Modeling and Numerical Simulation of Droplets with Variable Surface properties

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Introduction

- In multiphase flow systems, the fluid dynamics of bulk phases are strongly coupled with the dynamics of fluid interfaces, heat and mass transport across the interfaces, adsorption and transport effects on the interfaces, variable interface properties.
- Solid particles are attracted to fluid interfaces due to their hydrophilic or lipophilic character.
- For most of such systems, appropriate models are not available in literature. → Modeling issues are investigated.
- We concentrate on efficient and reliable numerical simulation of two-phase flows with dominating interfacial effects:
  - Variable surface tension coefficients.
  - Surface viscosity → Continuum model for particles at fluid interfaces.

Models

- Navier – Stokes equations describe dynamics in bulk phases for incompressible, viscous and Newtonian fluids.
- Sharp dividing surface model for immiscible fluids:

$$[\mathbf{T}\cdot\mathbf{n}]_\Gamma = -\tau\kappa\mathbf{n} + \nabla_\Gamma\tau = \mathrm{div}_\Gamma(\tau\mathbf{P})$$
$$[\mathbf{u}]_\Gamma = 0, \quad \mathbf{V}_\Gamma = \mathbf{u}\cdot\mathbf{n}_\Gamma$$

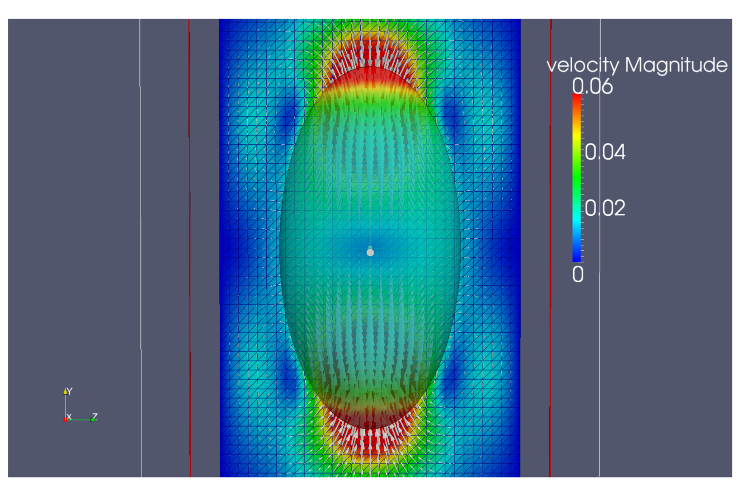
  with τ surface tension coefficient, κ curvature, $\mathbf{V}_\Gamma$ normal velocity of the interface, $\mathbf{P}$ projection onto interface.
- Mass transport and surfactant transport.
- Continuum description for effects of solid particles at fluid interface based on surface viscosity models.
  - Boussinesq-Scriven Law for viscous interface:

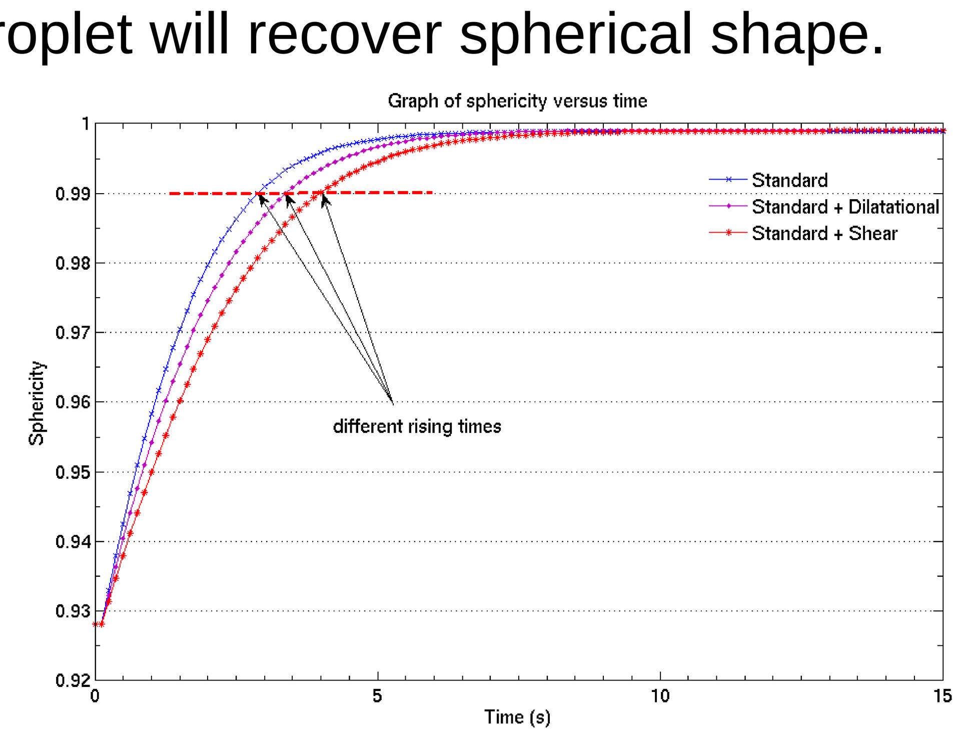
$$\mathbf{T}_\Gamma = [\tau + (\lambda_\Gamma - \mu_\Gamma)\,\mathrm{div}_\Gamma\,\mathbf{u}]\mathbf{P} + 2\mu_\Gamma\mathbf{D}_\Gamma$$
$$\mathbf{D}_\Gamma = \frac{1}{2}\mathbf{P}(\nabla_\Gamma\mathbf{u} + \nabla_\Gamma\mathbf{u}^T)\mathbf{P}, \quad [\mathbf{T}\cdot\mathbf{n}]_\Gamma = \mathrm{div}_\Gamma(\mathbf{T}_\Gamma)$$

  with λ_Γ surface dilatational viscosity, μ_Γ surface shear viscosity.
- Model validation with other groups in TMFB / other models?

Viscous Interface

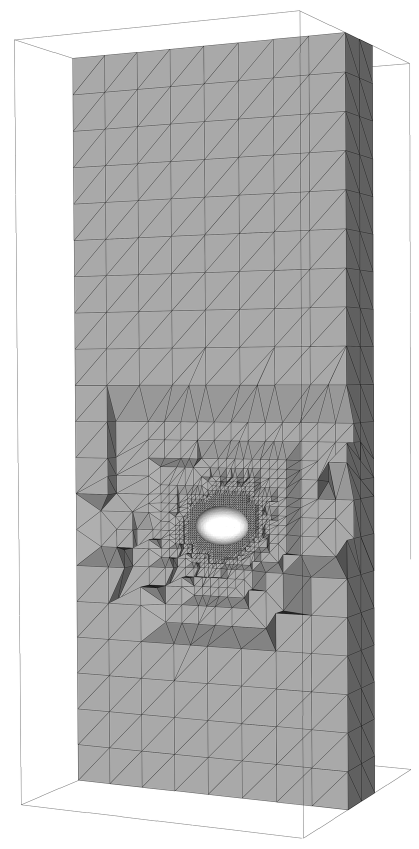
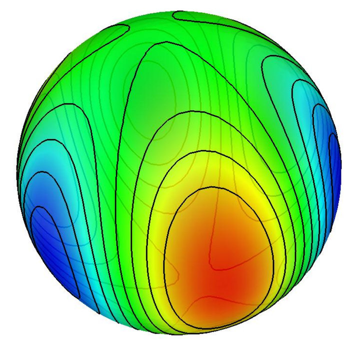
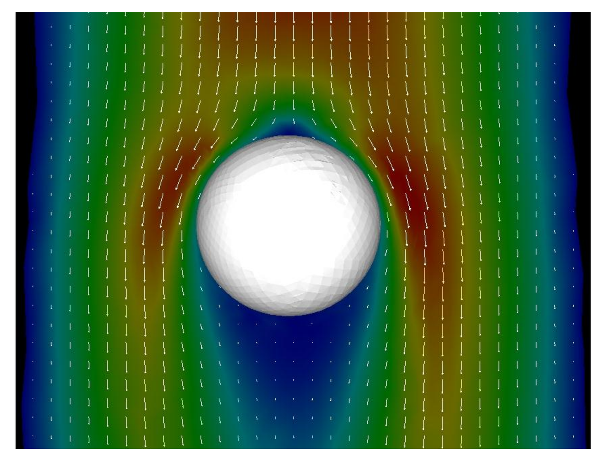
- Numerical experiment with single ellipsoidal droplet. Due to the surface tension force, the droplet will recover spherical shape.





