Unstructured Finite-Volume Arbitrary Lagrangian / Eulerian Interface Tracking computational framework for incompressible two-phase flows with surfactants

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This presentation

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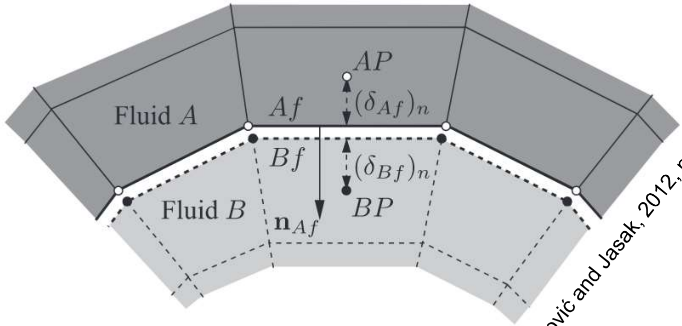
Interface-Tracking divides the domain with a sharp interface

- Finite volume
- Sharp interface
- Moving mesh
- Arbitrary cells



[Tuković and Jasak, 2012, p. 74]

Bulk equations

$$\oint_S \rho \boldsymbol{n} \cdot \boldsymbol{v}\, dS = 0$$

$$\frac{d}{dt}\int_V \rho \boldsymbol{v}\, dV + \oint_S \boldsymbol{n} \cdot \rho(\boldsymbol{v} - \boldsymbol{v_S})\boldsymbol{v}\, dS$$

$$= \oint_S \boldsymbol{n} \cdot (\mu \nabla \boldsymbol{v}) dS - \int_V \nabla p\, dV$$

Interfacial jump conditions

$$[\![p]\!] = -2[\![\mu]\!]\nabla_S \cdot \boldsymbol{v} + \sigma\kappa - 2[\![\rho \boldsymbol{g} \cdot \boldsymbol{r}]\!]$$

$$[\![\mu\, \boldsymbol{n} \cdot \nabla \boldsymbol{v}]\!] = -\nabla_S \sigma - [\![\mu(\nabla_S \boldsymbol{v}) \cdot \boldsymbol{n}]\!] - [\![\mu]\!]\boldsymbol{n}(\nabla_S \cdot \boldsymbol{v})$$

$$[\![\boldsymbol{v}]\!] = 0$$

$$\boldsymbol{n} \cdot \left[\!\!\left[\frac{1}{\rho}\nabla p\right]\!\!\right] = n \cdot \left[\!\!\left[\frac{D\boldsymbol{v}}{Dt}\right]\!\!\right] + \boldsymbol{n} \cdot \left[\!\!\left[\frac{\mu}{\rho}\Delta \boldsymbol{v}\right]\!\!\right]$$

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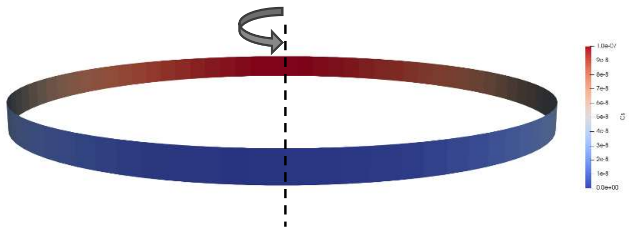
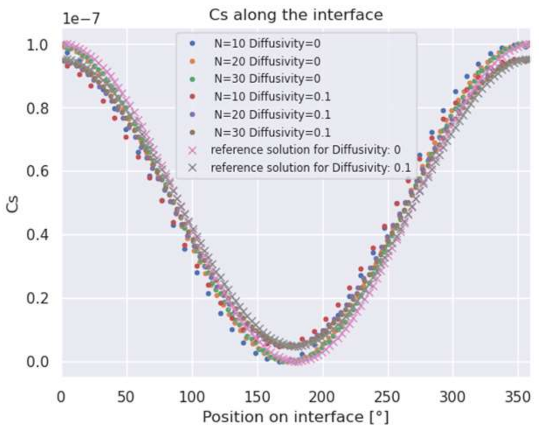
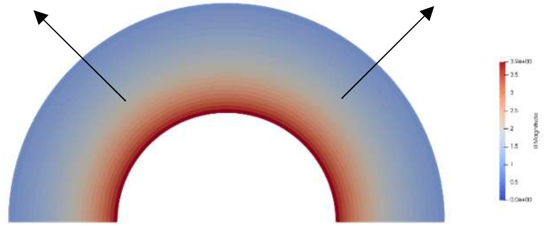
We verify surfactant capabilities

