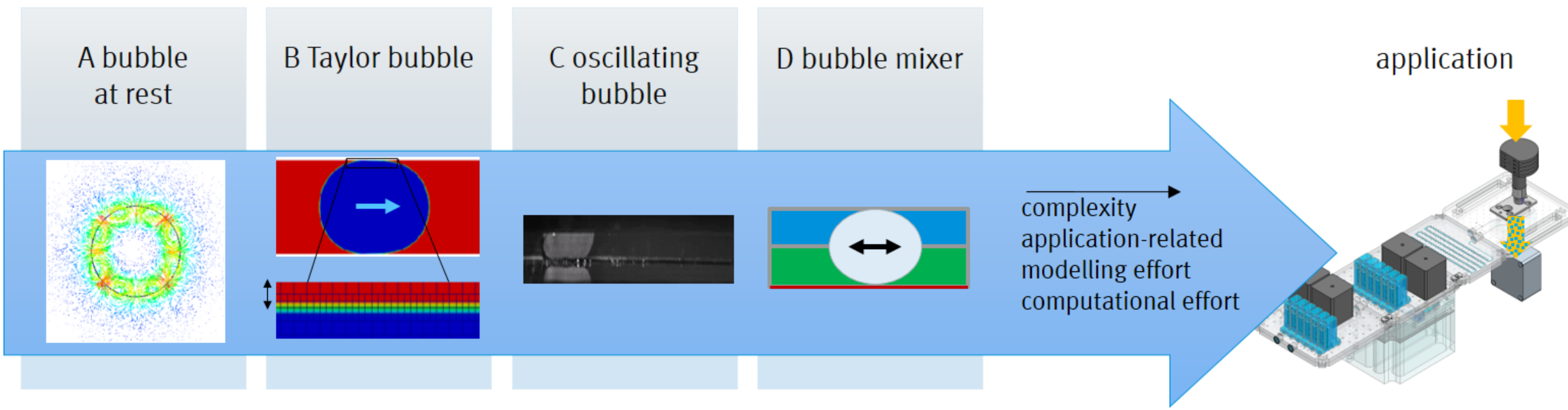
FESTO

From research to industry, Gerris for microfluidic multiphase application development

Hans Heimel[1]

Basilisk/Gerris Users' Meeting 2017

November 15-16, 2017 Princeton



[1]PhD student at IMTEK University Freiburg, Germany and Festo AG & Co. KG Esslingen, Germany

Outline

Introduction

- Festo
- Motivation
- Simulative challenges
- Simulative approach

Bubble at rest

- Case description
- Results

Taylor bubble

- Case description
- Results

Conclusions & Outlook

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Conclusions & Outlook

Festo

is a global market leader for Industry Automation

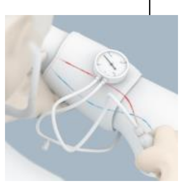
Festo

successfully invested in its fast growing MedLab business field

Medical Devices:

Controlling gas flow and pressure

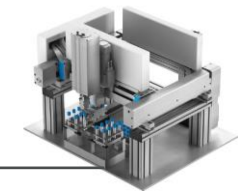
- Respiratory
- Dental station
- Ophthalmology
- Medical equipment

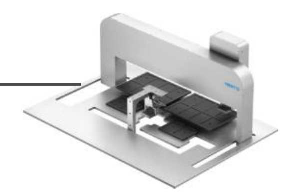


Laboratory Instruments:

From feeding, identifying and testing sample holders to moving, opening and closing test tubes and test carriers to feeding liquids and solids

- Sample handling
- Liquid handling
- Pre-/post-analytics





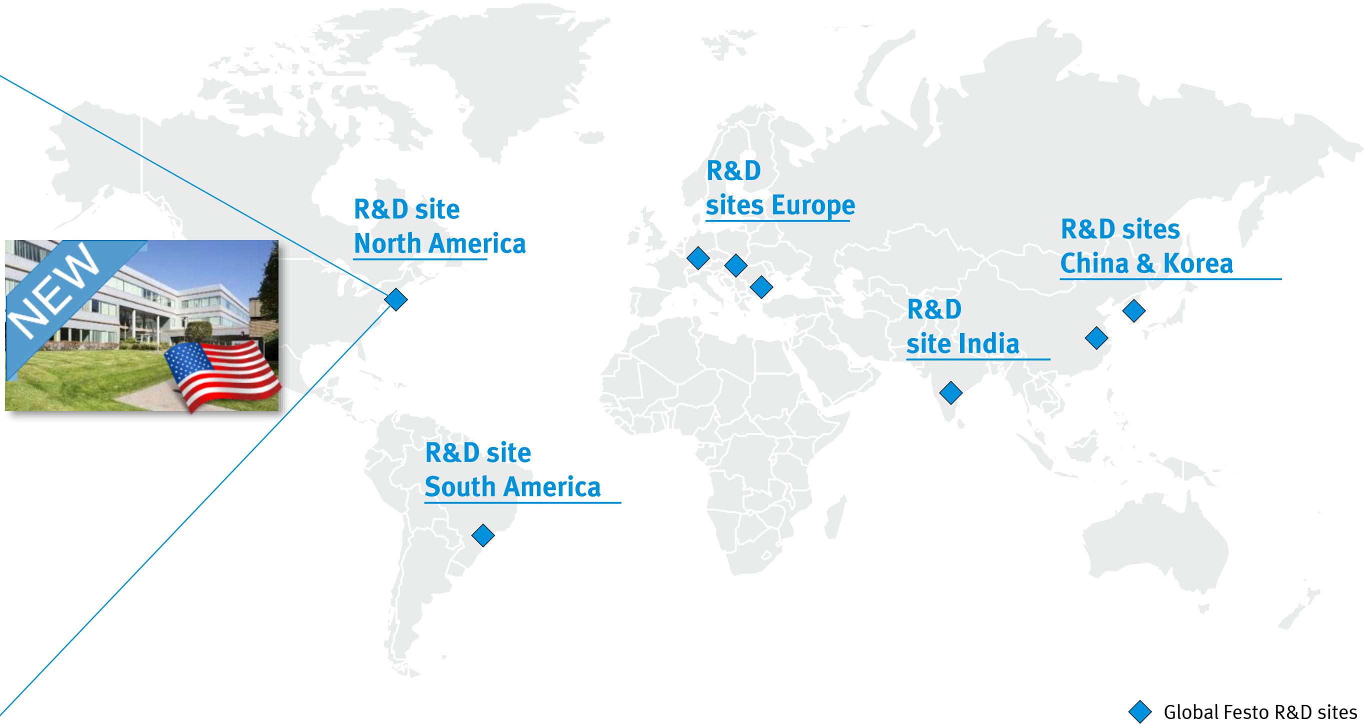
Festo

extends its global R&D footprint with a new R&D site for Liquid Handling near Boston, MA

New R&D site near Boston, MA

- Focus on our MedLab business field (Liquid and Sample Handling)
- Located in 298 Concord Road, Billerica, MA 01821
- Ramp up from beginning of 2018
- Development capacity for customer solutions and catalogue products

You are welcome to visit us in our new R&D site near Boston !



Motivation

Fast growth of microfluidic market -> desire for CFD assisted development

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- **Observation**: Microfluidic multiphase CFD has strong focus on research

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- Differences to macrofluidic industries (like automobile):

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    - Prototypes are cheap and quick to produce

Motivation

Fast growth of microfluidic market -> desire for CFD assisted development

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- Differences to macrofluidic industries (like automobile):
    - Prototypes are cheap and quick to produce
    - Cost per piece low

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Fast growth of microfluidic market -› desire for CFD assisted development

- **Observation**: Microfluidic multiphase CFD has strong focus on research

- Differences to macrofluidic industries (like automobile):
    - Prototypes are cheap and quick to produce
    - Cost per piece low
    - „Low hanging fruits“ in young microfluidic market

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- Differences to macrofluidic industries (like automobile):
    - Prototypes are cheap and quick to produce
    - Cost per piece low
    - „Low hanging fruits“ in young microfluidic market
    - Macrofluidic theorie and simulation methods well established for decades

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- Differences to macrofluidic industries (like automobile):
    - Prototypes are cheap and quick to produce
    - Cost per piece low
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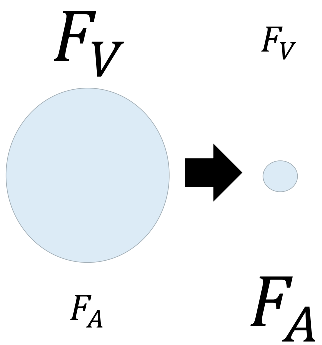
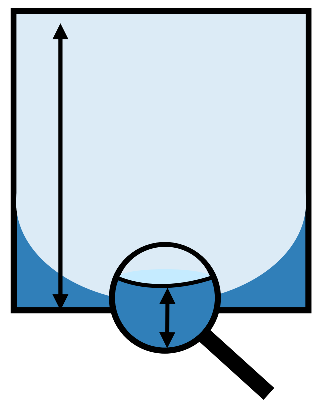
    - Macrofluidic theorie and simulation methods well established for decades

Can CFD simulations sucessfully be included into the development process of microfluidic multiphase applications?

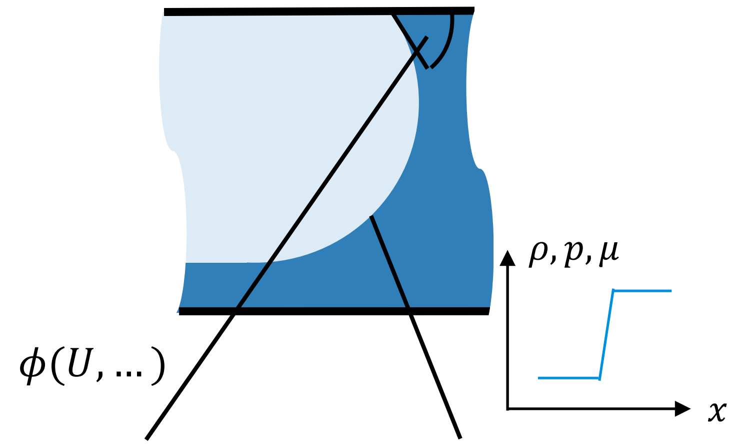
Simulative challenges – Overview



Surface forces



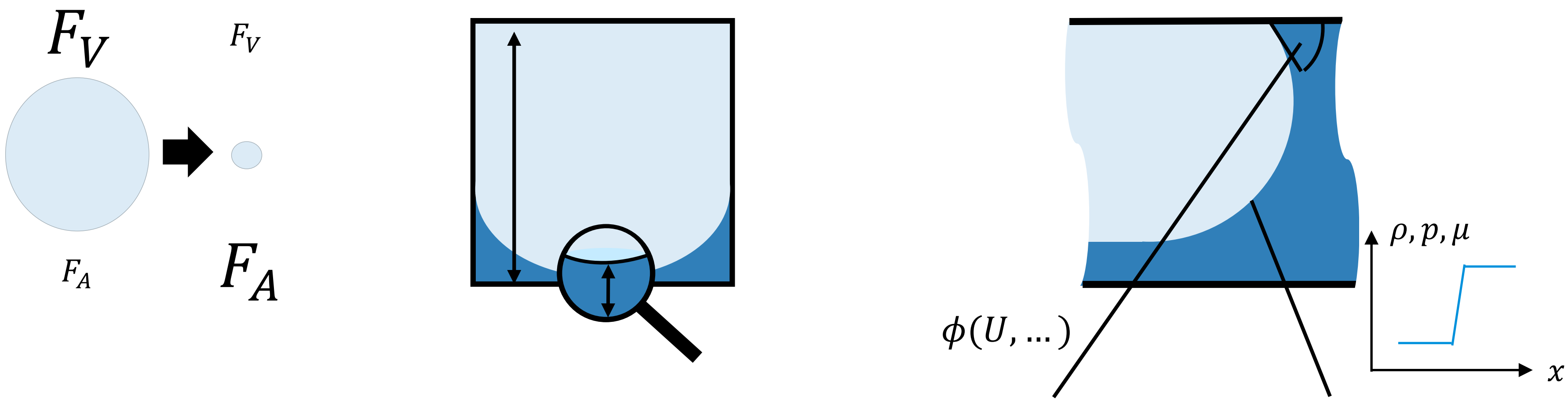
Multiple scales



Contact angles

Discontinuity

Simulative challenges – Overview



Surface forces | Multiple scales | Contact angles | Discontinuity

Volume of Fluid (VOF)
- sharp interface
- simple transport equation
- mass conservation **(+)**
- parasitic currents **(-)**

