RWTH AACHEN UNIVERSITY

igpm

DROPS Package

for Simulation of Two Phase Incompressible Flows

DROPS

Model

Fluid Dynamics

$\rho(\phi) = \rho_1 + (\rho_2 - \rho_1)H(\phi) \quad \mu(\phi) = \mu_1 + (\mu_2 - \mu_1)H(\phi)$

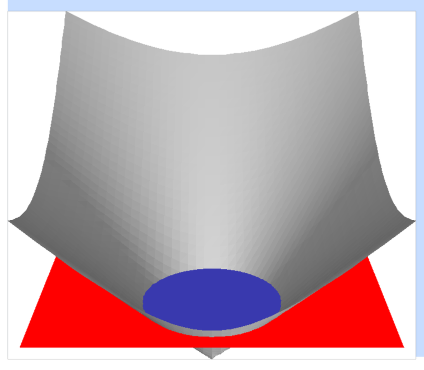
$$\begin{cases} \rho(\phi)\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) &= -\nabla p + \operatorname{div}(\mu(\phi)\mathbf{D}(\mathbf{u})) + \rho(\phi)\mathbf{g} \\ \operatorname{div}\mathbf{u} &= 0 \end{cases}$$

$$\text{in } \Omega_i, \quad i = 1,2,$$

$$[\boldsymbol{\sigma}\mathbf{n}]_\Gamma = -\tau\kappa\mathbf{n} - \nabla_\Gamma\tau, \quad [\mathbf{u}]_\Gamma = 0 \quad \text{on } \Gamma,$$

$$V_\Gamma = \mathbf{u}\cdot\mathbf{n}_\Gamma \quad \text{on } \Gamma,$$

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = 0 \quad \text{in } \Omega.$$



with proper boundary and initial conditions.

Mass Transport

$D(\phi) = D_1 + (D_2 - D_1)H(\phi) \quad \tilde{C}(\phi) = 1 + (C-1)H(\phi)$

$$\frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = \operatorname{div}(D(\phi)\nabla c) \qquad \text{in } \Omega_i, \quad i = 1,2,$$

$$[D(\phi)\nabla c]_\Gamma \cdot \mathbf{n} = 0, \quad \left[\tilde{C}c\right]_\Gamma = 0 \qquad \text{on } \Gamma.$$

with proper boundary and initial conditions.

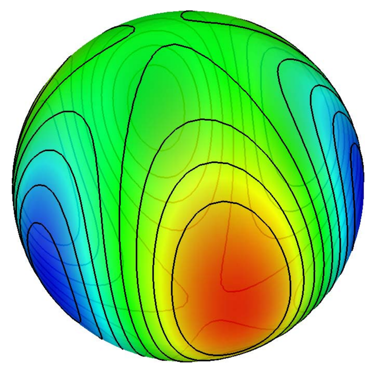
Transport of Surfactants

$$\frac{\partial S}{\partial t} + \mathbf{u}\cdot\nabla S + S\operatorname{div}_\Gamma\mathbf{u} = D_\Gamma\triangle_\Gamma S \qquad \text{on } \Gamma.$$

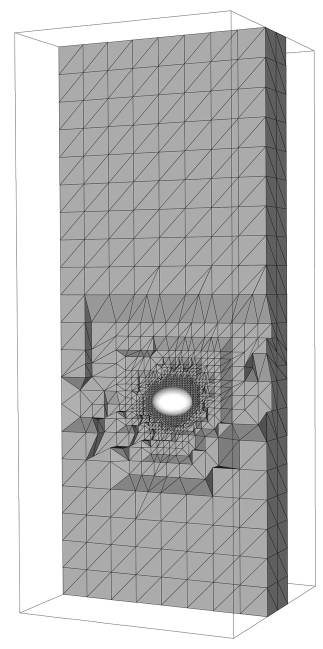
Aims

- Parallel simulation of coupled fluid dynamics, mass- and surfactant transport with variable surface property.
- Simulation of real physical systems; validation of numerics.
- Development and analysis of numerical methods.

Key Components



- Adaptive multilevel hierarchy of tetrahedral triangulations. Local refinement / coarsening.
- Level set method for interface representation.
- Finite Element methods. Extended-FEM(XFEM) for discretization of discontinuous quantities.
- Special Laplace-Beltrami method for surface tension force discretization.
- New FE method for discretization of surfactant transport equation.
- Method for treatment of variable surface tension coefficients.
- Implicit time discretization method with strong coupling of fluid dynamics and interface dynamics.
- Fast iterative solvers.
- Parallelization with MPI.