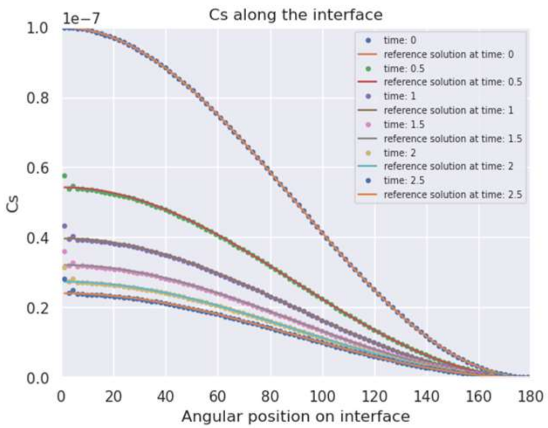
Transport with the interface



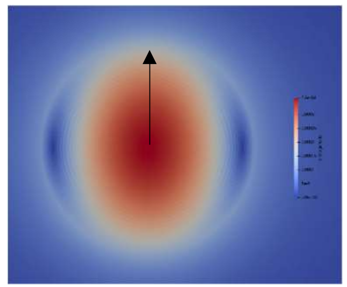


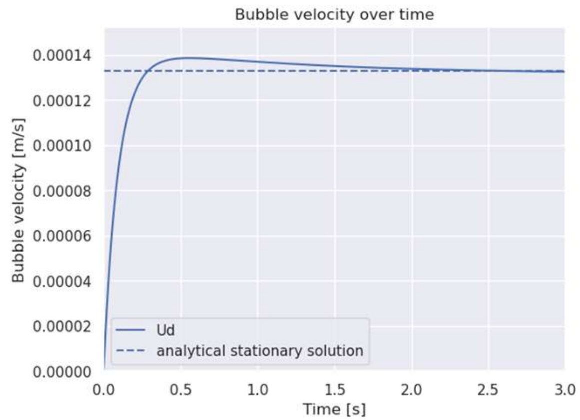
Changing interface





Surfactant induced Marangoni effect





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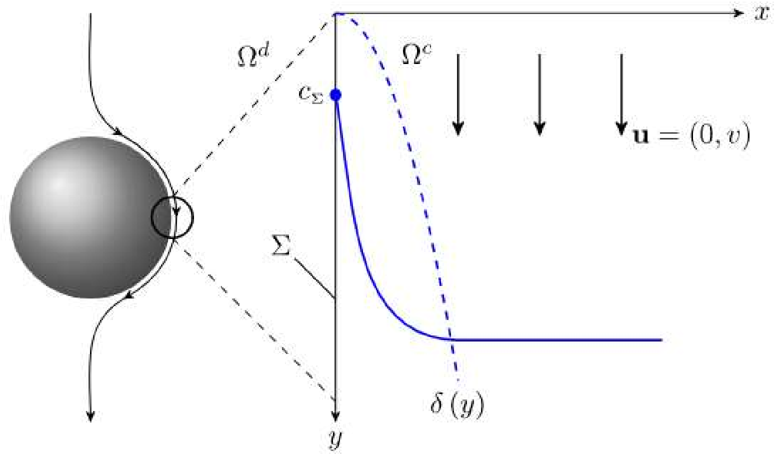
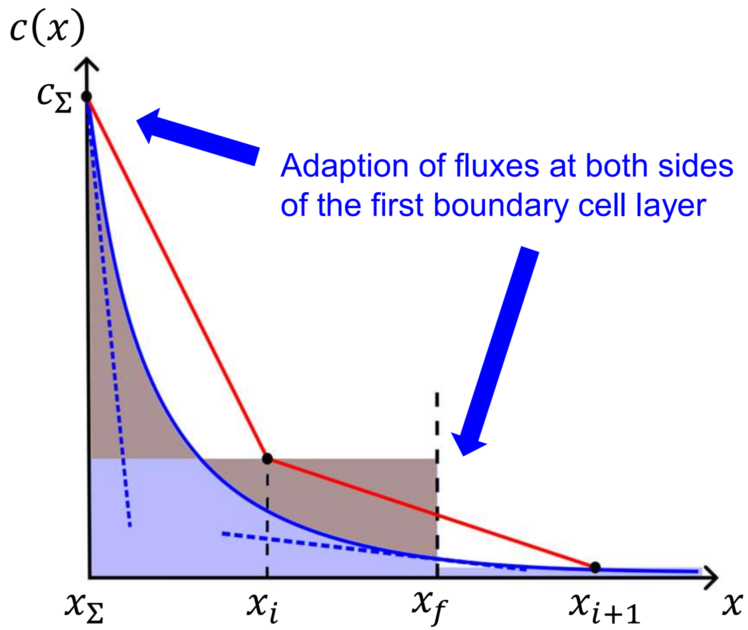
What is the SGS and why do we need it?

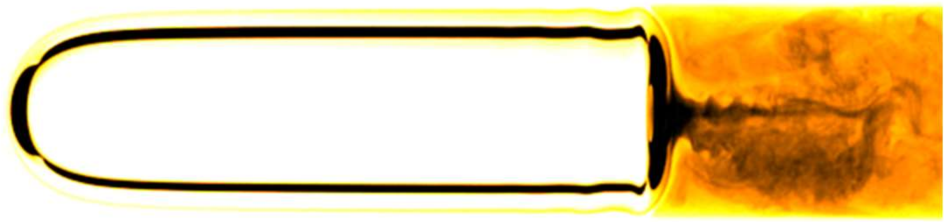


$$c(x, y) = c_\Sigma + (c_\infty - c_\Sigma)\,\mathrm{erf}\left(\frac{x}{\delta(y)}\right)$$

with

$$\delta(y) = \sqrt{4Dy/v}$$





Reactive Oxygen Taylor Bubble - Solution of Cu(btmgp)I (20 mM) in Acetonitrile at ambient pressure and temperature. Source: Project Group Prof. Dr.-Ing. Michael Schlüter, TU Hamburg: Experimental Investigation of Reactive Bubbly Flows - Influence of Boundary Layer Dynamics on Mass Transfer and Chemical Reactions

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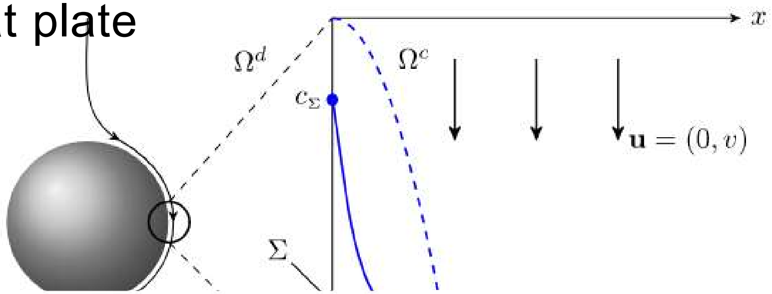
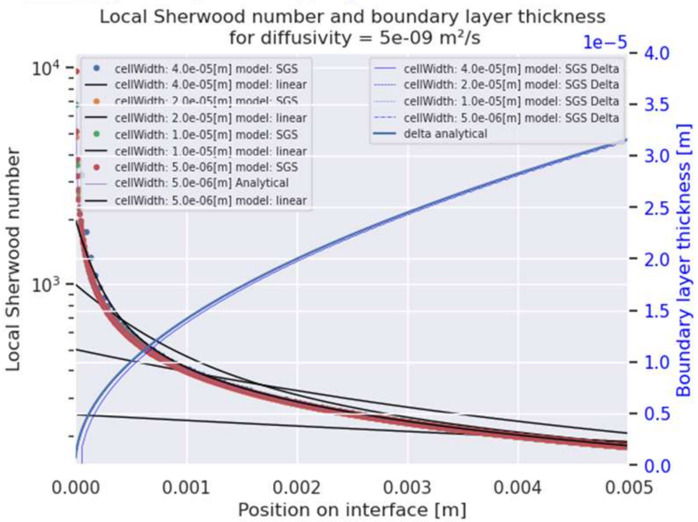
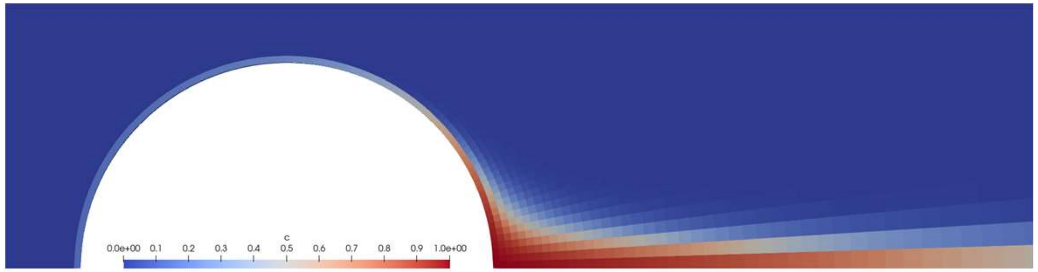
For development we have simple test cases