Gerris | interFoam (2.31) | StarCCM+ (10.4)

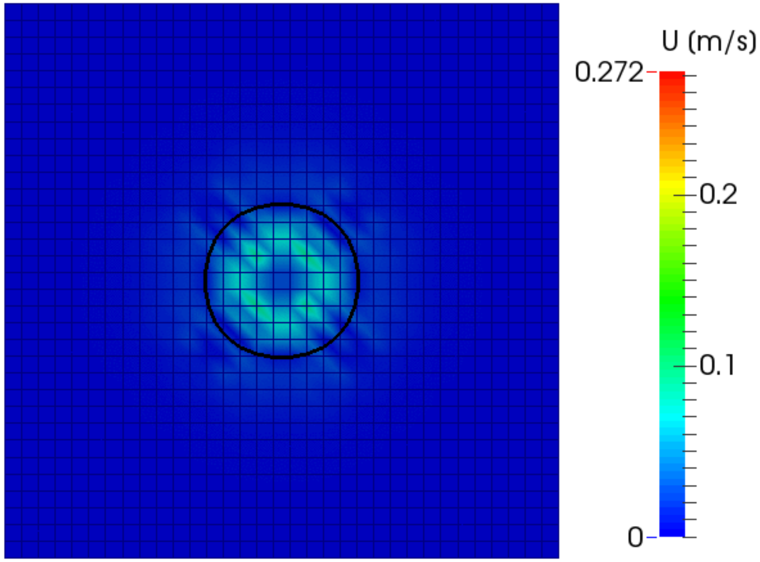
Phase Field (PF)
- diffuse interface
- complex transport equation
- mass conservation **(-)**
- parasitic currents **(+)**

phaseFieldFoam | COMSOL

Simulative challenges – Parasitic currents

- Undesired flow velocities
- **Worst case: $U_{parasitic} \gg U$**
  -> severe impact on microfluidic simulations

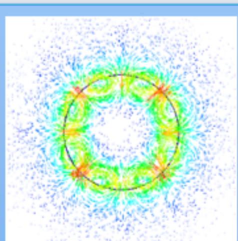
- Sources:
  1. Inconsistent implementation of
     ∇p and $\boldsymbol{f}_{\sigma} = \sigma\kappa\nabla\alpha$
  2. Inaccurate curvature estimation in
     $\boldsymbol{f}_{\boldsymbol{\sigma}} \approx \sigma\tilde{\kappa}\nabla\alpha$
  3. Residual tolerance of solver $\nabla\tilde{p}$
  4. Errors in interface advection
  5. Inaccurate initialization (capillary wave)



Simulative approach

Transition form research to industry

A bubble at rest

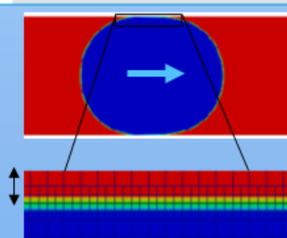


Parasitic currents
Bubble pressure
(Interface thickness)
(Mass error)

Simulation

+

B Taylor bubble



Lubrication film
Ca regime
Bubble dynamics

Simulation

+

C oscillating bubble

Surface effects
Contact angle dynamics/hysteresis

Simulation

Experiment

+

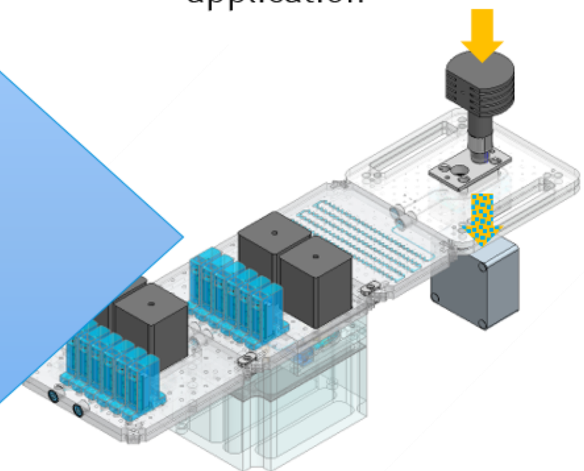
D bubble mixer

Verification mechanism

Simulation

Experiment

application



complexity
application-related modelling effort
computational effort

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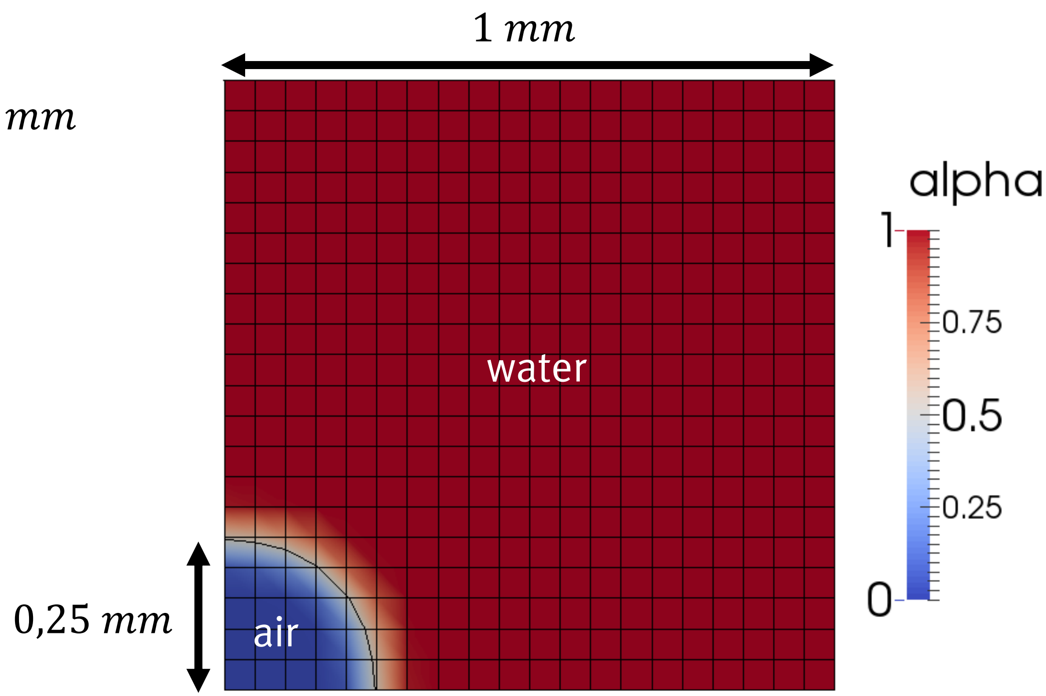
Bubble at rest – Case description

- 2D square domain, L $= 1\ mm$
- Centered air bubble (symmetry) $R = 0{,}25\ mm$ in **quiescent water**
- Water/air at standard conditions



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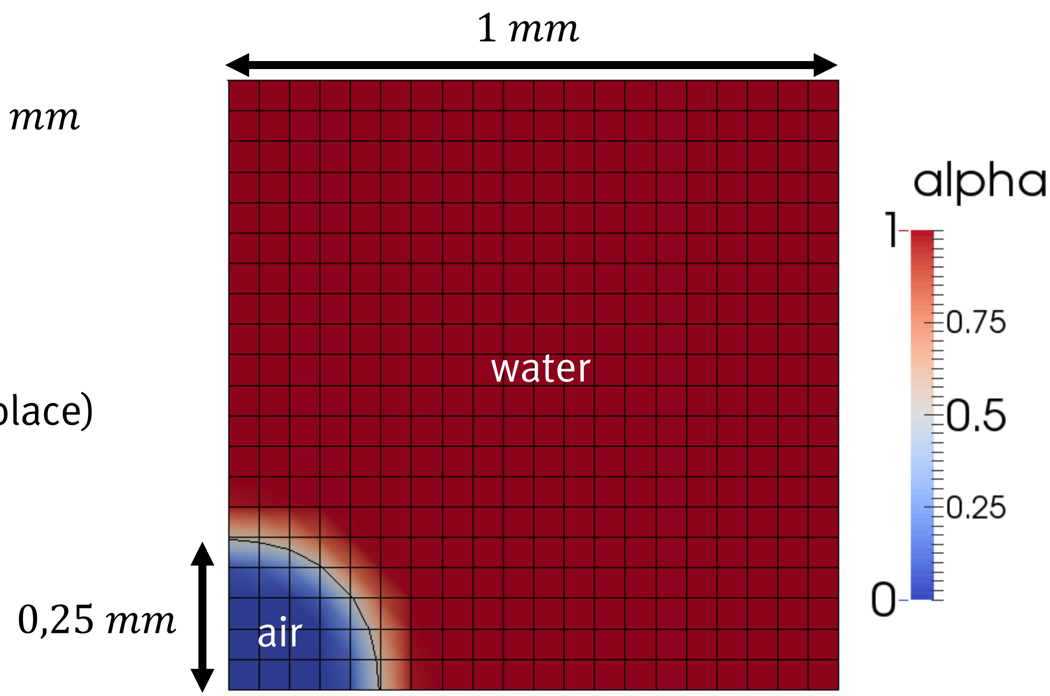
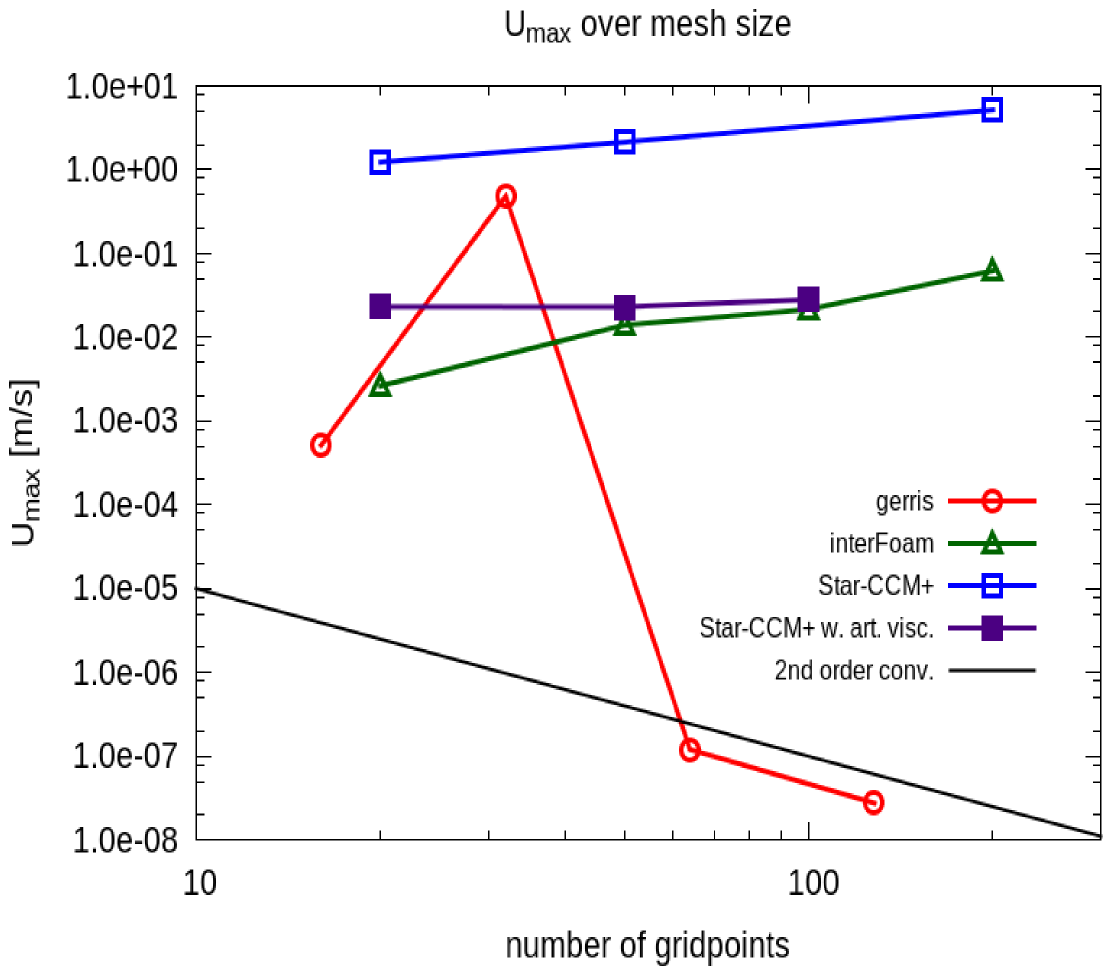
Bubble at rest – Case description

