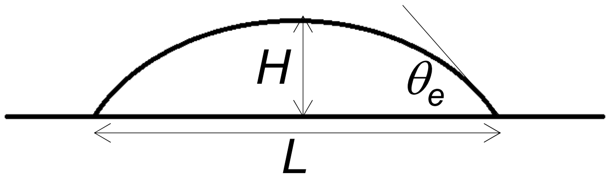
Hydrophilic surface



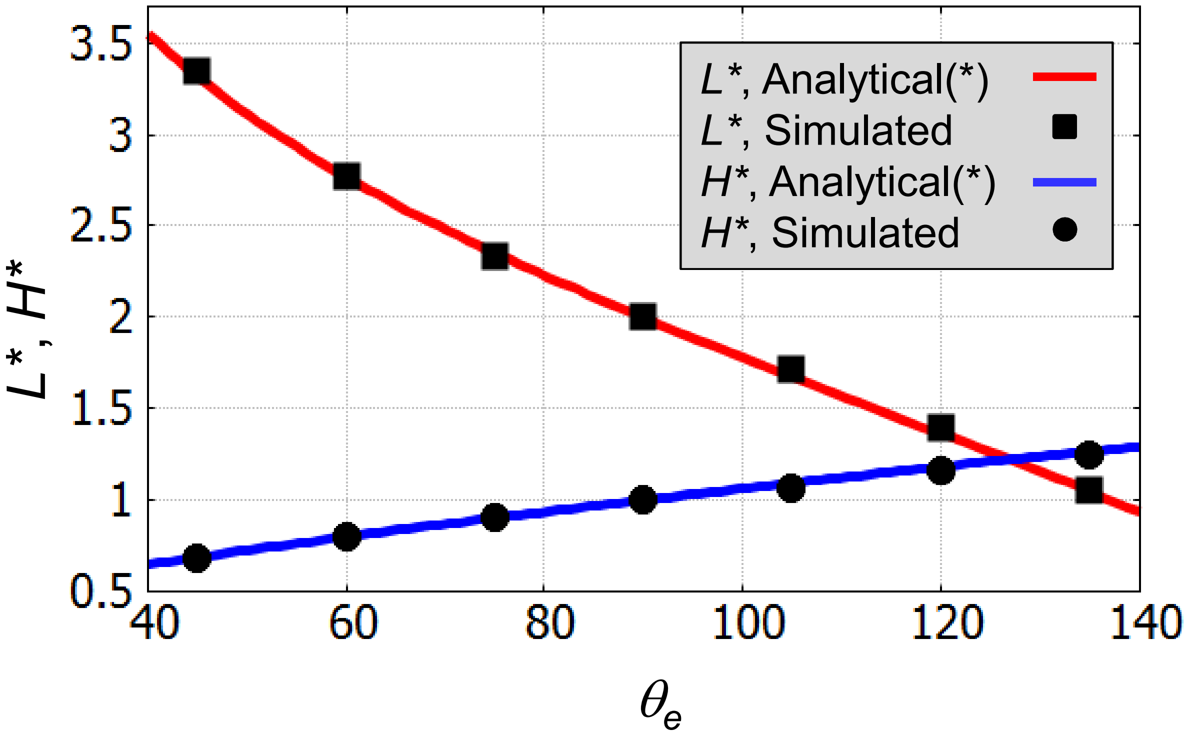
hydrophobic surface



Initial shape



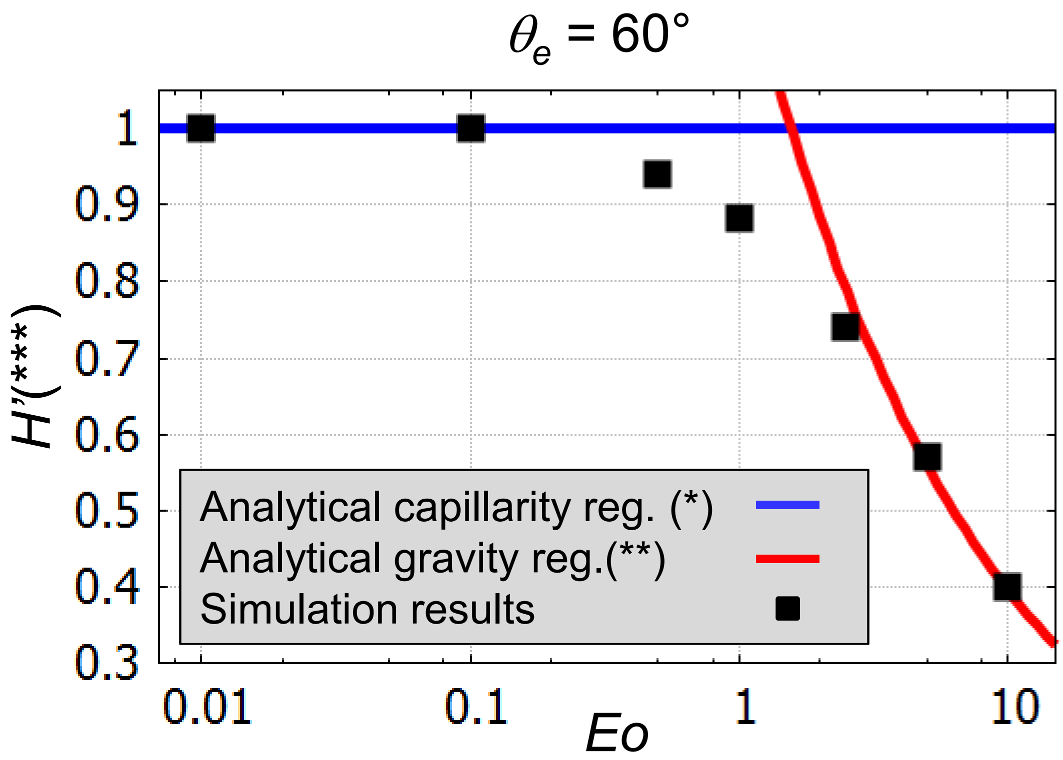
Final shape



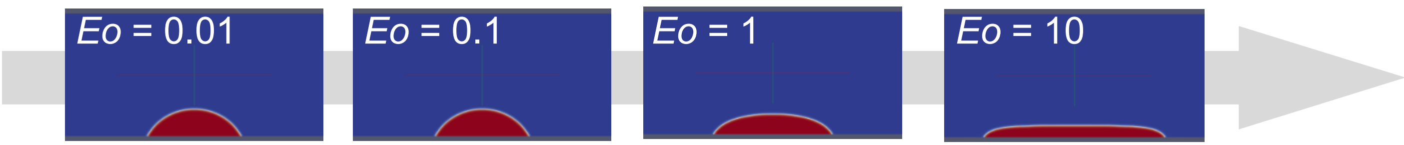
$L^* = L / R_0$
$H^* = H / R_0$

(*) Chen et al. 2009

Capillarity- / Gravity-driven Spreading



- Eötvös number (*Eo*):
  - *Eo* << 1
    capillarity-driven regime
  - *Eo* >> 1
    gravity-driven regime
  - *Eo* ≈ 1
    transitional regime



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

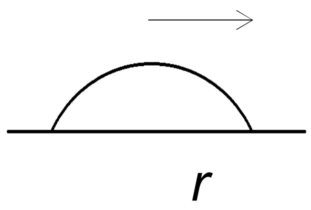
Capillarity-driven Droplet Spreading Process

