Numerical methods for interface PDEs in two-phase incompressible flows

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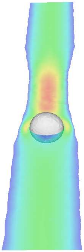
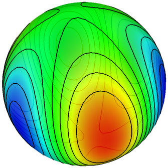
Chair for Numerical Mathematics
RWTH Aachen University

Freiburg, September 2009





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Joint work with: P. Esser, J. Grande, S. Groß, M. Olshanskii

Outline

- Standard model for two-phase flow.
- Challenges, examples of simulations.

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- Discretization of surface tension.
- Extended finite element space.
- Treatment of surfactant transport on the interface.

Standard model for two-phase flows

Domains: $\Omega_1 = \Omega_1(t)$ and $\Omega_2 = \Omega_2(t)$

Interface: $\Gamma = \Gamma(t) = \partial\Omega_1 \cap \partial\Omega_2$

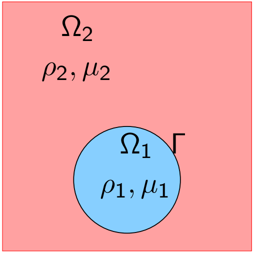
ρ_i: density in Ω_i

μ_i: viscosity in Ω_i

τ: surface tension coefficient

$\mathbf{D}(\mathbf{u}) = \nabla\mathbf{u} + \nabla\mathbf{u}^T$, $\sigma = -p\,\mathbf{I} + \mu\mathbf{D}(\mathbf{u})$

κ: curvature



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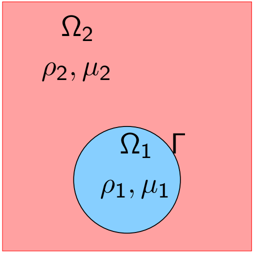

ρ_i: density in Ω_i
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τ: surface tension coefficient
$\mathbf{D}(\mathbf{u}) = \nabla\mathbf{u} + \nabla\mathbf{u}^T$, $\sigma = -p\,\mathbf{I} + \mu\mathbf{D}(\mathbf{u})$
κ: curvature

$$\begin{cases} \rho_i(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}) = \mathrm{div}\,(\sigma) + \rho_i\mathbf{g} \\ \qquad\qquad = -\nabla p + \mathrm{div}\,(\mu_i\mathbf{D}(\mathbf{u})) + \rho_i\mathbf{g} \quad \text{in } \Omega_i \quad \text{for } i = 1,2 \\ \mathrm{div}\,\mathbf{u} = 0 \qquad\qquad\qquad\qquad \text{in } \Omega_i \end{cases}$$

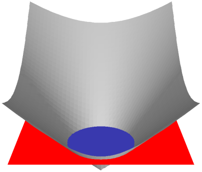
$$[\sigma\mathbf{n}]_\Gamma = \tau\kappa\mathbf{n}, \quad [\mathbf{u}]_\Gamma = 0\ .$$

Interface capturing: Level set approach

$\Gamma(t)$ = zero-level of a scalar function:

the level set function $\varphi(x,t)$

$$\varphi(x,t) = \begin{cases} < 0 & \text{for } x \text{ in phase } \Omega_1 \\ > 0 & \text{for } x \text{ in phase } \Omega_2 \\ = 0 & \text{at the interface} \end{cases}$$



should be an *"approximate signed distance function"*.

$$x(t) \in \Gamma(t) \quad \Rightarrow \quad \varphi(x(t),t) = 0.$$

Level set equation

$$\varphi_t + \mathbf{u} \cdot \nabla\varphi = 0$$

Model: Navier-Stokes + level set equation

Navier-Stokes equations coupled with level set equation

$$\begin{aligned} \rho(\varphi)\Big(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}\Big) - \operatorname{div}\Big(\mu(\varphi)\,\mathbf{D}(\mathbf{u})\Big) + \nabla p &= \rho(\varphi)\,g - \tau\,\kappa(\varphi)\,\delta_\Gamma \mathbf{n}_\Gamma \\ \nabla\cdot\mathbf{u} &= 0 \\ \varphi_t + \mathbf{u}\cdot\nabla\varphi &= 0 \end{aligned}$$

where ρ, μ and $\kappa, \delta_\Gamma, \mathbf{n}_\Gamma$ depend on φ, e.g.:

$$\kappa(\varphi) = \nabla\cdot\left(\frac{\nabla\varphi}{||\nabla\varphi||}\right)$$ second derivatives.