- 2D square domain, L $= 1\ mm$
- Centered air bubble (symmetry) $R = 0{,}25\ mm$ in **quiescent water**
- Water/air at standard conditions
- Mesh influence in solvers on
  - parasitic currents $\rightarrow U_{max} = U_{pc}$
  - Bubble physics $\rightarrow \Delta\text{p} = \sigma/R$ (Laplace)
- Grid refinement study
  - 16 … 200 cells / L
  - 4 … 50 cells / R



-> Scaling behaviour of parasitic currents and bubble physics with mesh size

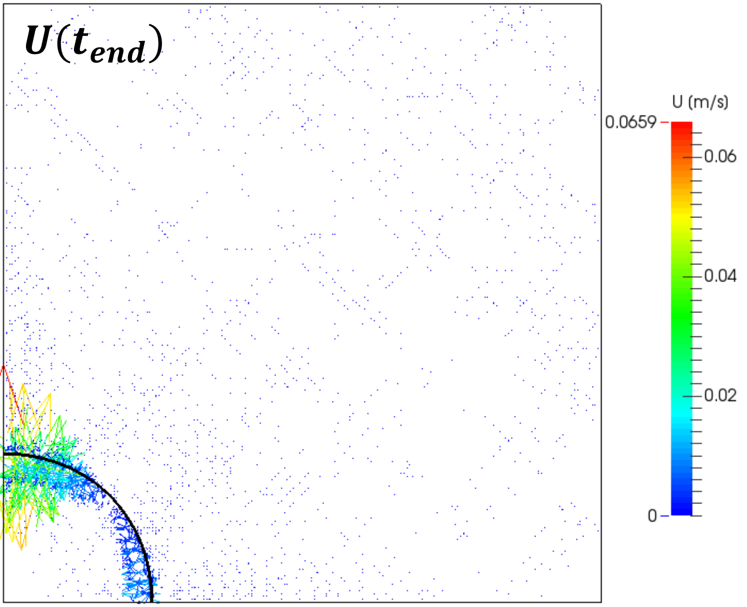
Bubble at rest – Parasitic currents over resolution

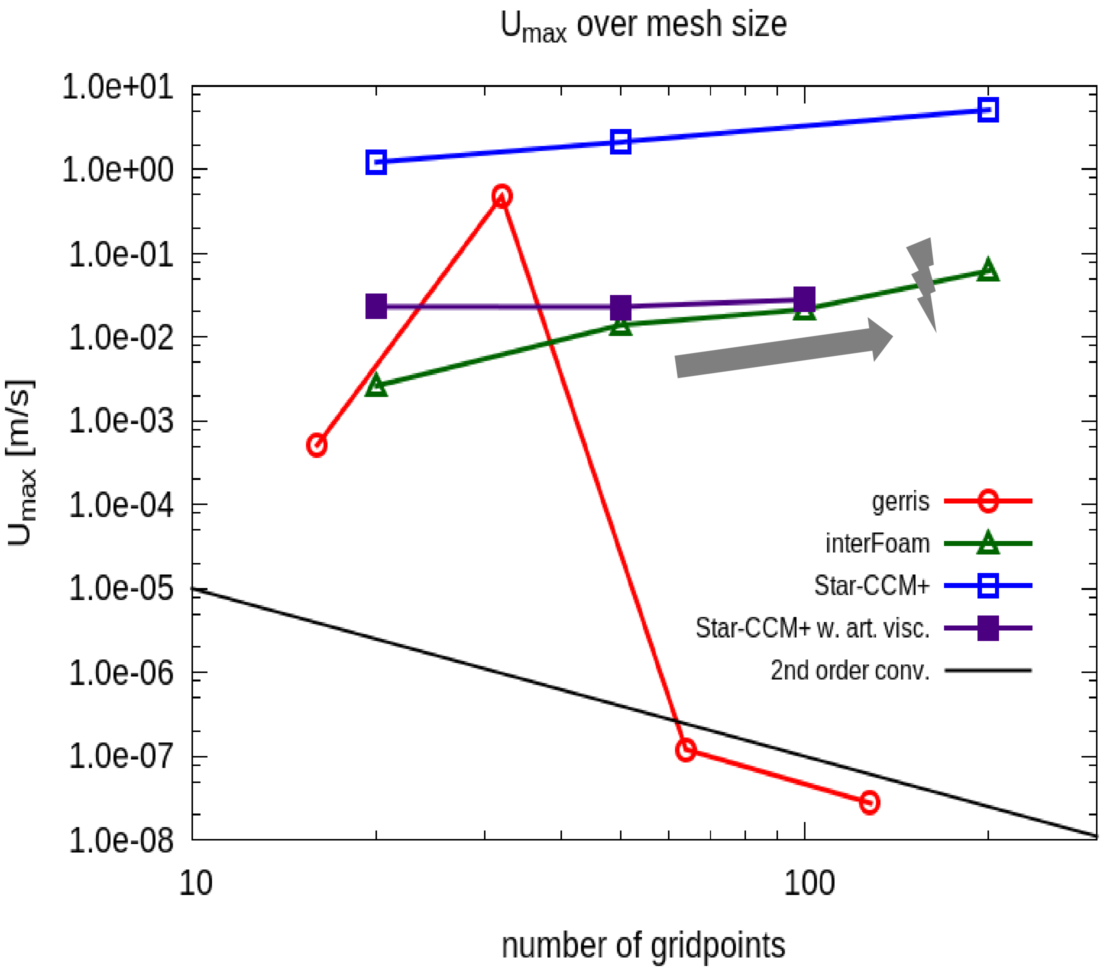


Bubble at rest – Parasitic currents over resolution

interFoam

- U_{pc} increase with $\Delta x \rightarrow 0$
- $O(U_{pc}) \approx 10^{-3} - 10^{-1}\ m/s$

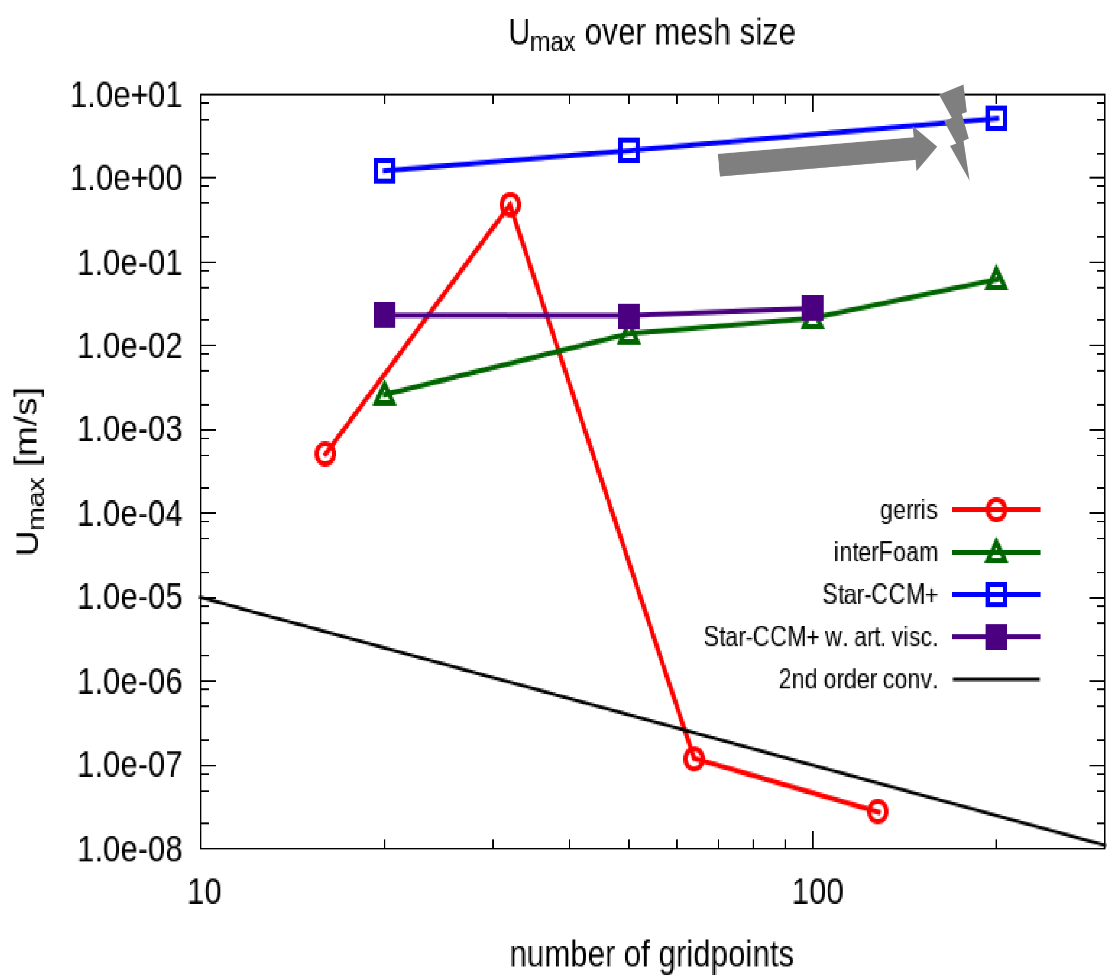




Bubble at rest – Parasitic currents over resolution

Star-CCM+

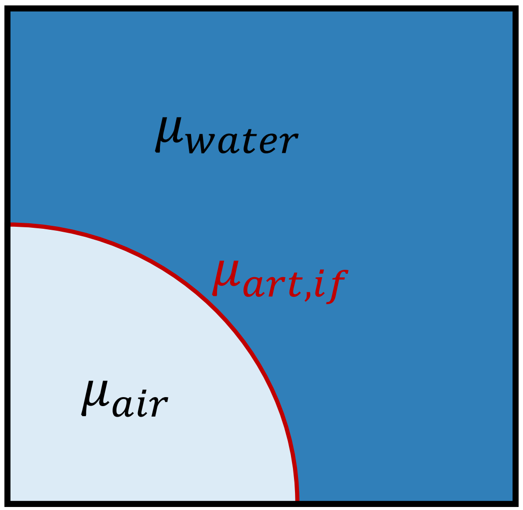
- U_{pc} increase with $\Delta x \rightarrow 0$