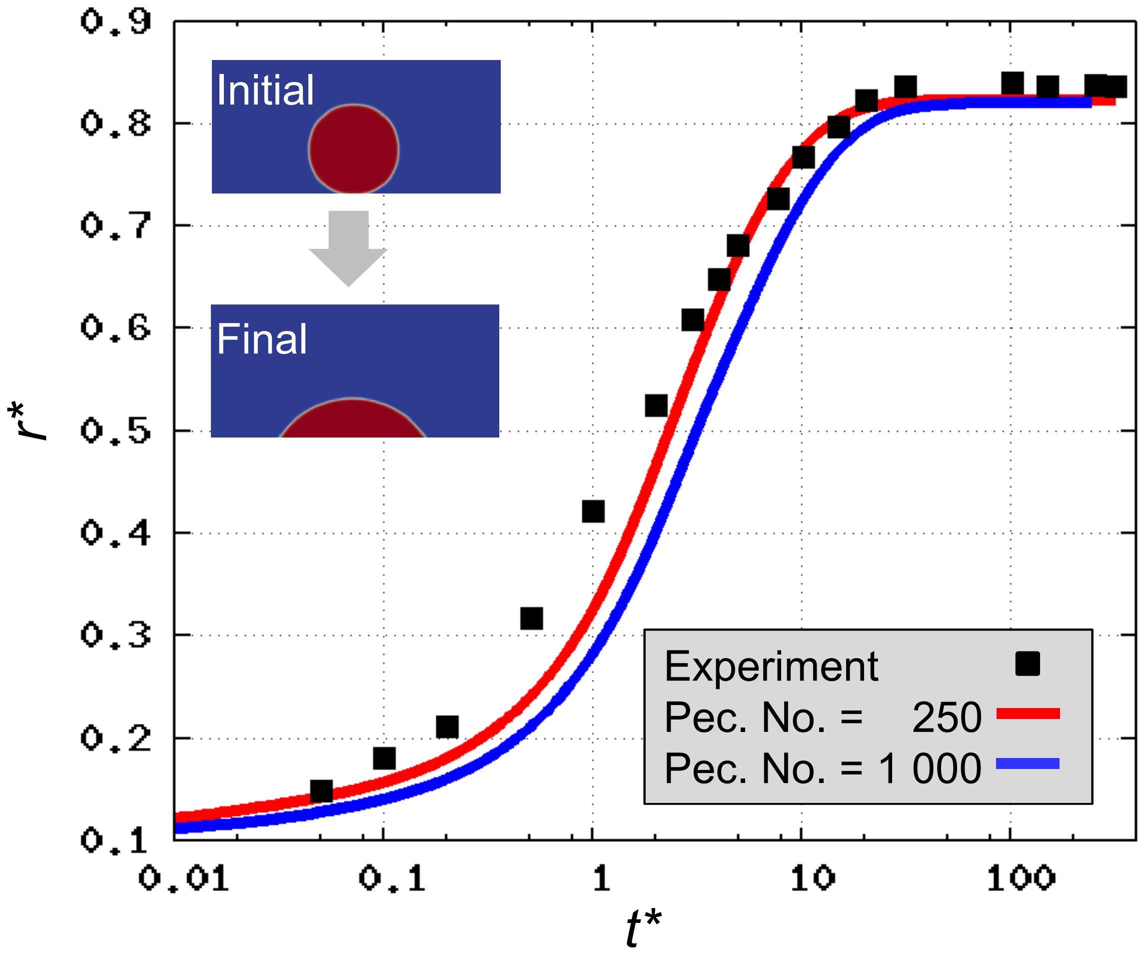
Experiment by Zosel 1993:

– Droplet spreading on flat smooth surface

– $D_{droplet}$ = 1.5 mm → Gravity effect negligible

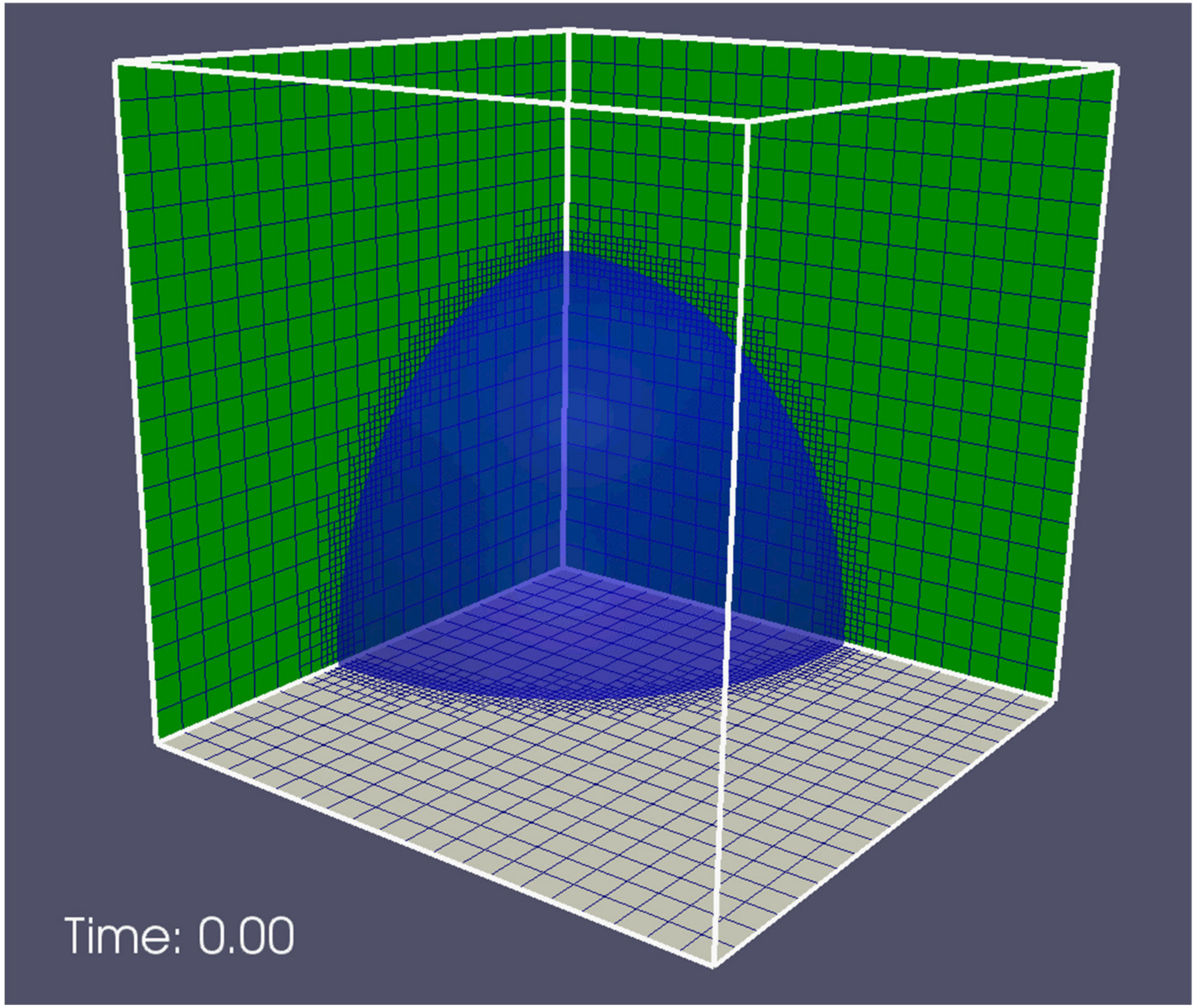
– Variable of interest: time evolution of base radius