Localized force term in weak formulation

$$f_\Gamma(\mathbf{v}) = \tau\int_\Gamma \kappa\mathbf{n}_\Gamma\cdot\mathbf{v}\;ds, \qquad f_\Gamma \in H^{-1}(\Omega)$$

Accurate discretization of f_Γ is essential!.

Fluid dynamics + mass- and surfactant transport

Mass transport

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D(\varphi)\Delta c,$$
$$[D(\varphi)\nabla c \cdot \mathbf{n}] = 0 \quad \text{on} \quad \Gamma(t),$$
$$c_1 = C_H c_2 \quad \text{on} \quad \Gamma(t)$$

D: piecewise constant. Henry condition: discontinuity in c.

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Transport of surfactants

$$\dot{S} + S\,\mathrm{div}_\Gamma \mathbf{u} = \mathrm{div}_\Gamma(D_\Gamma \nabla_\Gamma S) \quad \text{on} \quad \Gamma(t)$$

with $\dot{S}$: material derivative $\dot{S} = \frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S$.

Challenges

- Unknown interface.
- Highly nonlinear couplings between $\mathbf{u}$, φ, f_Γ, c, S.
- Multiscale phenomena close to the interface.
- Interesting modeling aspects, e.g.: $\tau = \tau(c, S)$ (SFB 540).
  Inverse problems!

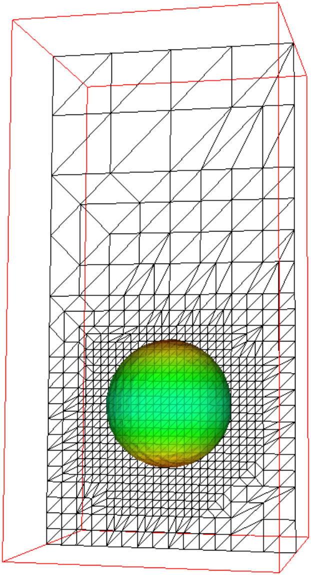
Numerical key issues:

- Accurate resolution of unknown interface.
- Treatment of surface tension force.
- Discretization of transport equation with discontinuous c.
- Discretization of transport equation on $\Gamma(t)$.
- Coupling of flow + interface dynamics + transport equations.
- Efficiency/robustness of iterative solvers.
- High complexity: parallelization needed.

Key components in DROPS:

- Discretization of surface tension force f_Γ: Laplace-Beltrami.
- Finite element space for discontinuous pressure: XFEM .
- Surfactant transport equation: Interface FE method.

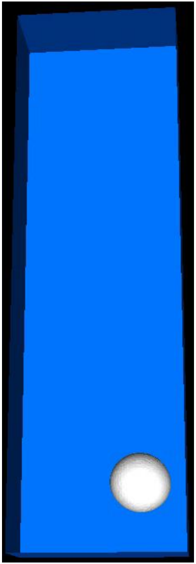
Examples of fluid dynamics simulations



Rising droplet

system: n-butanol/water

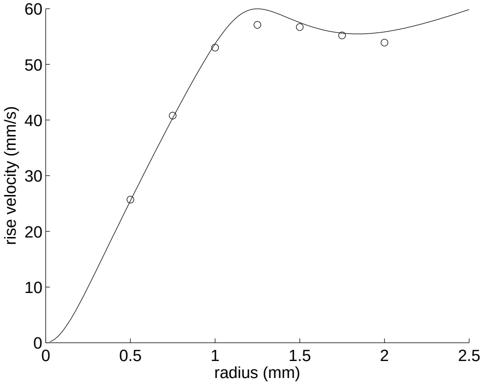
drop radius $r = 3\,mm \quad \rightsquigarrow$ wobbling

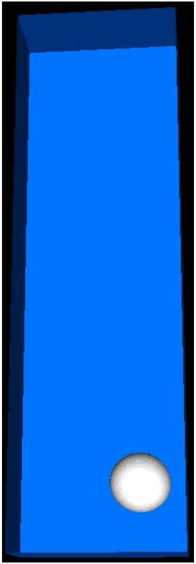


Rising droplet

system: n-butanol/water

rise velocity vs. drop radius





Surface tension discretization

Approximation of Γ by Γ_h

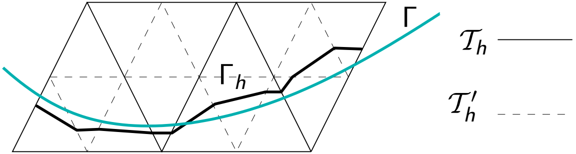
Γ = zero level of ϕ (= level set function = signed distance function)

ϕ_h = piecewise quadratic FE approximation of ϕ.