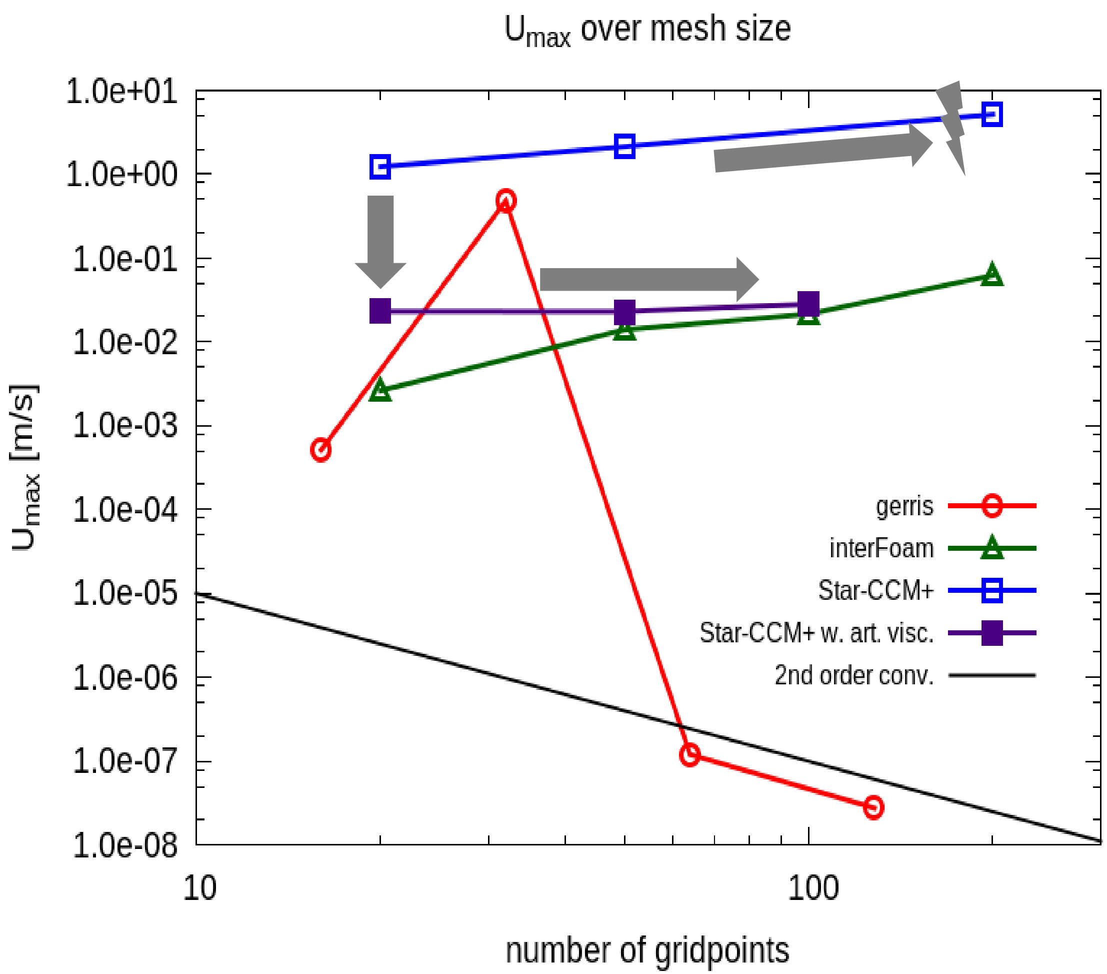
Bubble at rest – Parasitic currents over resolution

Star-CCM+

- U_{pc} increase with $\Delta x \rightarrow 0$
- Artificial interface viscosity



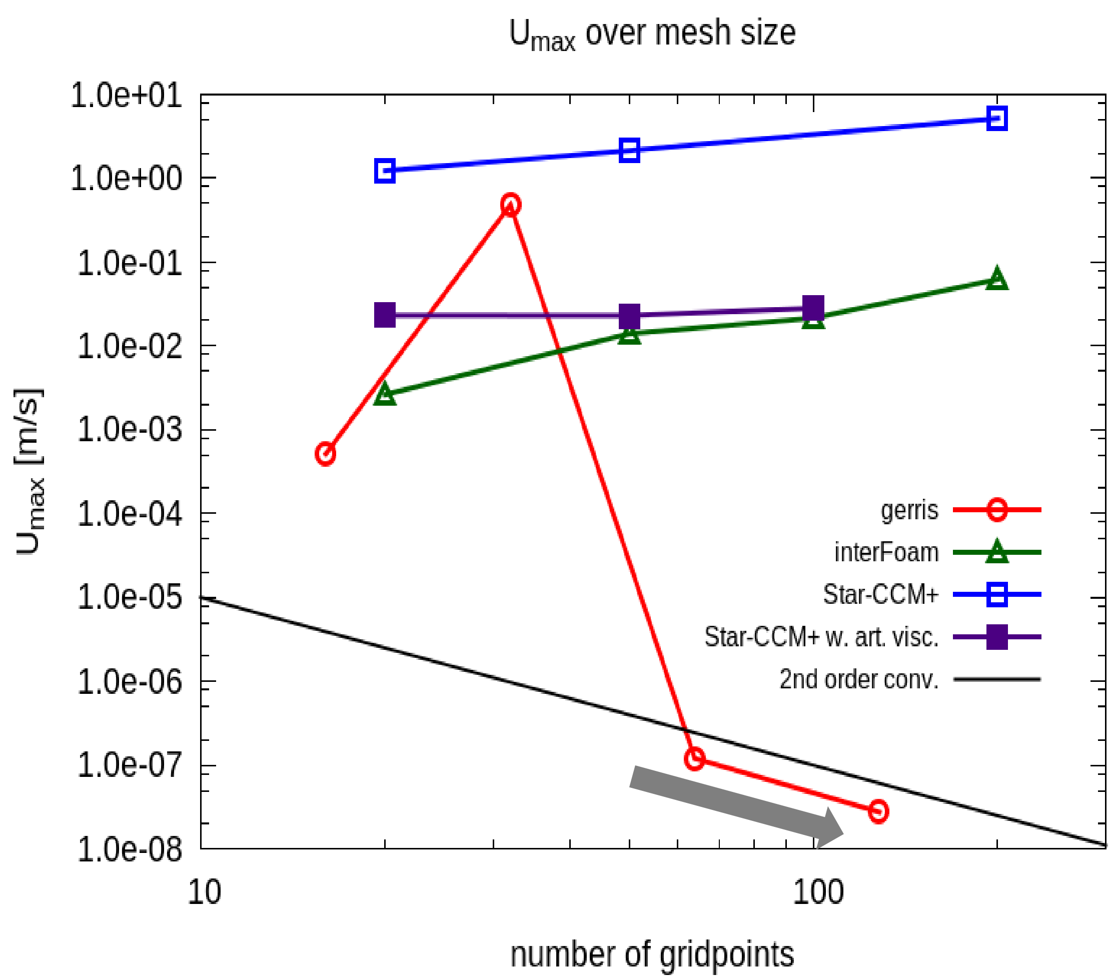
- $\mu_{art,if} \gg \mu_{water}$
- reduces U_{pc} by 10^2
- U_{pc} stagnates with $\Delta x \rightarrow 0$
- $O(U_{pc}) \approx 10^{-2} - 1\ m/s$



Bubble at rest – Parasitic currents over resolution

Gerris

- $U_{pc} \sim \Delta x^2$ for $\mathrm{R}/\Delta x \geq 16$



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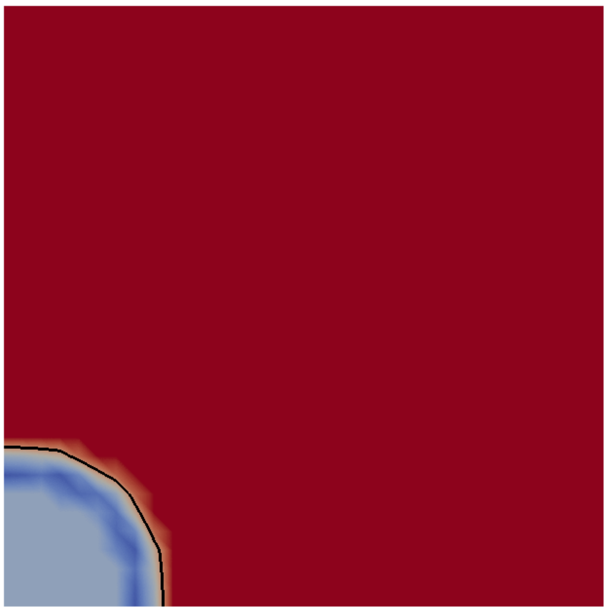