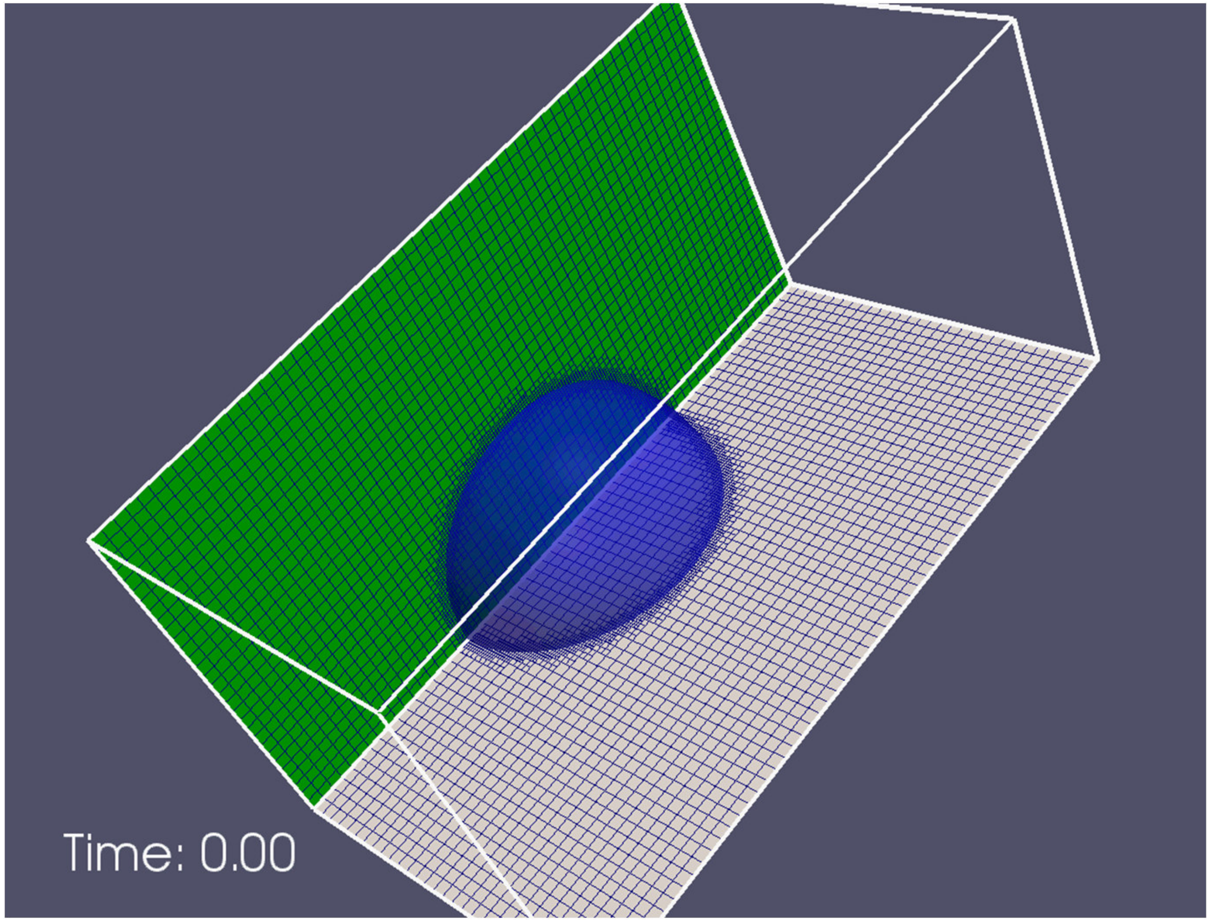
(*)Zosel 1993

3D Adaptive Mesh Refinement (AMR) Simulation



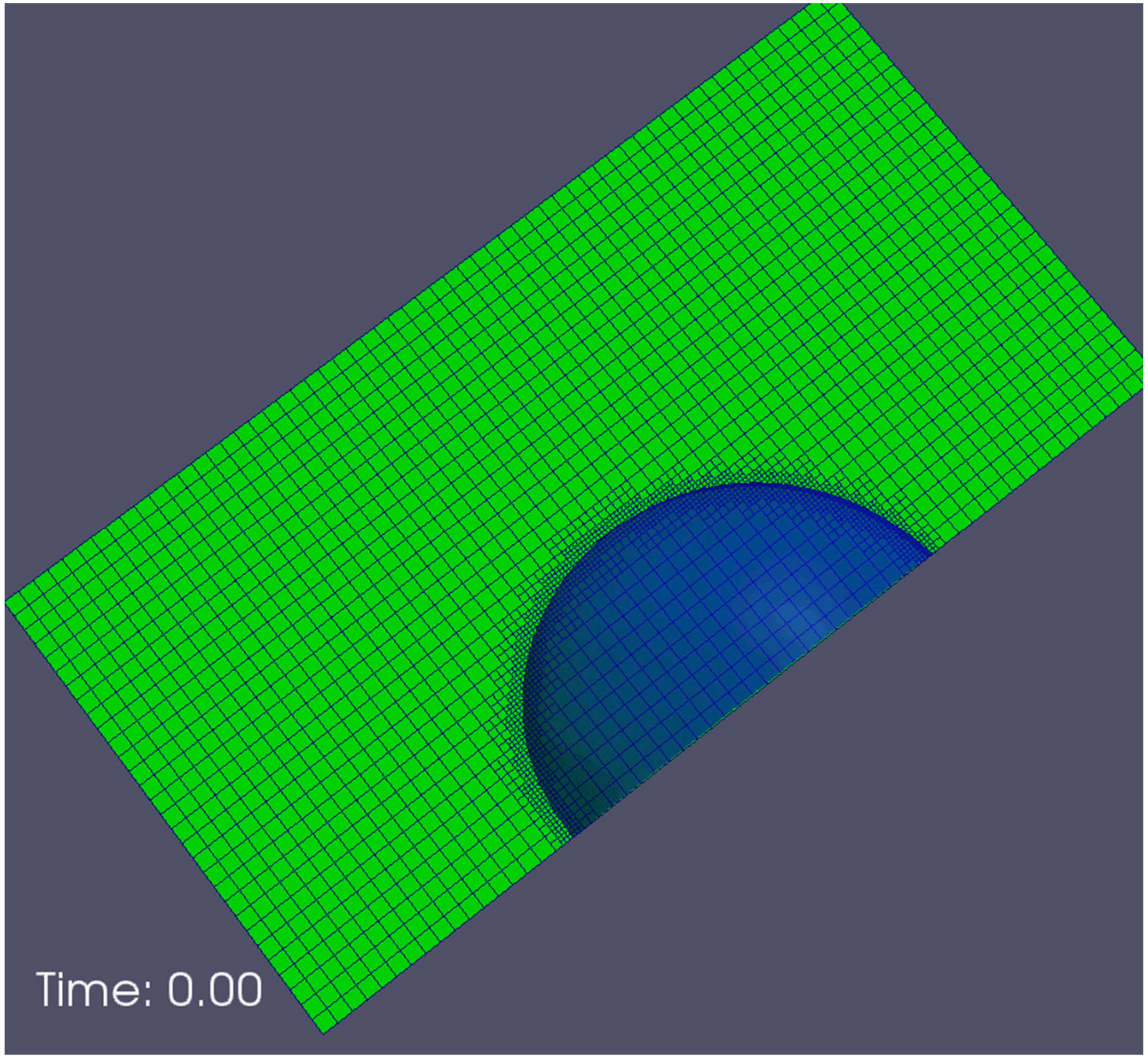
- On flat surface
- Quarter-symmetry
- AMR near interface (two-level refinement)
- $\theta_{initial}$ = 90° θ_{equi} = 75°
- Spreading driven by capillary effect

3D Adaptive Mesh Refinement (AMR) Simulation



- 45° inclined surface
- Semi-symmetry
- AMR near interface (two-level refinement)
- $\theta_{initial}$ = 90°
- First spreading driven by combined capillary and gravity effect
- Then sliding due to gravity effect

3D Adaptive Mesh Refinement (AMR) Simulation



- 45° inclined surface
- Semi-symmetry
- AMR near interface (two-level refinement)
- $\theta_{initial}$ = 90°
- First spreading driven by combined capillary and gravity effect
- Then sliding due to gravity effect