Our strategy:

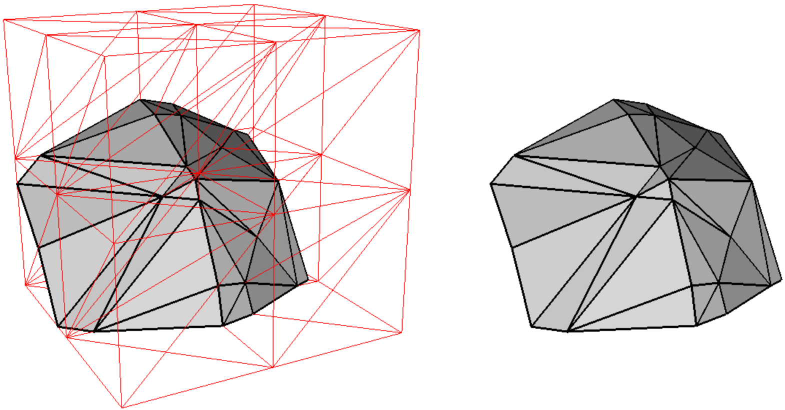
$\phi \approx \phi_h$ (piecewise P_2) $\rightarrow$ $I(\phi_h)$ (piecewise P_1 on refined mesh).

$\Gamma \approx \Gamma_h :=$ zero level of $I(\phi_h)$ (planar segments).



Under reasonable assumptions: $\mathrm{dist}(\Gamma, \Gamma_h) \leq c\, h^2$.

Approximation of Γ by Γ_h: 3D illustration



Surface tension approximation with Laplace-Beltrami

Surface tension force:

$$f_\Gamma(\mathbf{v}) = \tau \int_\Gamma \kappa \mathbf{n}_\Gamma \cdot \mathbf{v} \; ds,$$

Tangential derivative (along Γ):

$$\nabla_\Gamma g = (I - \mathbf{n}_\Gamma \mathbf{n}_\Gamma^T)\nabla g.$$

The *Laplace-Beltrami operator* of g on Γ is defined by

$$\Delta_\Gamma g := \nabla_\Gamma \cdot \nabla_\Gamma g.$$

Basic result from differential geometry:

$$\int_\Gamma \kappa \, \mathbf{n}_\Gamma \cdot \mathbf{v} \, ds = -\int_\Gamma (\Delta_\Gamma \, \mathrm{id}_\Gamma) \cdot \mathbf{v} \, ds = \int_\Gamma \nabla_\Gamma \, \mathrm{id}_\Gamma \cdot \nabla_\Gamma \mathbf{v} \, ds.$$

Discretization of surface tension

Obvious approximation method ($\mathbf{v}_h \in \mathbf{V}_h$):

$$f_\Gamma(\mathbf{v}_h) = \tau \int_\Gamma \nabla_\Gamma \, \mathrm{id}_\Gamma \cdot \nabla_\Gamma \mathbf{v}_h \, ds \approx \int_{\Gamma_h} \nabla_{\Gamma_h} \mathrm{id}_{\Gamma_h} \cdot \nabla_{\Gamma_h} \mathbf{v}_h \, ds =: f_{\Gamma_h}(\mathbf{v}_h)$$

This technique was introduced by Dziuk, Bänsch, used by others.

Analysis and improvement of this method ([Groß, AR: SINUM 07]):

$$\sup_{\mathbf{v}_h \in \mathbf{V}_h} \frac{|f_\Gamma(\mathbf{v}_h) - \tilde{f}_{\Gamma_h}(\mathbf{v}_h)|}{\|\mathbf{v}_h\|_1} \leq c h_\Gamma \qquad (h_\Gamma = \text{mesh size in } U \supset \Gamma)$$

Extended FE: XFEM

XFEM

Motivation

Piecewise smooth solutions, nonsmooth across the interface:

- Pressure is discontinuous across Γ.
- Velocity has discontinuous normal derivative across Γ.
- Discontinuity of concentration (mass transport) across Γ.