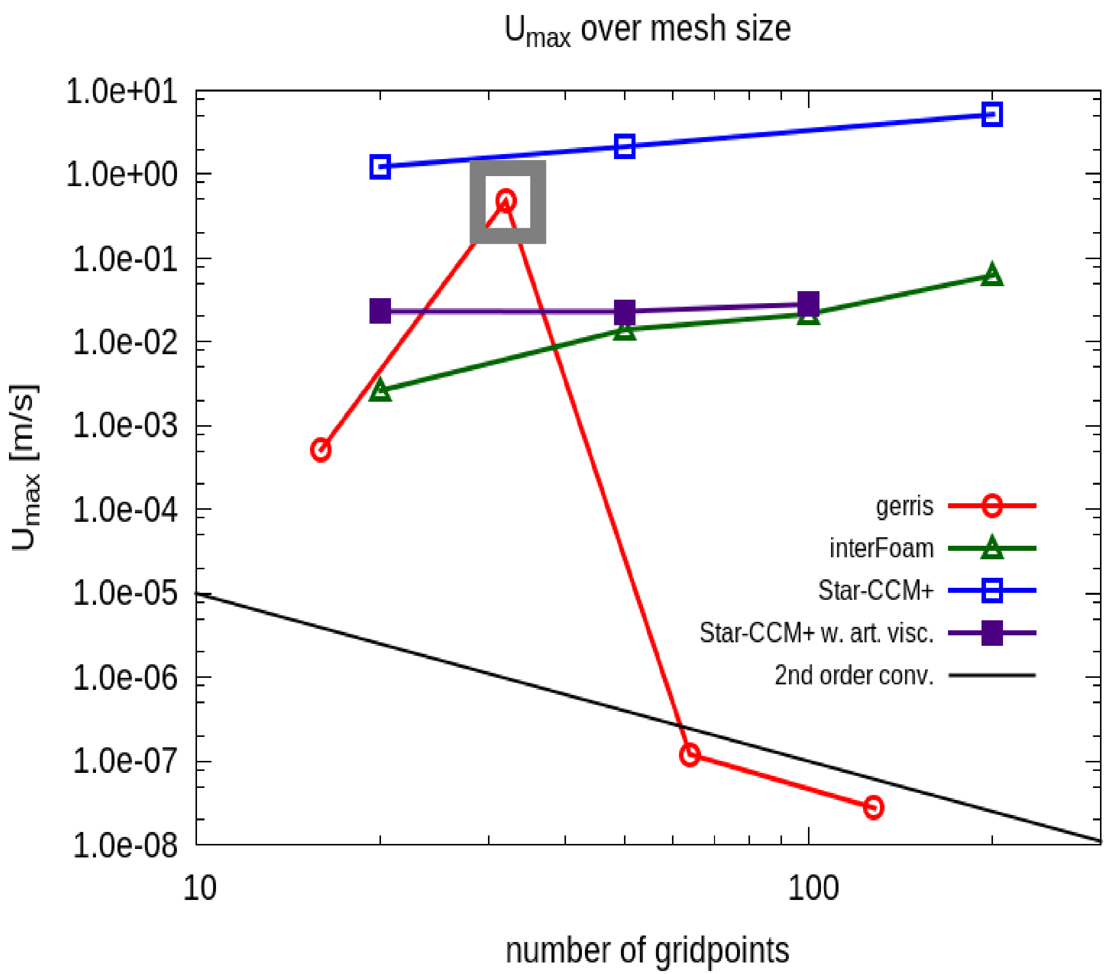

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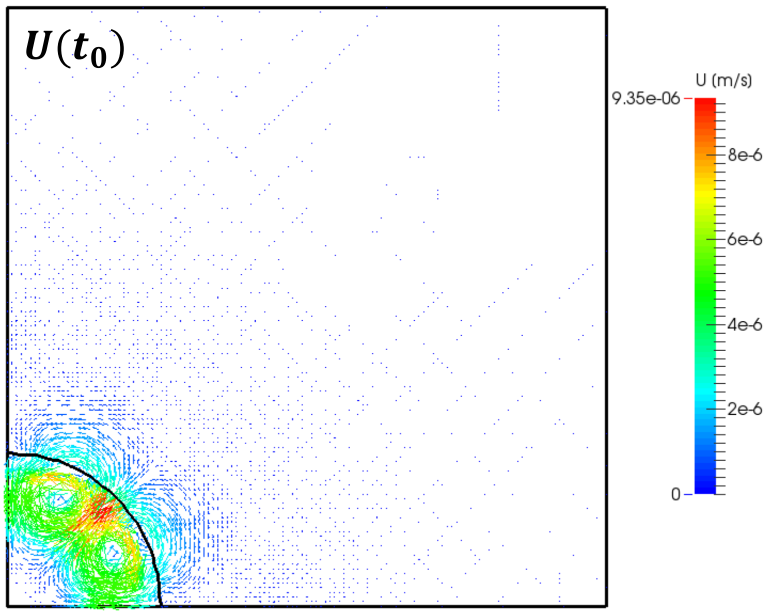
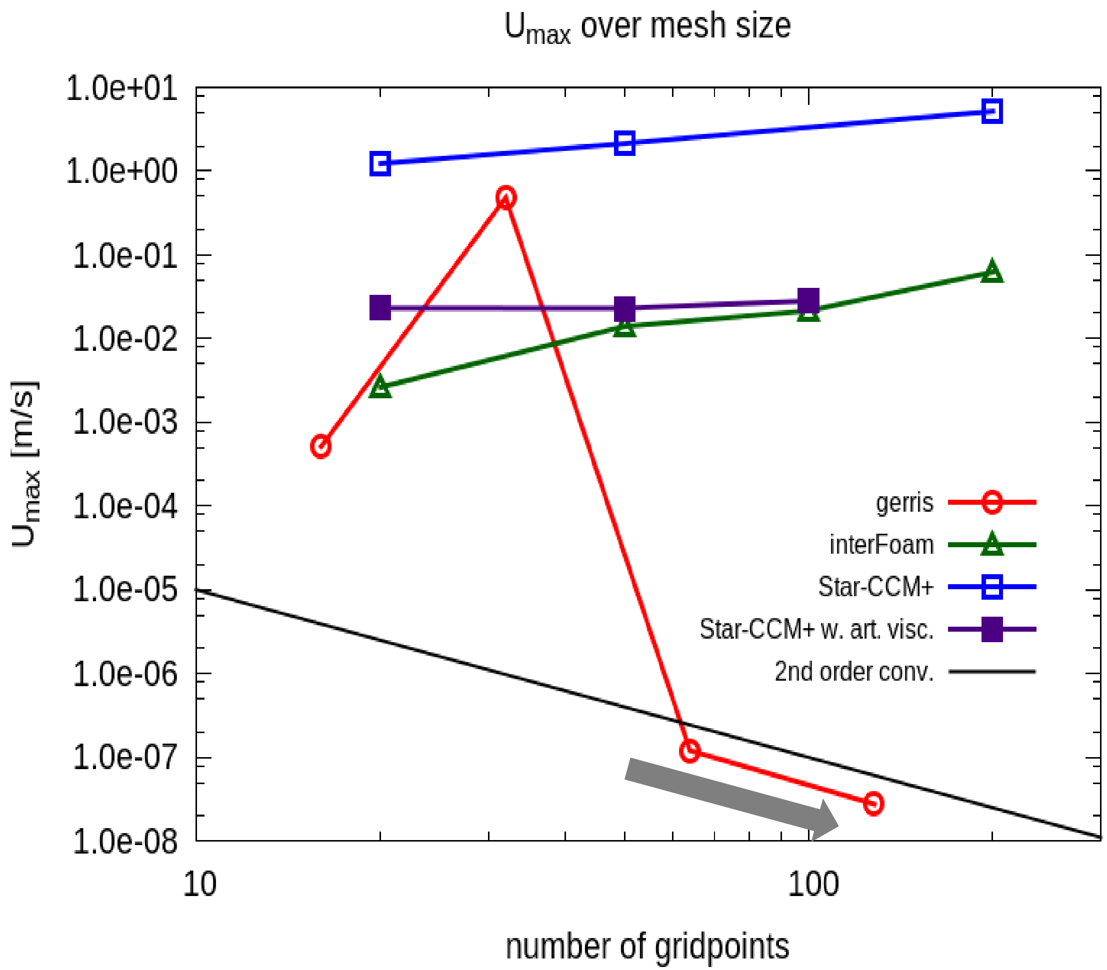


- U_{pc} as capillary wave
  - $U_{pc}(t) \rightarrow 0 \; for \; t \rightarrow \infty$
  - $U_{pc}(t_0, initialization)$



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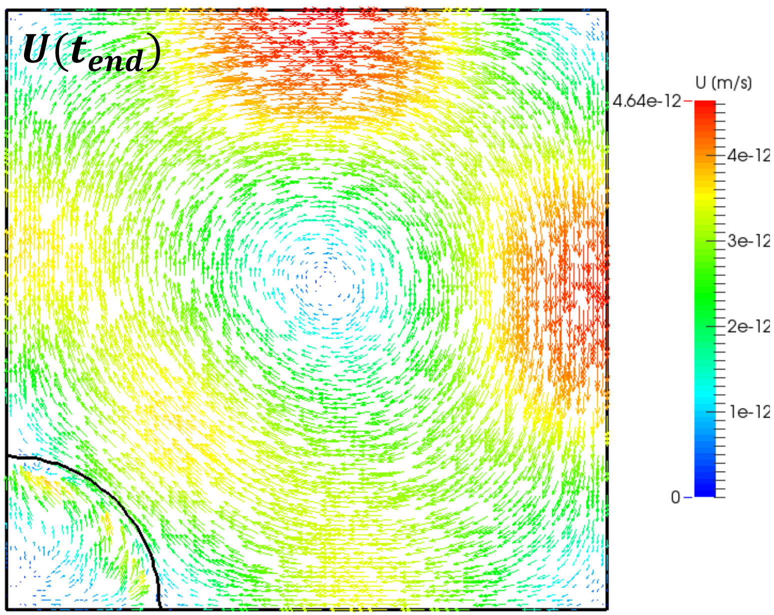

- U_{pc} as capillary wave
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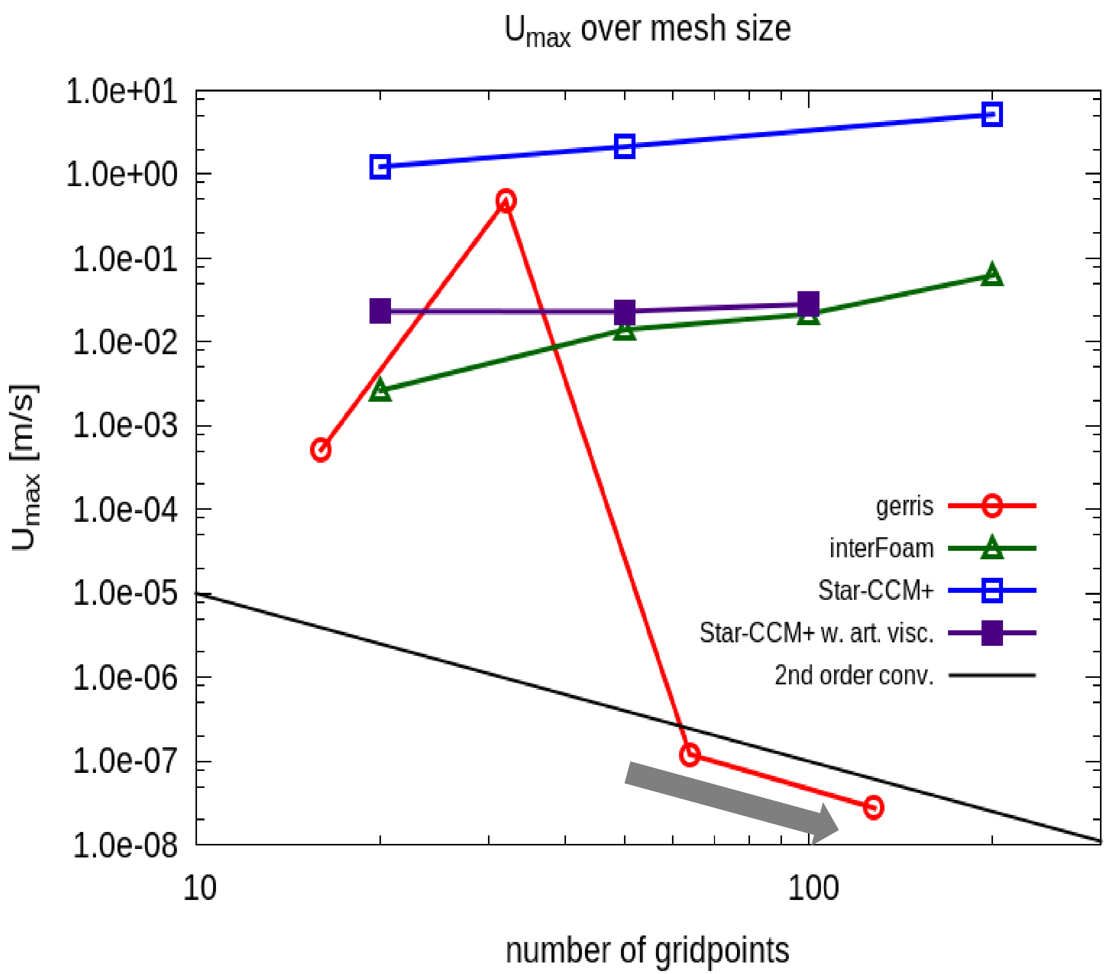
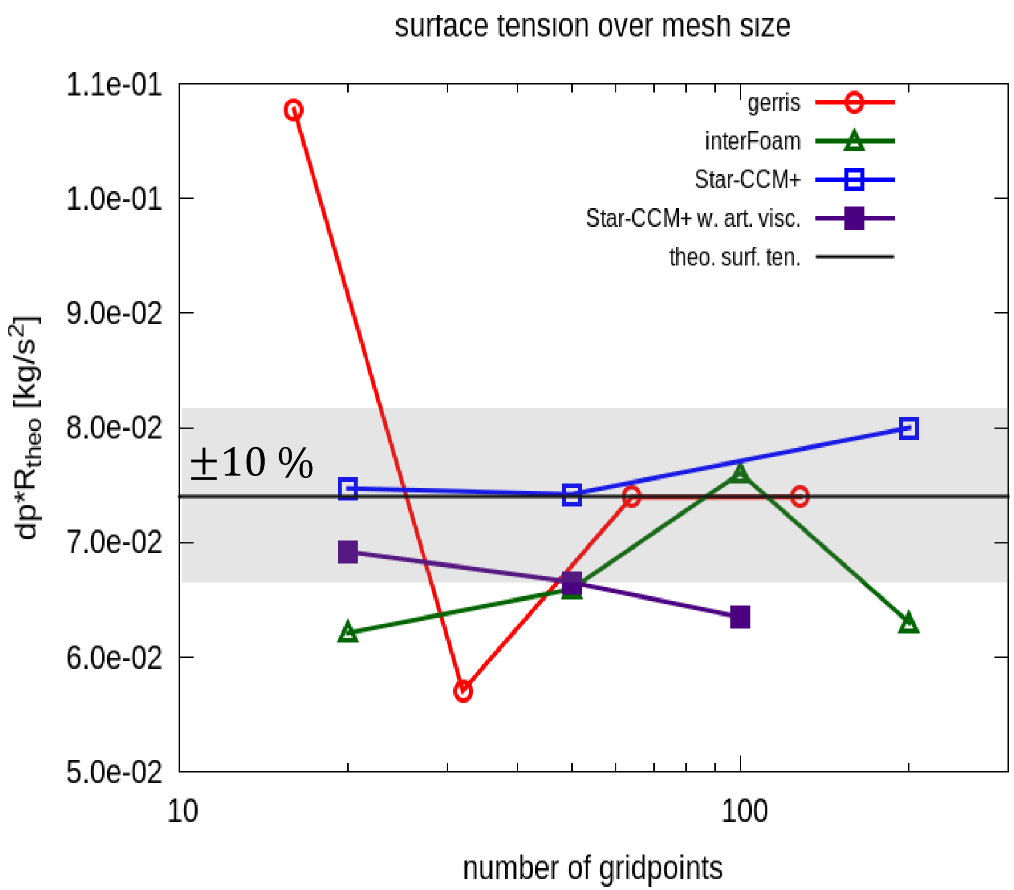