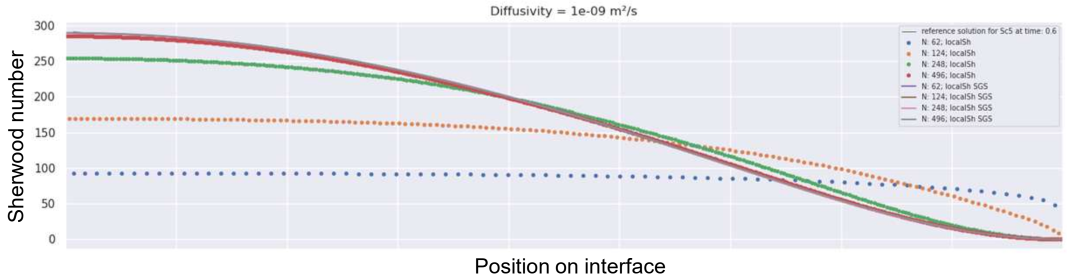
Flat plate





Axisymmetric bubble





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We added extensive evaluation possibilities, e.g.

Concentration

The concentration boundary layer is embedded into the first layer of cells adjacent to the interface over a large portion of the bubble.

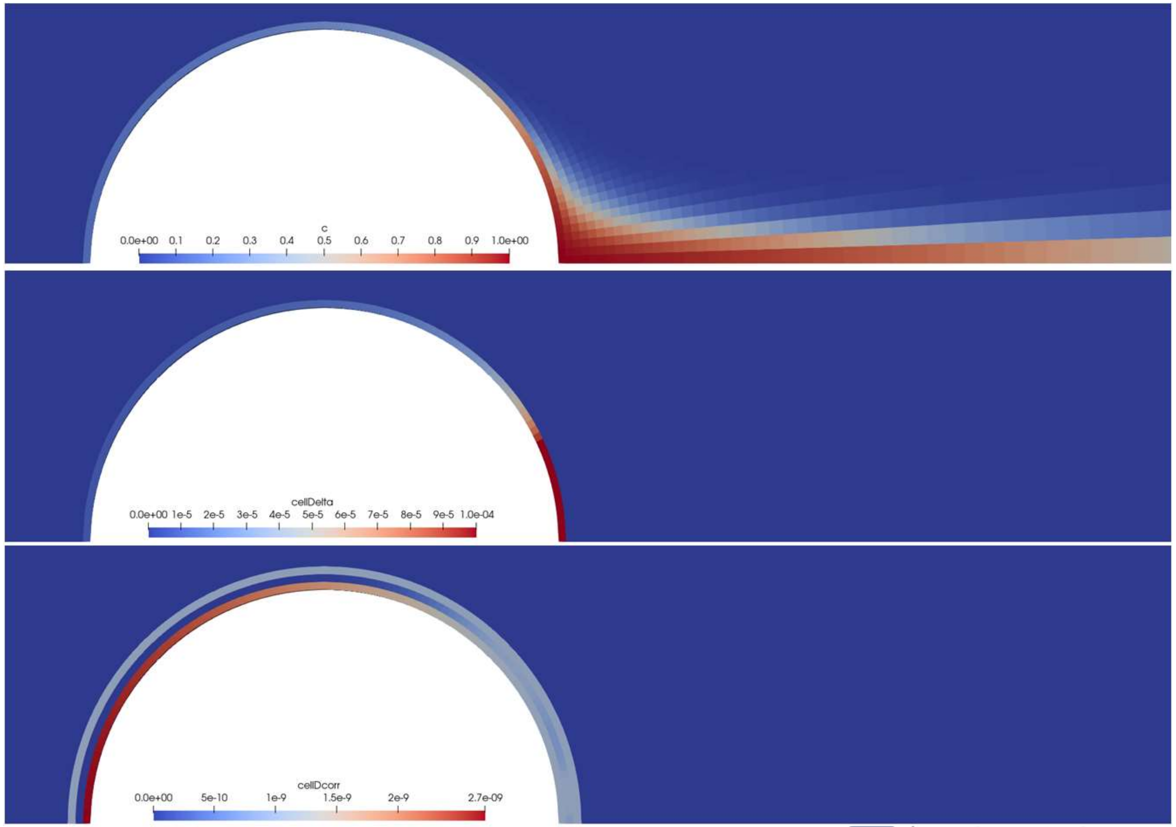
Boundary layer thickness

The boundary layer thickness grows slowly, where the flow is adjacent. It is big, where the flow is separated.

Diffusivity coefficient

(from inside out: at the interface, the 2nd layer, original)

In the impingement area, the flow at the interface is increased, but decreased at the cell faces between first and second cell layer. Not much correction is needed where the boundary layer thickness is big.



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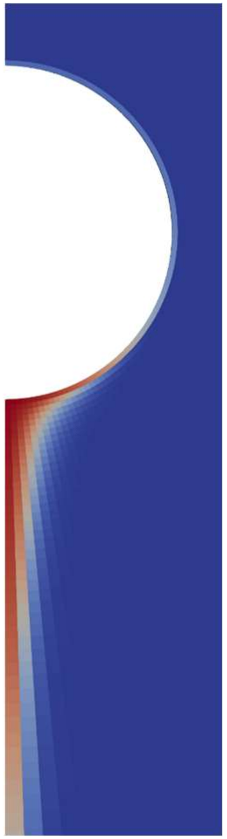
Wrap-up



- We provide an Arbitrary Lagrangian/Eulerian Interface Tracking (ALE-IT) framework for OpenFOAM
- We implemented our Subgrid-scale model library
  - Calculate very thin passive scalar boundary layers
  - Correct diffusive and convective fluxes at the boundary and the faces next to the interface
    - The fluxes at the interface are increased
    - The fluxes at the faces next to the interface are decreased
  - Visualisation of Subgrid-scale model internal parameters enables understanding and further developments
- Publicly available soon

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Further reading

- This presentation
  DOI: 10.48328/tudatalib-1266.6
- Preprint
  (currently in preparation)
- Code repository
  (currently private, going public soon)
  https://gitlab.com/interface-tracking/

This presentation

Code repository is coming soon

- Papers
  - Interface Tracking: Zeljko

    - Tuković, Ž. & Jasak, H. A moving mesh finite volume interface tracking method for surface tension dominated interfacial fluid flow. *Computers & Fluids* **55**, 70–84 (2012).

  - Subgrid-scale model

    - Pesci, C., Weiner, A., Marschall, H. & Bothe, D. Computational analysis of single rising bubbles influenced by soluble surfactant. *J. Fluid Mech.* **856**, 709–763 (2018).
    - Weiner, A. & Bothe, D. Advanced subgrid-scale modeling for convection-dominated species transport at fluid interfaces with application to mass transfer from rising bubbles. *Journal of Computational Physics* **347**, 261–289 (2017).