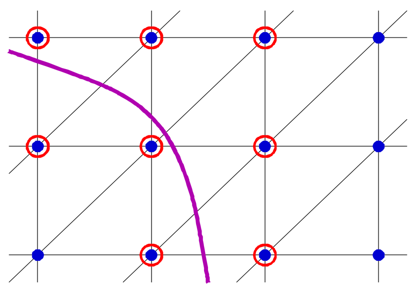


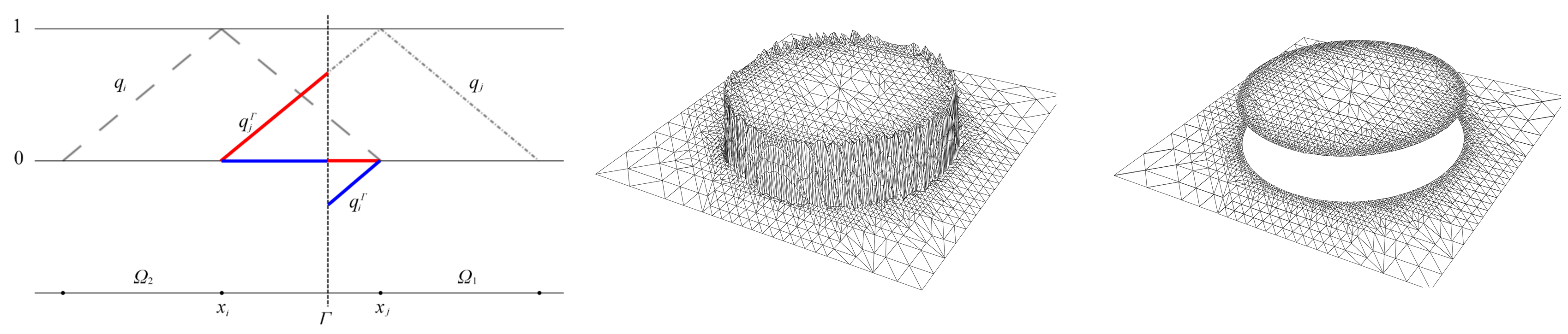
Fluid Dynamics

XFEM (Extended FEM)

•By extending the standard finite element space with additional basis functions, the jump at the interface can be formulated as

$$q_j^\Gamma = q_j\Phi_j^H = q_j\left(H_\Gamma(x) - H_\Gamma(x_j)\right)$$



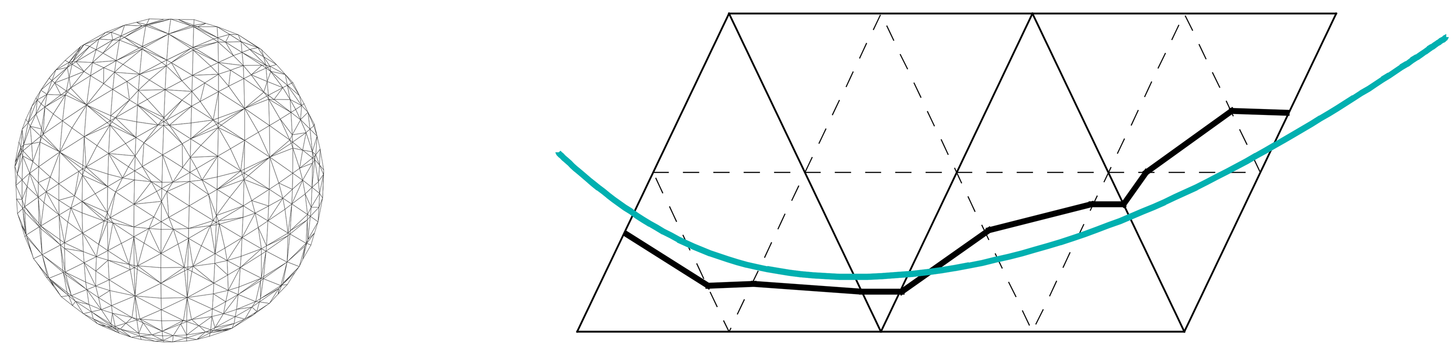


Approximation quality for $p \in L_2(\Omega) \cap H^1(\Omega_1 \cup \Omega_2)$

$$\inf_{q\in Q_h} \|q - p\|_{L_2(\Omega)} \leq \begin{cases} \mathcal{O}(\sqrt{h}), & \text{Standard P1-FE} \\ \mathcal{O}(h^2), & \text{XFEM} \end{cases}$$