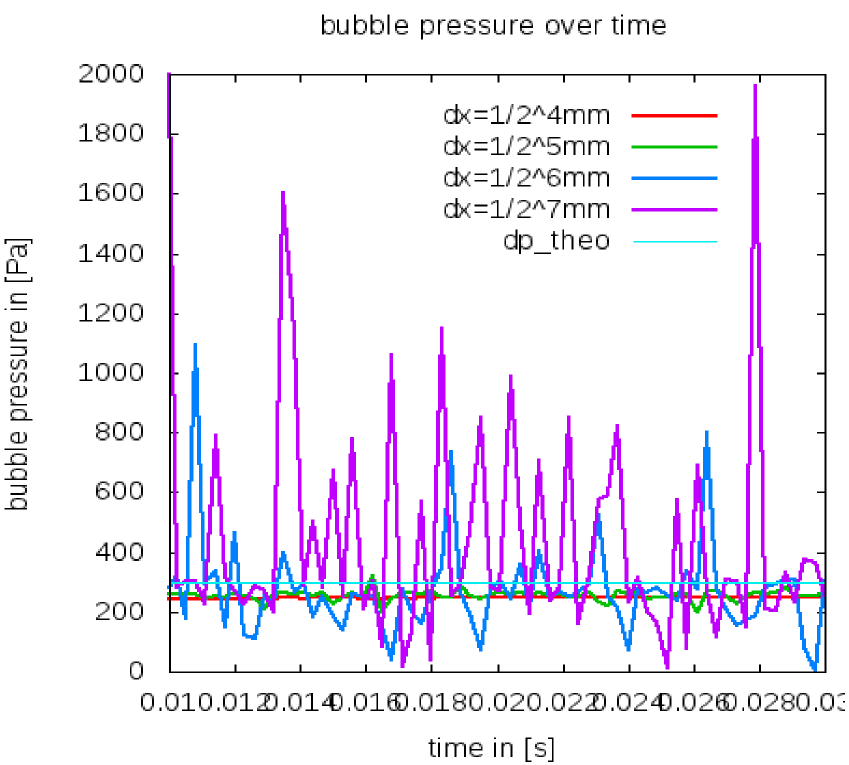
Bubble at rest – Laplace pressure over resolution

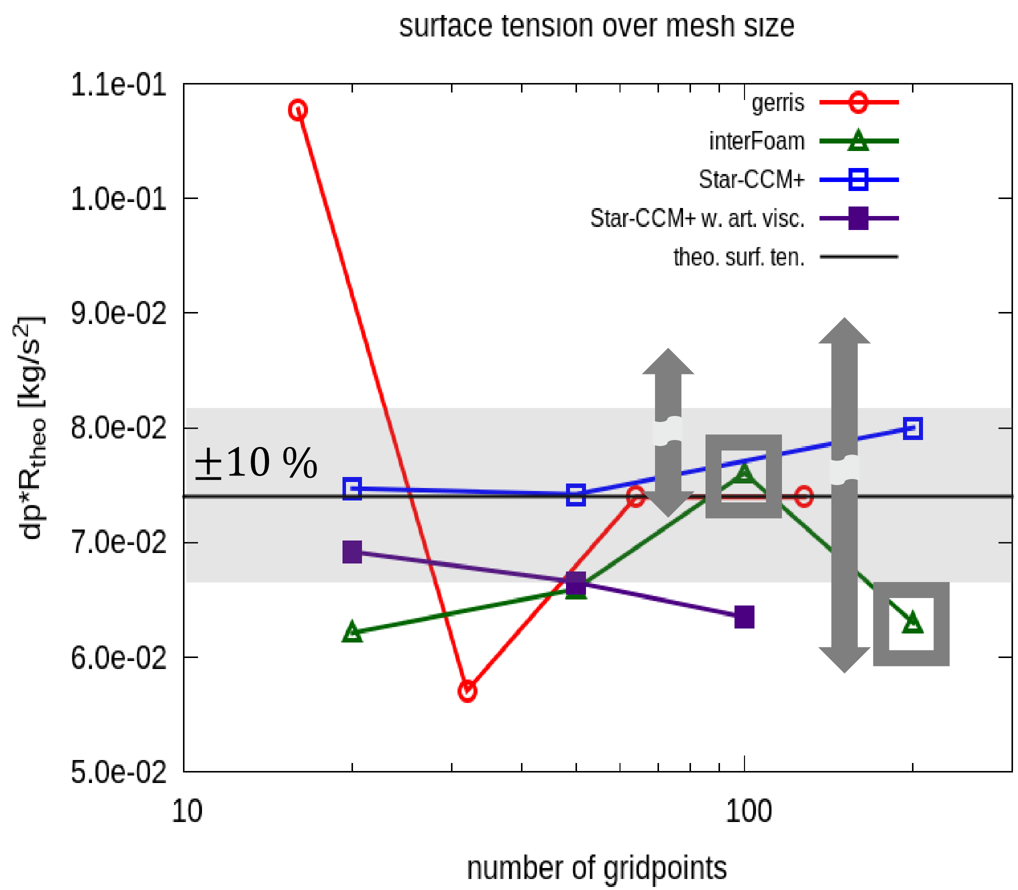


Bubble at rest – Laplace pressure over resolution

InterFoam

- **Extreme oscillations** for $\Delta x \rightarrow 0$
- $\epsilon(\Delta p \cdot R)$ rises for $\Delta x \rightarrow 0$

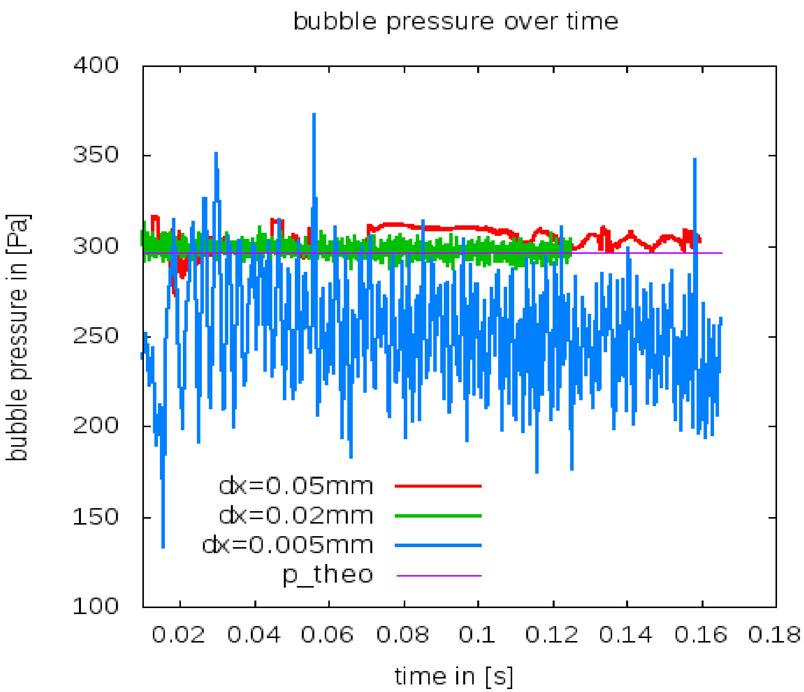


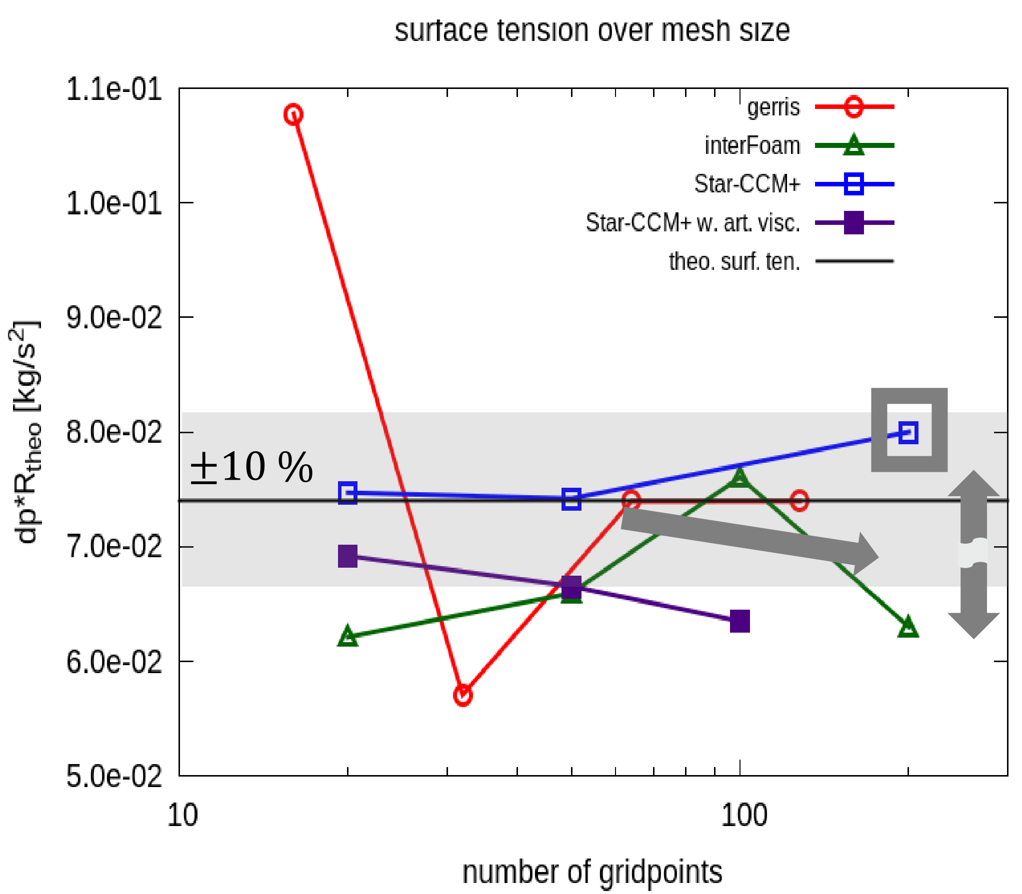


Bubble at rest – Laplace pressure over resolution

Star-CCM+

- Strong oscillations for $\Delta x \rightarrow 0$
- $\epsilon(\Delta p \cdot R)$ rises for $\Delta x \rightarrow 0$