XFEM applications in other fields:

- Belytschko (1999 -$>$): elasticity problems.
- Hansbo (2002 -$>$): interface problems + analysis.

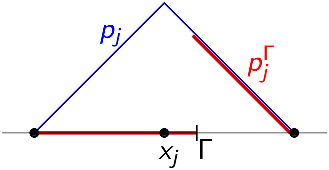
XFEM

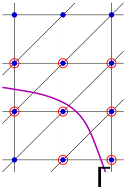
Piecewise smooth discontinuous p^* and standard FE spaces Q_h:

$$\inf_{q_h \in Q_h} \|q_h - p^*\|_{L^2} = \mathcal{O}(\sqrt{h})$$

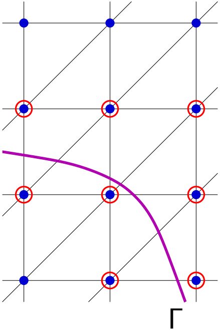
Reason: Grid not aligned with interface!

Remedy: Extend P_1 FE space with discontinuous basis functions near Γ:





XFEM



$$V_h^\Gamma := V_h \oplus \mathrm{span}\{\, R\phi_k \mid k \in \mathcal{I}^\Gamma \,\}$$

with R: restriction; ϕ_k nodal basis function;
$\mathcal{I}^\Gamma$: "interface nodes".

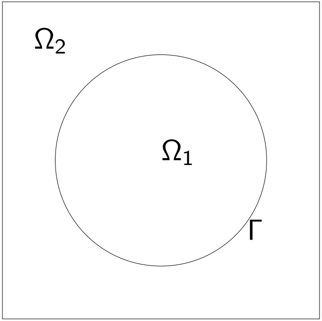
Remarks:

- In practice: Γ_h instead of Γ.
- $\dim(V_h^\Gamma)$ depends on Γ.
- LBB stability of the $\mathcal{P}_2, V_h^\Gamma$ pair ?
- Stability issues: in discretization, in iterative solvers.
- Implementation not straightforward.

Analyses: [Groß, AR: JCP 2007], [AR: Comp. Vis. Sci. 2008].

Numerical experiment: static bubble

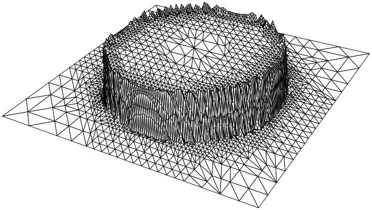
$\Omega_1 = \{ x \in \mathbb{R}^3 \mid \|x\| \leq \frac{2}{3} \}$.



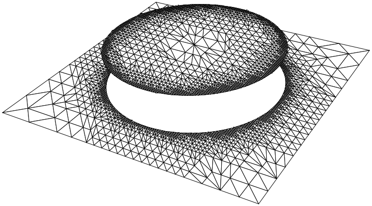
$f_\Gamma(\mathbf{v}) = \tau \int_\Gamma \kappa \mathbf{n}_\Gamma \cdot \mathbf{v} \, ds$ with $\tau = 1$. Note $\kappa = 2/r = 3$.

Solution: $u^* = 0, \qquad p^* = \begin{cases} C & \text{in } \Omega_2, \\ C + \tau\kappa & \text{in } \Omega_1. \end{cases}$

Results of experiment



f_{Γ_h} and V_h (linear FE)



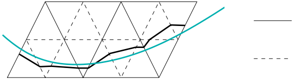
$\tilde{f}_{\Gamma_h}$ and V_h^{Γ} (XFEM)

Results of experiment

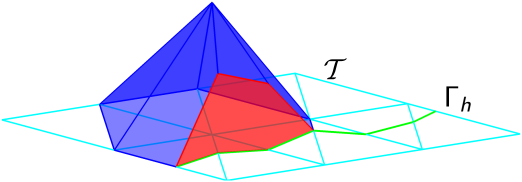
ref.	$\|e_p\|_{L^2}$ for $p_h \in V_h$				$\|e_p\|_{L^2}$ for $p_h \in V_h^\Gamma$			
	f_{Γ_h}	order	$\tilde{f}_{\Gamma_h}$	order	f_{Γ_h}	order	$\tilde{f}_{\Gamma_h}$	order
0	1.60E+00	–	1.60E+00	–	3.12E-01	–	1.64E-01	–
1	1.07E+00	0.57	1.07E+00	0.57	1.00E-01	1.64	4.97E-02	**1.73**
2	8.23E-01	0.38	8.23E-01	0.38	6.24E-02	0.68	1.66E-02	**1.58**
3	5.80E-01	0.51	5.80E-01	0.51	4.28E-02	0.54	7.16E-03	**1.22**
4	4.13E-01	0.49	4.13E-01	0.49	2.95E-02	0.54	2.83E-03	**1.34**

Surfactant transport equation

Interface FE-space



Γ_h: piecewise planar approximation of Γ.