Improved Laplace-Beltrami discretization

$$\tilde{f}_{\Gamma_h}(\mathbf{v}_h) = -\tau\int_{\Gamma_h} \tilde{\mathbf{P}}_h\nabla\mathrm{id}_{\Gamma_h}\cdot\nabla_{\Gamma_h}\mathbf{v}_h ds, \quad \tilde{\mathbf{P}}_h(x) = \mathbf{I} - \tilde{\mathbf{n}}_h(x)\tilde{\mathbf{n}}_h(x)^T$$



$$\mathcal{O}(\sqrt{h}) \rightsquigarrow \mathcal{O}(h)$$

Variable surface tension coefficients

$$f_\Gamma(\mathbf{v}) = \int_\Gamma \kappa\mathbf{n}\cdot(\gamma\mathbf{v}) - \nabla_\Gamma\gamma\cdot\mathbf{v}ds$$

$$\approx \int_{\Gamma_h}\left[\gamma\tilde{\mathbf{P}}_h\nabla(\mathrm{id}_{\Gamma_h})\cdot\nabla_{\Gamma_h}\mathbf{v} + v_i\mathbf{P}_h\tilde{\mathbf{P}}_h\nabla(\mathrm{id}_{\Gamma_h})_i\cdot\nabla_{\Gamma_h}\gamma - (\nabla_{\Gamma_h}\gamma)\cdot\mathbf{v}\right]ds$$

Parallelization

- Implementation based on MPI.
- Distributed multilevel hierarchy of tetrahedral triangulations.
- Dynamic load-balancing.
- Treatment of distributed unknowns.