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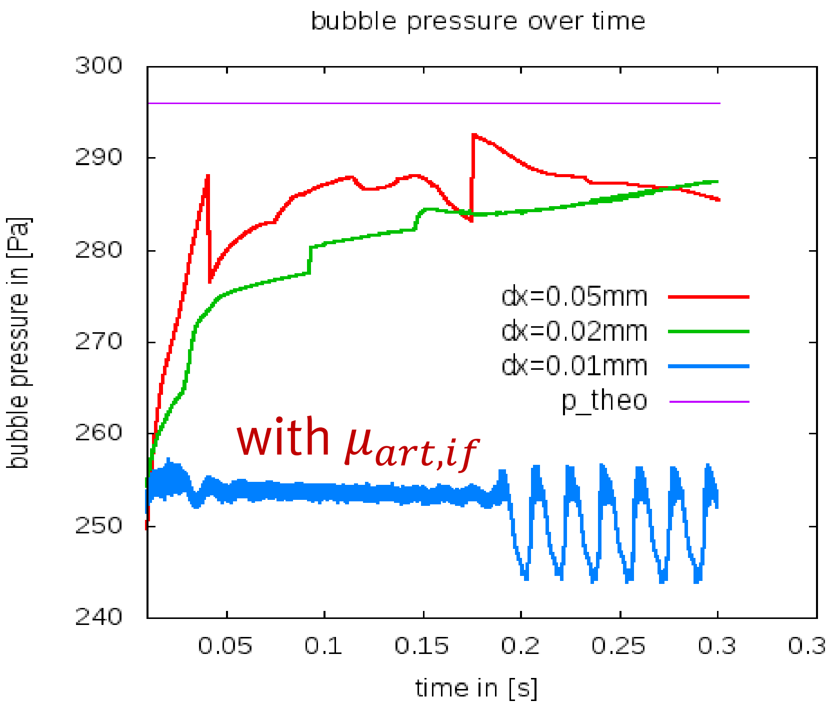
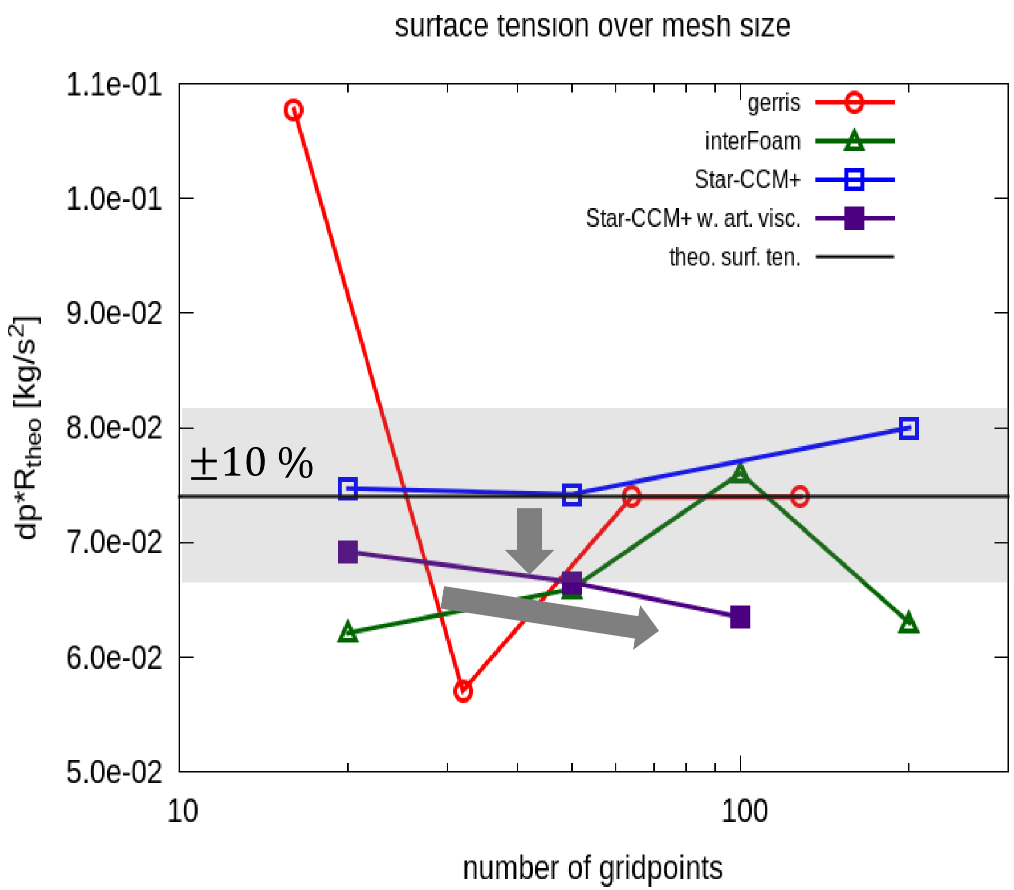


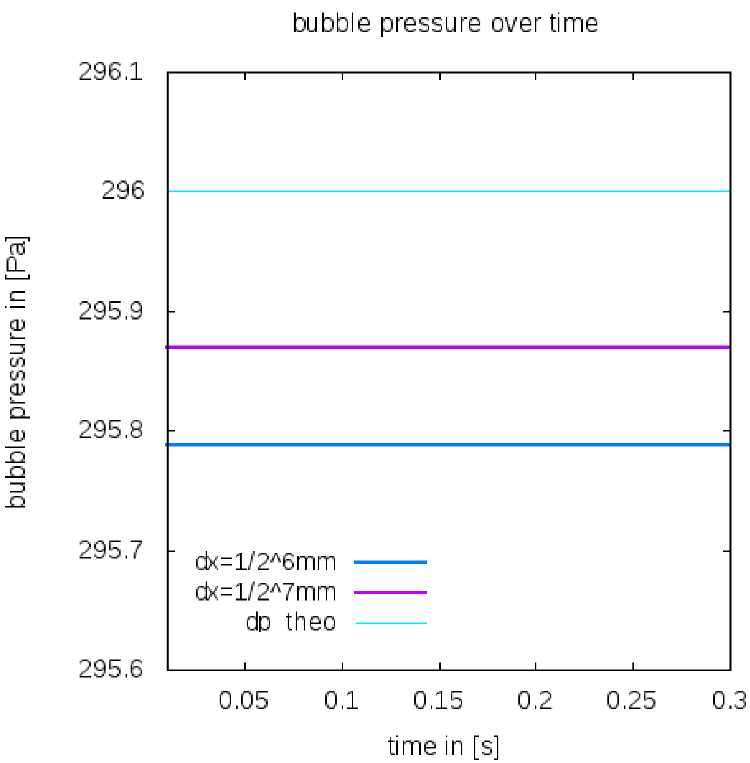


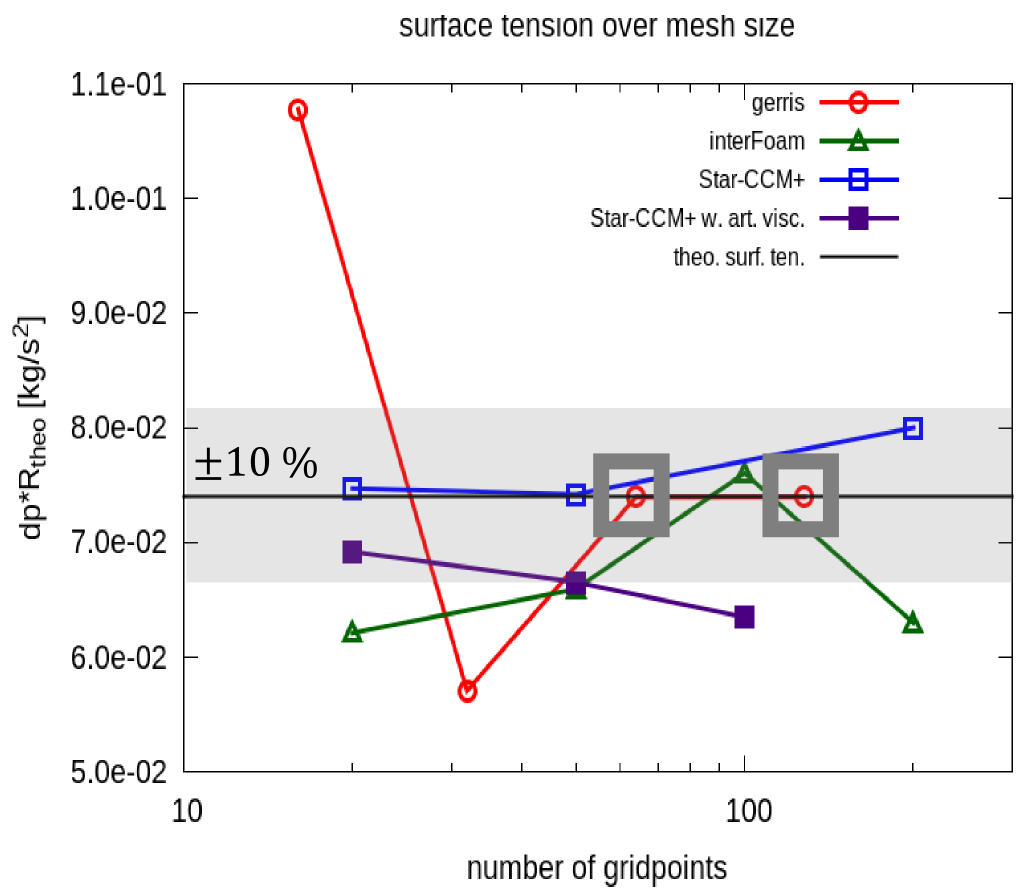
- **$\mu_{art,if}$ damps oscillations and Δp**

Bubble at rest – Laplace pressure over resolution

Gerris

- ‹ **0.1 %** deviation for $R/\Delta x \geq 16$





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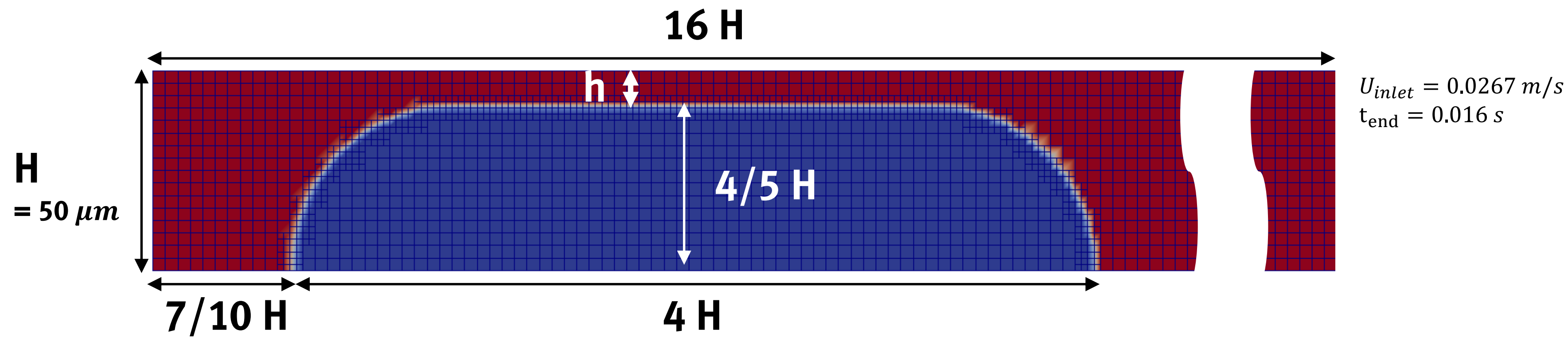
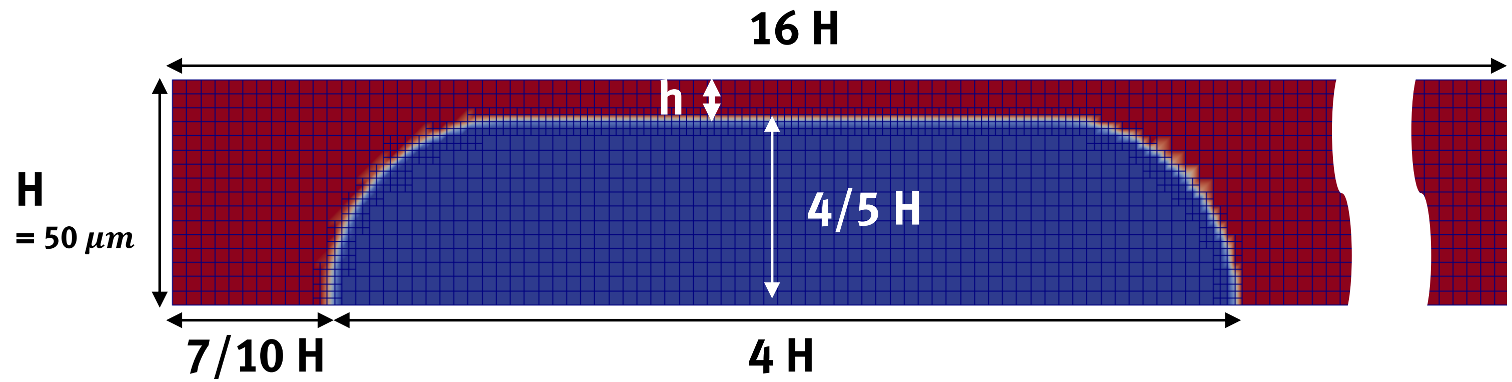
Taylor bubble – Case description



- 2D rectangular half channel (symmetry), constant inflow U_{inlet}
- Two fluid combinations (density, viscosity ratios): 1. Liquid – Liquid // 2. Water – Air