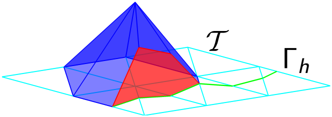
ω_h: local "outer" triangulation.
Use FE space on Γ_h induced by FE on ω_h.

$$V_h := \{ v_h \in C(\omega_h) \mid v|_T \in P_1 \ \text{ for all } \ T \in \omega_h \} \quad \textbf{outer space.}$$

Interface space

$$V_h^\Gamma := \{\psi_h \in H^1(\Gamma_h) \mid \text{there is } v_h \in V_h : \ \psi_h = v_h|_{\Gamma_h}\}$$

Discretization with V_h^Γ



Choosing the standard ansatz-functions ϕ_i in V_h yields a frame for V_h^Γ that is almost always a basis.

Galerkin method leads to a consistent linear system with

$$M_{i,j} = \oint_{\Gamma_h} \phi_j \phi_i, \quad A_{i,j} = \oint_{\Gamma_h} \nabla_{\Gamma_h} \phi_j \cdot \nabla_{\Gamma_h} \phi_i.$$

Implementation: Only quadrature on Γ_h is needed.

Analysis: Discretizaton error bounds.
Conditioning of mass and stiffness matrix.

Example: Laplace-Beltrami equation

Model problem:

$$-\Delta_\Gamma u + u = f \quad \text{on } \Gamma$$

with the unit sphere $\Gamma = \{\mathbf{x} \in \mathbb{R}^3 \mid \|\mathbf{x}\|_2 = 1\}$ and $\Omega = (-2, 2)^3$.

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$$-\Delta_\Gamma u + u = f \quad \text{on } \Gamma$$

with the unit sphere $\Gamma = \{\mathbf{x} \in \mathbb{R}^3 \mid \|\mathbf{x}\|_2 = 1\}$ and $\Omega = (-2, 2)^3$.

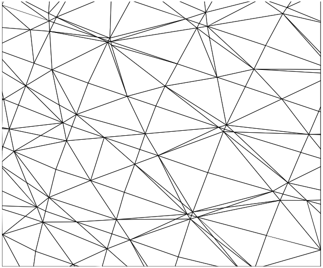
- Tetrahedral triangulations $\{\mathcal{T}_\ell\}_{\ell \geq 0}$ constructed by local refinement.
- Level-set function $\phi(\mathbf{x}) = \|\mathbf{x}\|^2 - 1$; $\phi_h := I(\phi)$ piecewise linear on $\mathcal{T}_h$, $\Gamma_h := \{\, \mathbf{x} \in \Omega \mid I(\phi_h)(\mathbf{x}) = 0 \,\}$,

Galerkin: Determine $u_h \in V_h^\Gamma$ such that

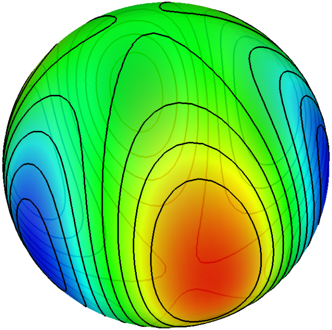
$$\int_{\Gamma_h} \nabla_{\Gamma_h} u_h \nabla_{\Gamma_h} \psi_h + u_h \psi_h \, ds_h = \int_{\Gamma_h} f_h \psi_h \, ds_h \qquad \text{for all} \quad \psi_h \in V_h^\Gamma,$$

with f_h an extension of f.