  - Surfactant verification cases

    - Antritter, T. Numerical Simulation of Coupled Wetting and Transport Phenomena in Inkjet Printing. (Technische Universität Darmstadt, 2022). doi:10.26083/tuprints-00021326.

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Appendix

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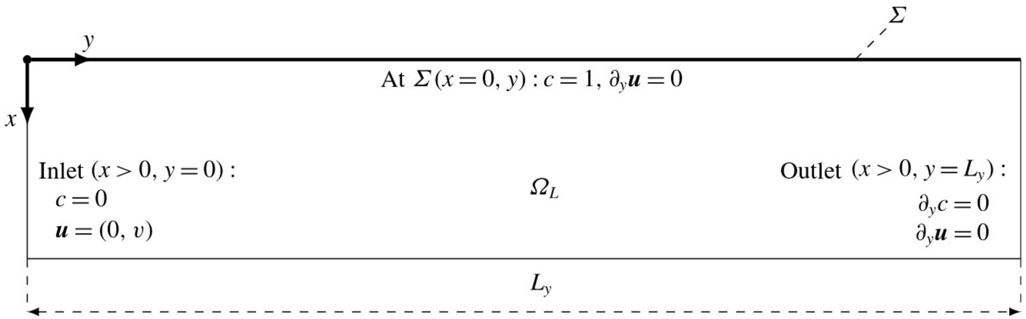
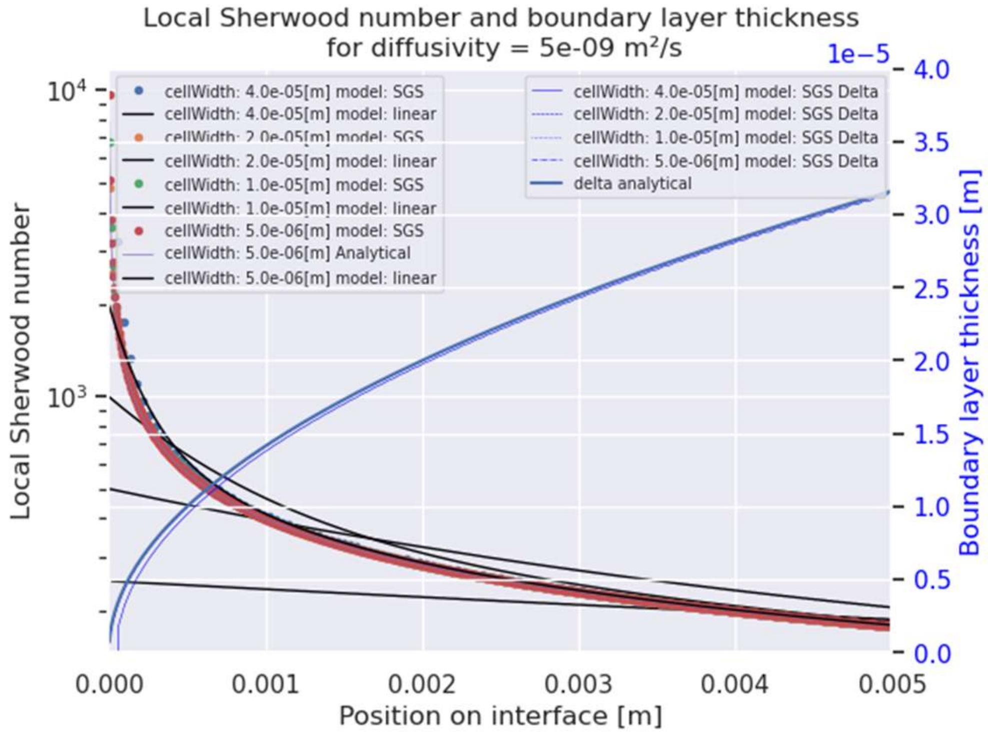
Flat plate





- Prescribed velocity = 0.1 m/s
- No velocity boundary layer
- Peclet number 10^5
  - Tested with $10^4 – 10^7$

$$Pe = \frac{L \cdot u}{D}$$

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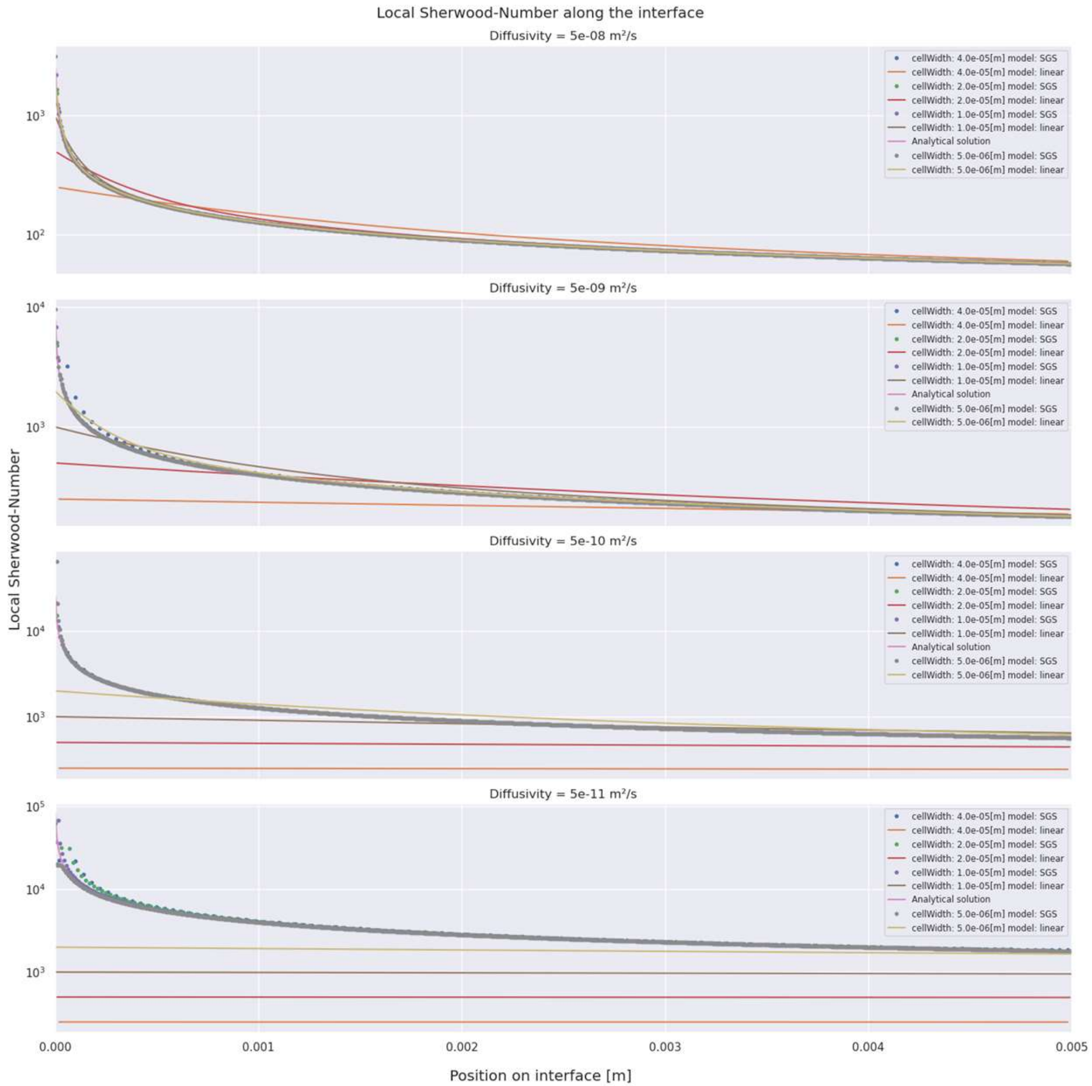
Flat plate