Conclusions

- Phase field method has been implemented in OpenFOAM®

- The method has been verified in terms of
  - Mobility term
  - Surface tension force
  - Equilibrium contact angle boundary condition

- The method is capable of simulating wetting phenomena
  - predicting spreading/dewetting process
  - reproducing two spreading regimes (capillarity and gravity regimes)
  - achieving good agreement with experimental data
  - 3D adaptive-mesh-refinement simulation of droplet spreading and sliding

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Ongoing work – Numerical Method Development

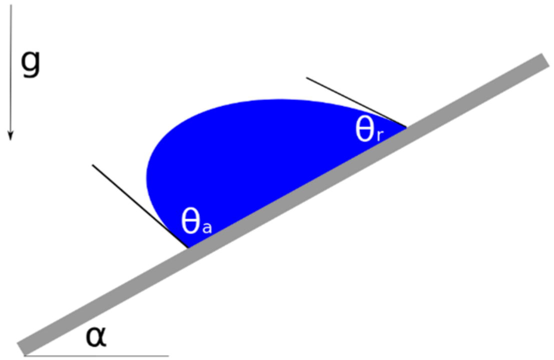
- Current state:
  - **Novel top-level solver**: `phaseFieldFoam`, supporting foam-typical algorithmic flexibility, e.g.

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

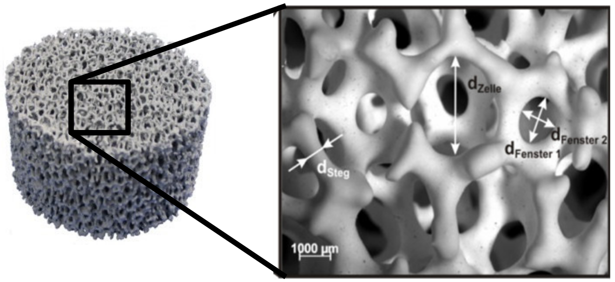
  - **3 new model libraries**
    (following common strategy design pattern; run-time selection via factory method)
    - `diffuseInterfaceModels`
      Abstract base class for diffuse interface models.
    - `diffuseInterfaceProperties`
      Diffuse interface mixture properties from phase transport properties.
    - `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).

Ongoing work – Next Steps towards Application

- Pinning effect of droplet on inclined surface

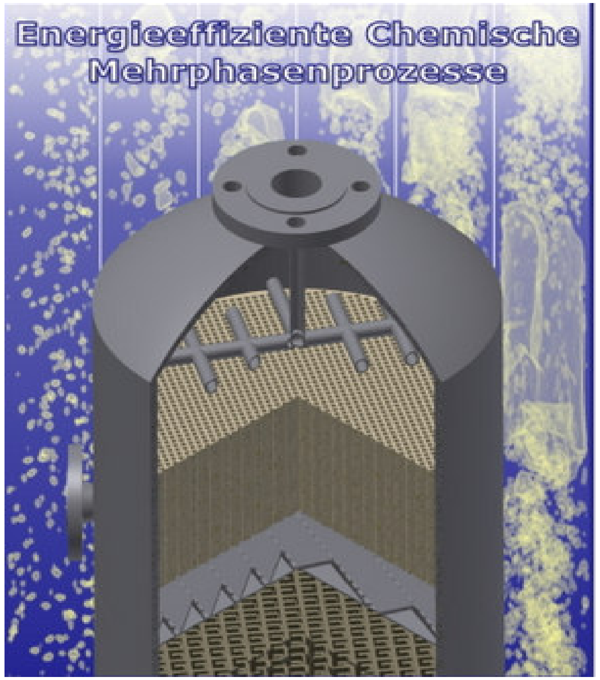


- Droplet wetting on chemically heterogeneous surface / on rough surface
- Wetting process on representative complex geometry of sponge structure



Acknowledgement

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



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