Numerical results



The induced interface "triangulation" Γ_h is not shape-regular.



solution u_h

Results

$\ell,\ h = 2^{-\ell}$	$\|u^e - u_h\|_{L_2(\Gamma_h)}$	factor	# SSOR-CG
1	0.1124	–	14
2	0.03244	3.47	26
3	0.008843	3.67	53
4	0.002186	4.05	104
5	0.0005483	3.99	201
6	0.0001365	4.02	435
7	3.411e-05	4.00	849

Analysis

Theorem

Let $I_h : H^2(\omega_h) \to V_h$ be linear interpolation. For $u \in H^2(\Gamma)$ we have:

$$\inf_{v_h \in V_h^\Gamma} \|u^e - v_h\|_{L^2(\Gamma_h)} \leq \|u^e - (I_h u^e)_{|\Gamma_h}\|_{L^2(\Gamma_h)} \leq C\, h^2 \|u\|_{H^2(\Gamma)},$$

$$\inf_{v_h \in V_h^\Gamma} \|u^e - v_h\|_{H^1(\Gamma_h)} \leq \|u^e - (I_h u^e)_{|\Gamma_h}\|_{H^1(\Gamma_h)} \leq C\, h \|u\|_{H^2(\Gamma)}.$$

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$$\inf_{v_h \in V_h^\Gamma} \|u^e - v_h\|_{H^1(\Gamma_h)} \leq \|u^e - (I_h u^e)_{|\Gamma_h}\|_{H^1(\Gamma_h)} \leq C\, h \|u\|_{H^2(\Gamma)}.$$

Corollary

$$\|u_h - u^e\|_{L^2(\Gamma_h)} \leq ch^2 \|f\|_{L^2(\Gamma)}$$

Cf. [Olshanskii, Grande, AR, SINUM 2009].

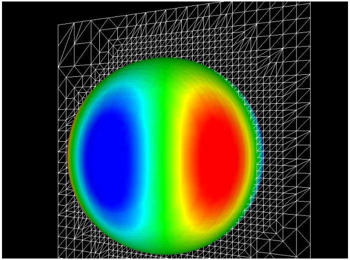
Nonstationary model problem

Convection-diffusion equation for $S(x, t)$

$$\dot{S} - D_\Gamma \Delta_\Gamma S + (\nabla_\Gamma \cdot \mathbf{v}) S = 0, \quad \Gamma(t), t \in (0,1)$$

with the unit sphere $\Gamma(0) = \{\mathbf{x} \in \mathbb{R}^3 \mid \|\mathbf{x}\|_2 = 1\}$ moving with constant velocity $\mathbf{v} = 0.5\mathbf{e}_y$ in $\Omega = (-2, 2)^3$, $D_\Gamma = 0.05$.

inital configuration:

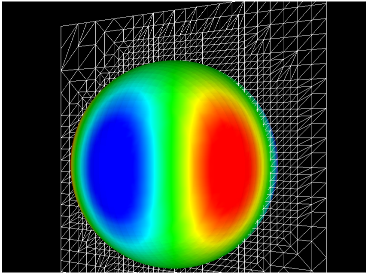


- Transport takes place **on** the interface.

Numerical experiment

- Special time integration method.
- error measure:
  $\Delta := \|S_{h,dt} - S_{\text{ref}}\|_{L_2(\Gamma_h(1))}$

solution



Quadratic convergence in h **and** dt

h = dt	**Δ**	**factor**
0.25	0.1799	-
0.125	0.0442	4.07
0.0625	0.0101	4.38

Application to a rising droplet

- gravity-driven butanol-droplet (diam. 4mm) in water, interfacial tension 1.63mN/m
- Velocity field determined from NS-equations.

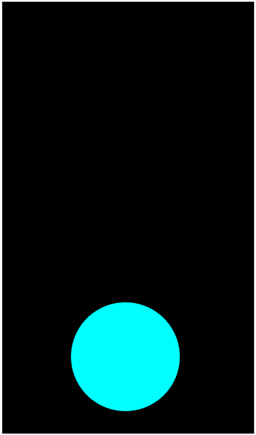
+ surfactant eqn. $\dot{S} - D_\Gamma \Delta_\Gamma S + (\nabla_\Gamma \cdot \mathbf{v})S = 0$

- τ does **not** depend on S.

Observation

- accumulation of surfactant at the bottom.

solution



Concluding remarks

- DROPS: FE techniques for two-phase incompressible flows.
- Hierarchical tetrahedral triangulations.
- Level set method.
- Variational Laplace-Beltrami discretization of surface tension.
- XFEM space for discretization of discontinuous functions.
- Interface FE space for PDE on the interface.
- Special preconditioners for efficient solvers.
- MPI parallelization.

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More information: www.igpm.rwth-aachen.de/DROPS