Diffusivity [m²/s]	Peclet number [ ]
$5e^{-08}$	$1e^{4}$
$5e^{-09}$	$1e^{5}$
$5e^{-10}$	$1e^{6}$
$5e^{-11}$	$1e^{7}$



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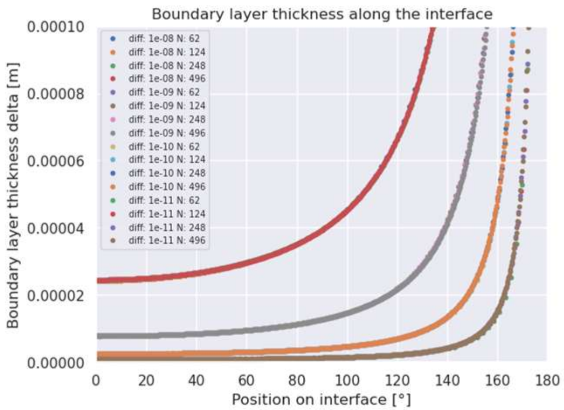
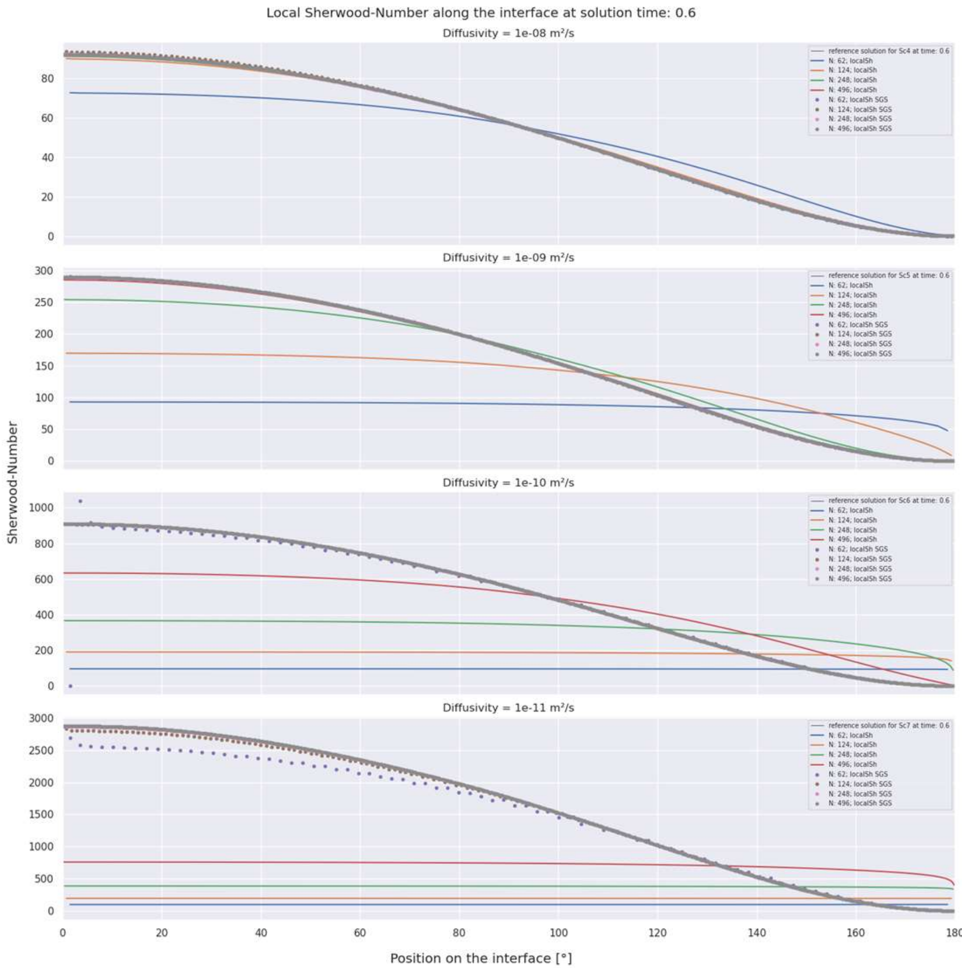
Axisymmetric bubble

- Prescribed velocity based on solution by Satapathy & Smith
- Spherical bubble (Ø 2mm) with rigid interface
- Axisymmetric setup
- Schmidt-numbers of real-world problems $Sc = \frac{\mu}{D}$

Diffusivity [m²/s]	Schmidt number [ ]
5e^{-08}	**1e^{4}**
5e^{-09}	**1e^{5}**
5e^{-10}	**1e^{6}**
5e^{-11}	**1e^{7}**





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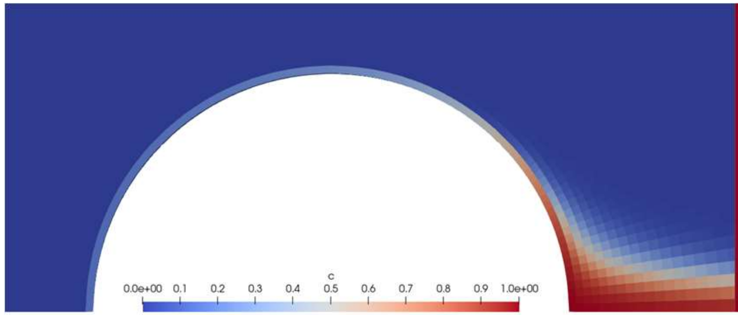
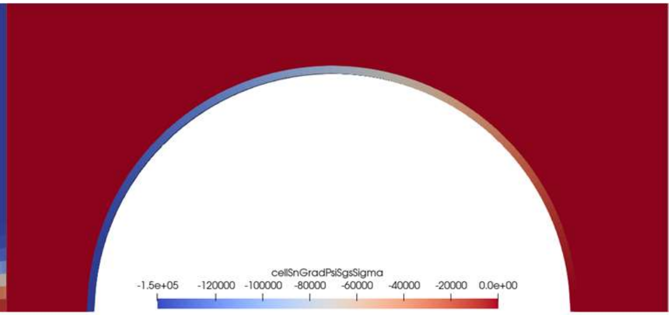
Axisymmetric bubble