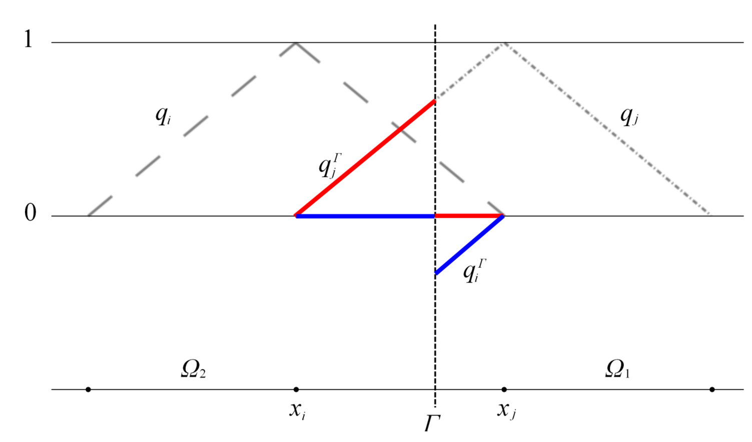
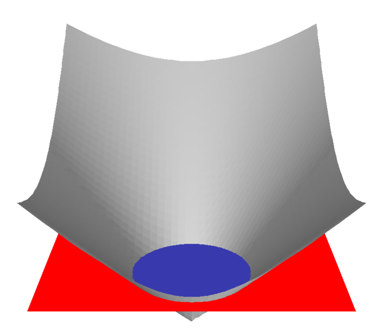
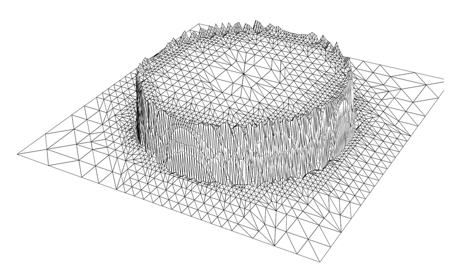
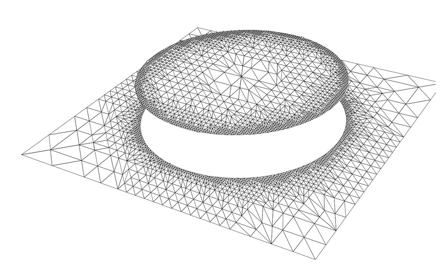
DROPS

- Numerical solver for two phase flows with transport phenomena and surface properties.
- Own development; Open source; Object oriented.
- Algorithms + Data structures + Post-processing.

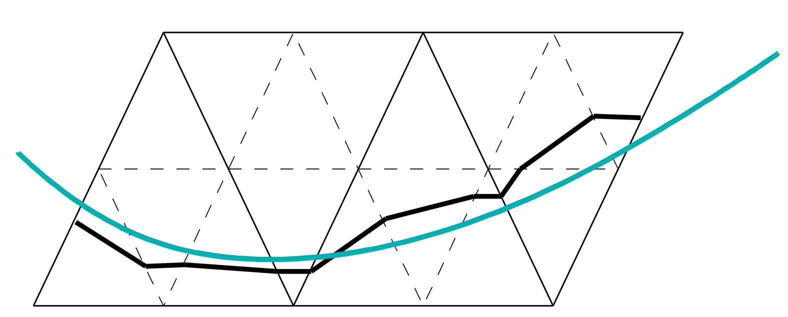
Numerical Methods

- Finite element methods with multilevel tetrahedral grid hierarchy.
- Level set method for interface representation.
- Extended-FEM for discontinuous quantities.

- Interface condition represented as localized force term:

$$f_\Gamma(\mathbf{v}) := \int_\Gamma \mathrm{div}_\Gamma(\mathbf{T}_\Gamma)\cdot\mathbf{v}\,\mathrm{d}s = -\int_\Gamma \mathrm{tr}(\mathbf{T}_\Gamma\nabla_\Gamma\mathbf{v})\mathrm{d}s$$



Literature

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[2] **P. Esser, J. Grande, A. Reusken**, *An extended finite element method applied to levitated droplet problems*, J. Numer. Methods Engrg., 2010.

[3] **Drops package**, *http://www.igpm.rwth-aachen.de/DROPS*