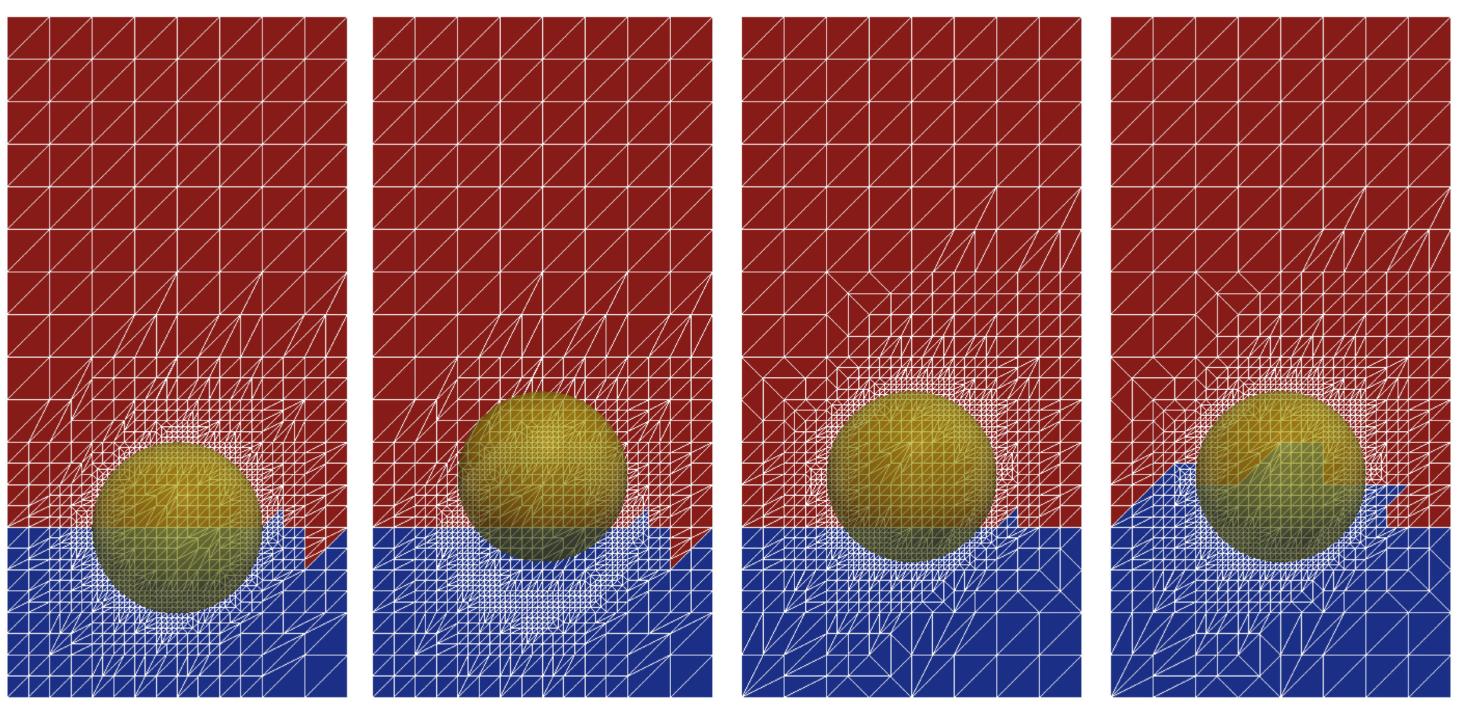


Fig: Simulation evolution with refinement and load-balancing

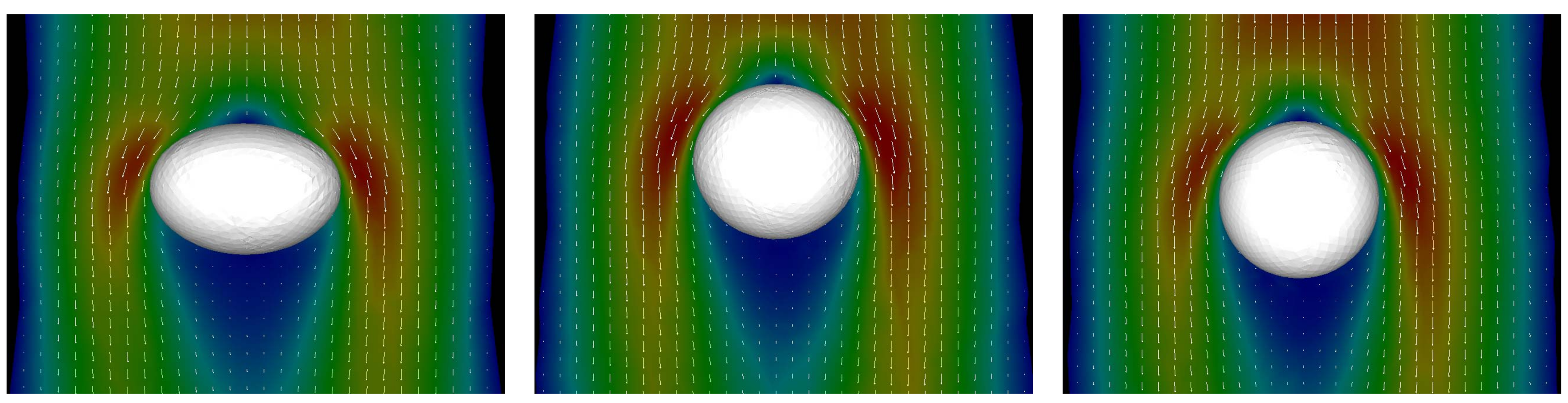


Fig: From left to right : interfacial tension τ = 1.63e-3N/m, 8.15e-3N/m, 32.6.e-3N/m

Publications

- **P. Esser, J. Grande, A. Reusken,** *An extended finite element method applied to levitated droplet problems,* J. Numer. Methods Engrg., 2010.
- **A.Reusken, T.H.Nguyen**, *Nitsche's method for a transport problem in two-phase incompressible flows,* Journal of Fourier Analysis and Applications, 2009
- **E. Bertakis, S. Gross, J. Grande, O. Fortmeier, A. Reusken, A. Pfennig**, *Validated simulation of droplet sedimentation with finite-element and level-set methods,* Comp. Eng. Sci., 2009.
- **S. Groß**, *Numerical methods for three-dimensional incompressible two-phase flow problems*, doctoral thesis, IGPM, RWTH Aachen, 2008.
- **Drops package for simulation of two phase incompressible flows, http://www.igpm.rwth-aachen.de/DROPS/.**