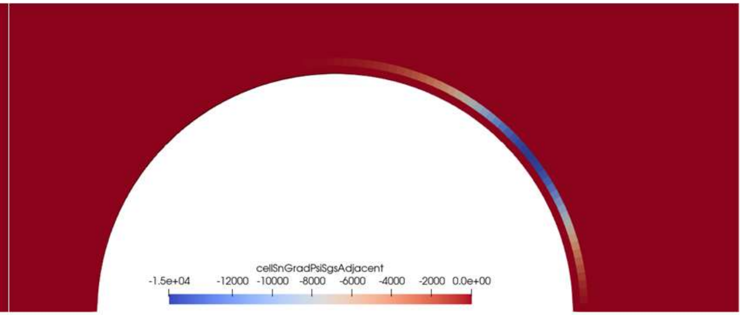
- Concentration

Accumulates pronounced in the wake of the bubble.



- Surface normal gradient at the surface

Decreases over the run length to almost zero in the wake.



- Surface normal gradient at outward-faces of the 1st cell layer

Is highest where the flow is still adjacent. Is almost zero in the impingement area and in the center of the wake.

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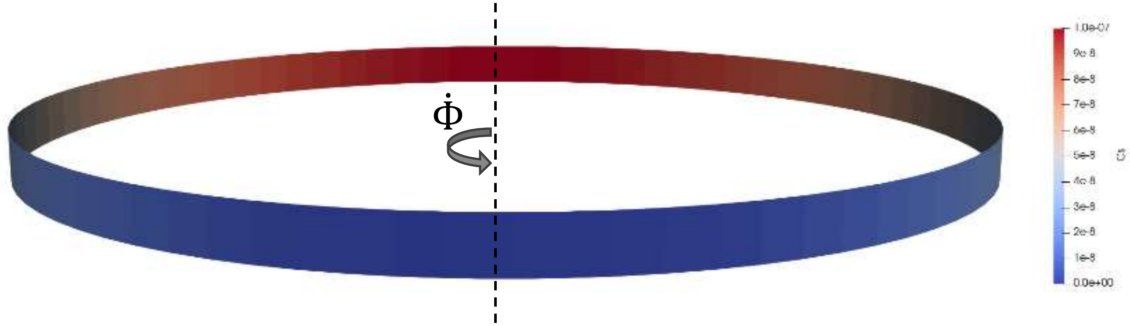
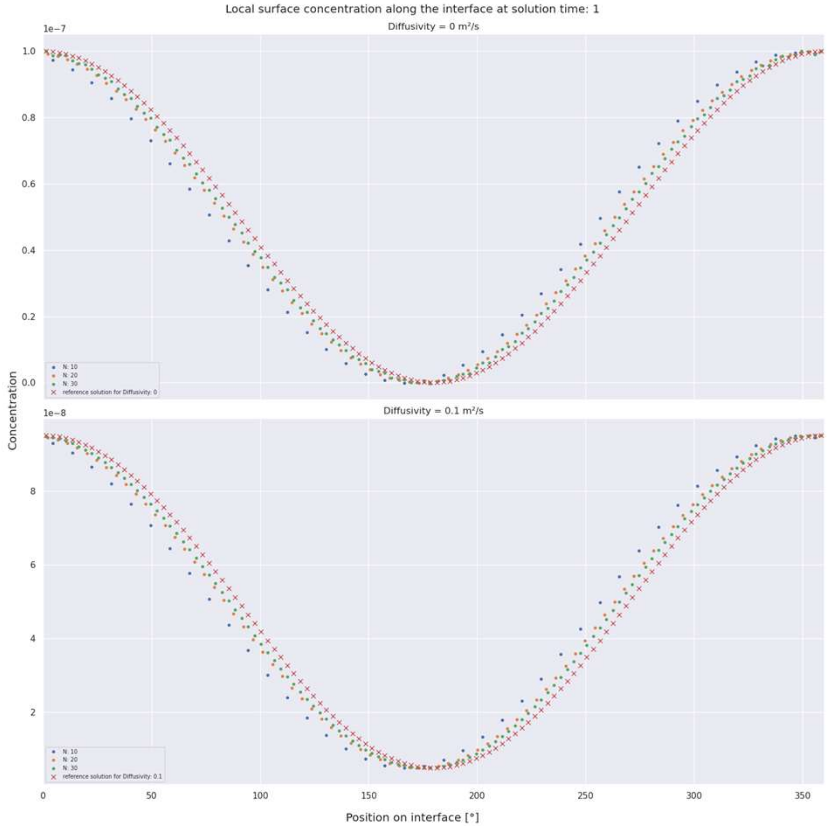
Rotating contaminated droplet



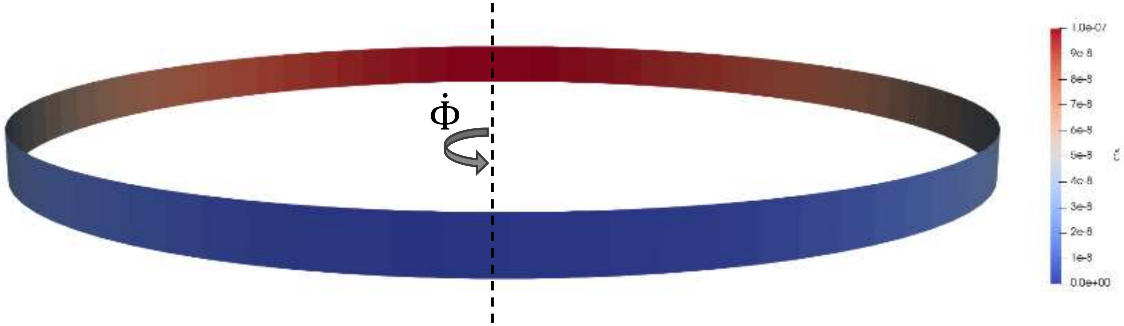


$$\Gamma(\Phi,\tau) = \frac{e^{-D*r_0^{-2}\tau}\cos\left(\Phi - \dot{\Phi}\tau\right) + 1}{2}\Gamma_0$$

cf. [Antritter, 2022]

- Prescribed rotation $\dot{\Phi}$
- No mesh motion
- With/without diffusivity

Rotating contaminated droplet



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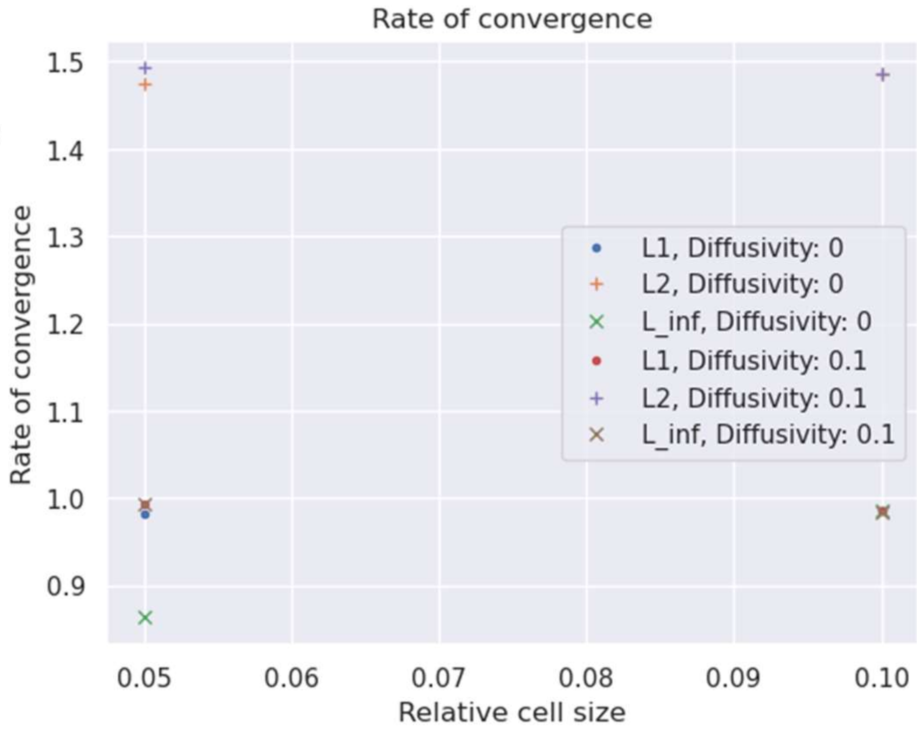

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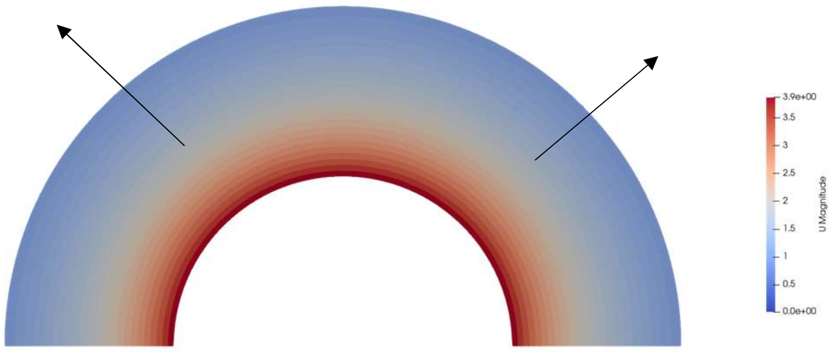
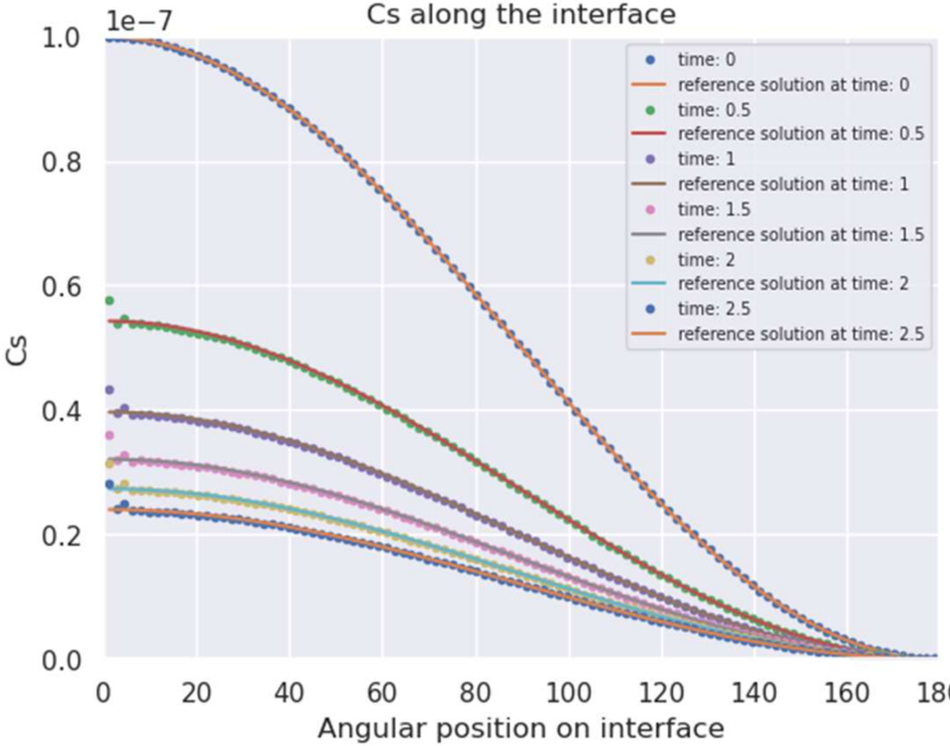
Expanding contaminated droplet



$$\Gamma\big(\Phi,\tau(t)\big) = \frac{\cos(\Phi)+1}{2}\Gamma_0\frac{r_0^2}{\big(r(t)\big)^2}$$

cf. [Antritter, 2022]



- Prescribed velocity
- Prescribed mesh motion
- No diffusion

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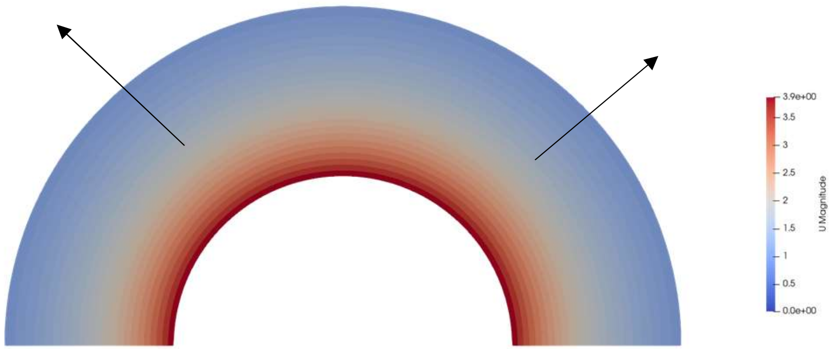
Expanding contaminated droplet



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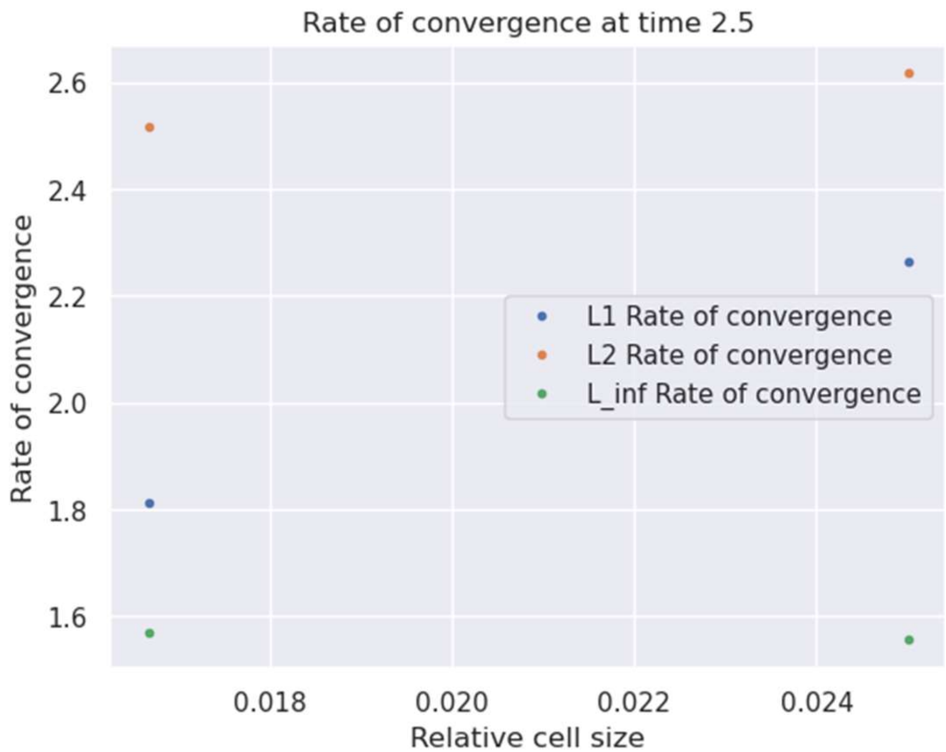

- Prescribed velocity
- Prescribed mesh motion
- No diffusion

cf. [Antritter, 2022]

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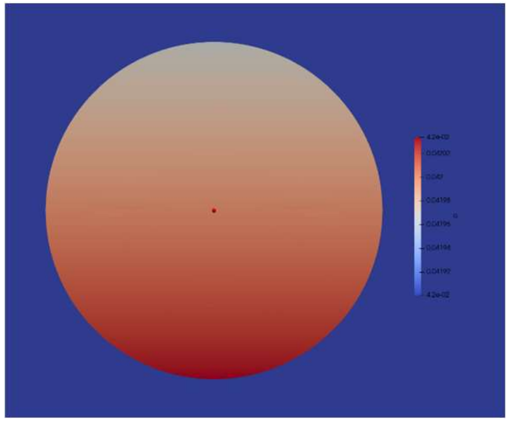
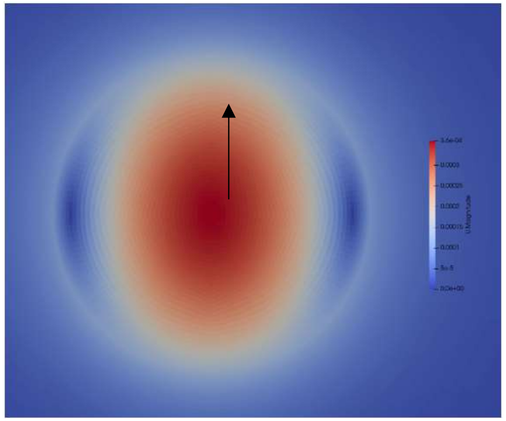
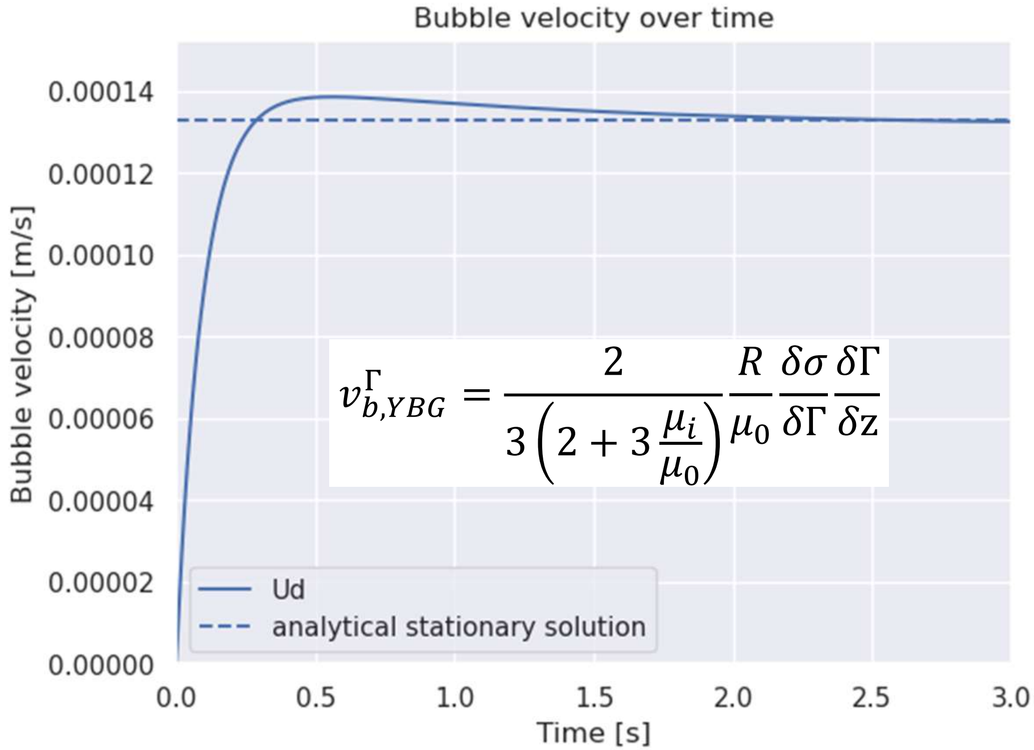
Surfactant induced Marangoni effect driven bubble







- No (mesh) motion, rigid bubble
- Fixed surfactant concentration leads to pressure gradient

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