Taylor bubble – Case description



$U_{inlet} = 0.0267\ m/s$
$t_{end} = 0.016\ s$

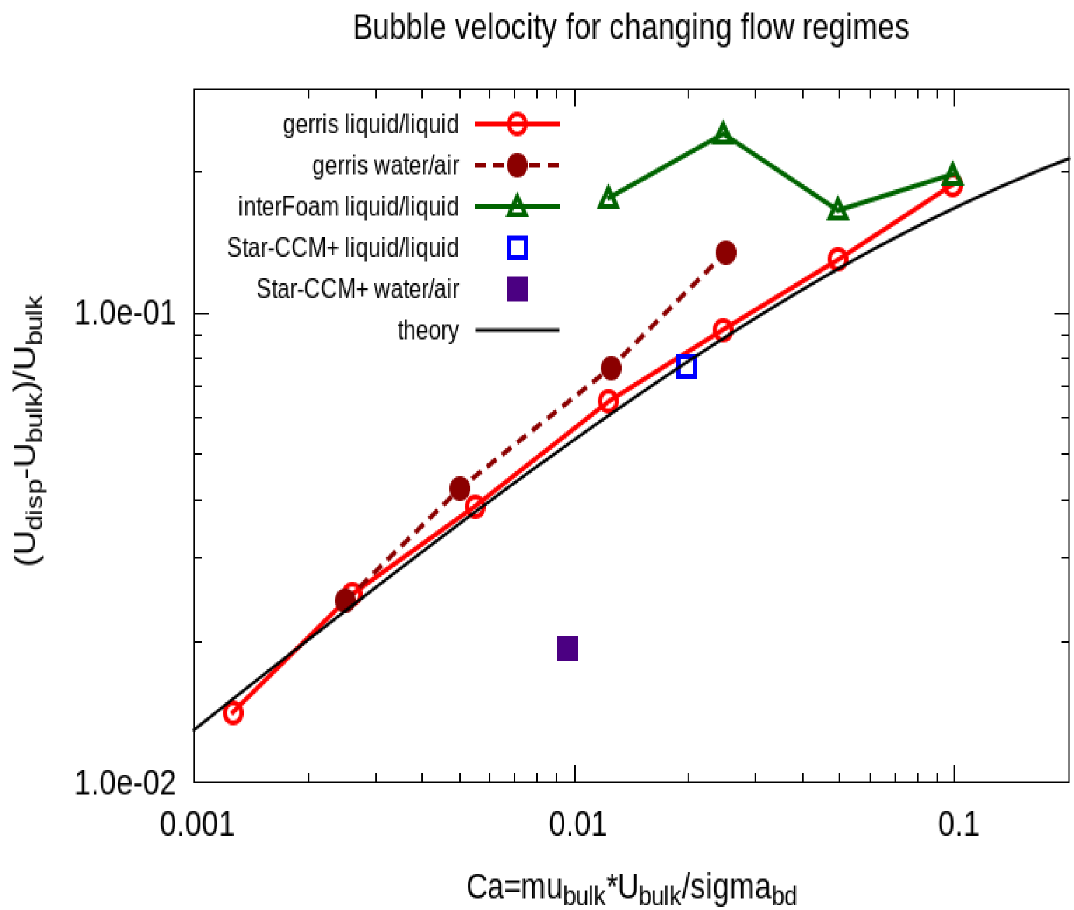
- 2D rectangular half channel (symmetry), constant inflow U_{inlet}
- Two fluid combinations (density, viscosity ratios): 1. Liquid – Liquid // 2. Water – Air
- Investigate film thickness and droplet velocity[1]: $\frac{h}{H} = \frac{\overline{U} - U_{bubble}}{\overline{U}} = \frac{0.643(3Ca)^{\frac{2}{3}}}{1+0.643 \cdot 2.5(3Ca)^{\frac{2}{3}}}$

[1]Aussillous P, Quere D. Phys Fluids 2000;12:2367–71

- For Ca: $10^{-3} - 10^{-1}$
  - Liquid – Liquid // Water – Air

Accuracy of film thickness and bubble velocity for changing Ca?

Taylor bubble – Bubble velocity over Ca

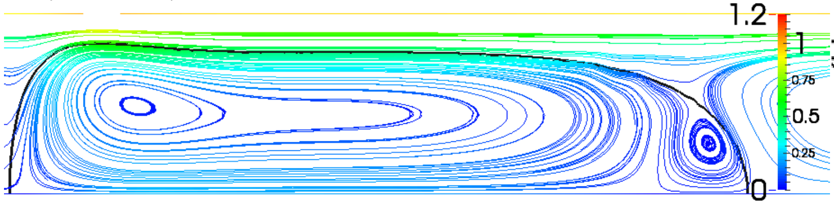


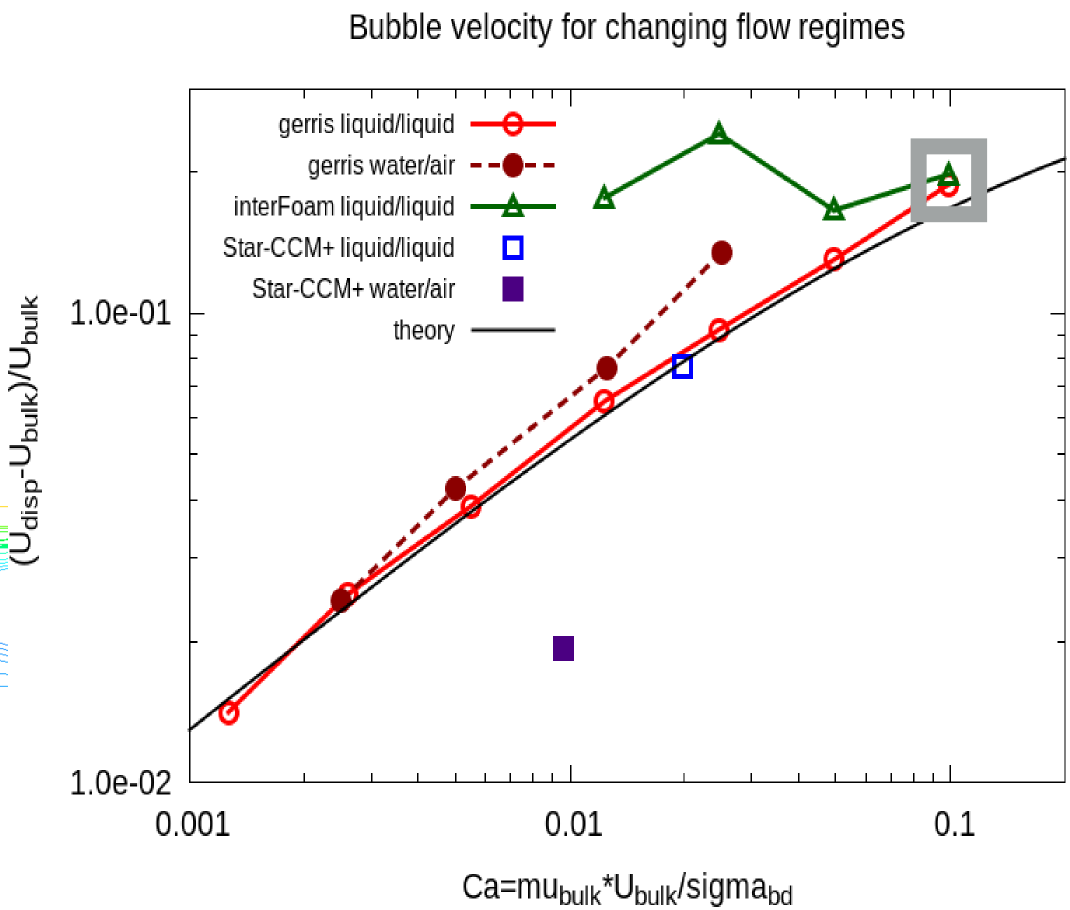
Taylor bubble – Bubble velocity over Ca

interFoam

- Good agreement at $Ca \geq 0.06$

Liquid/liquid at $Ca = 0.1$



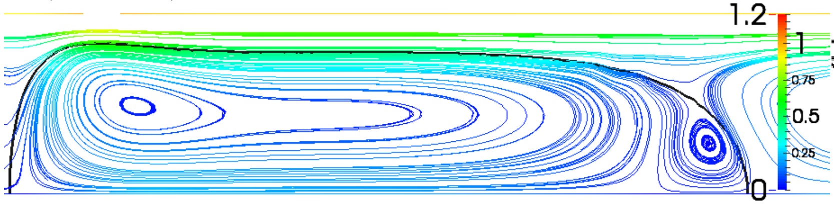


Taylor bubble – Bubble velocity over Ca

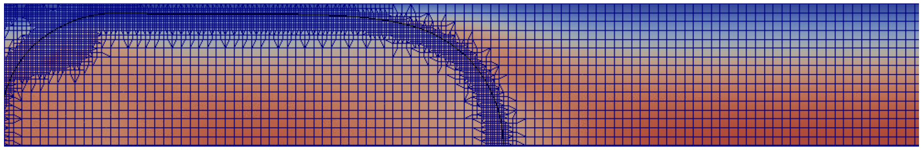
interFoam

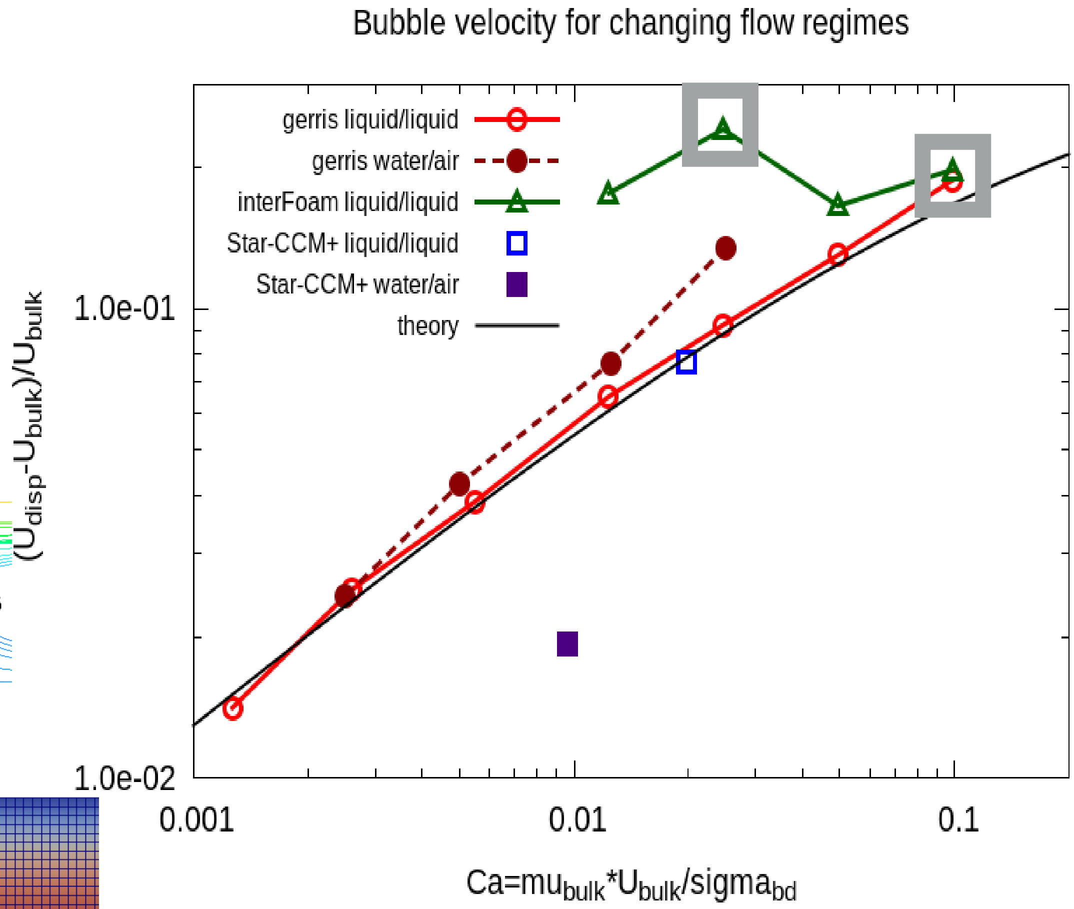
- Good agreement at $Ca \geq 0.06$
- Large deviation $Ca < 0.06$
    - Parasitic currents at rear
    - Detachement at rear
    - Computationally expensive

Liquid/liquid at $Ca = 0.1$



Fluid/fluid at $Ca = 0.03$



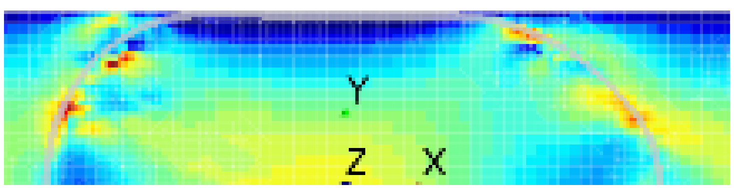


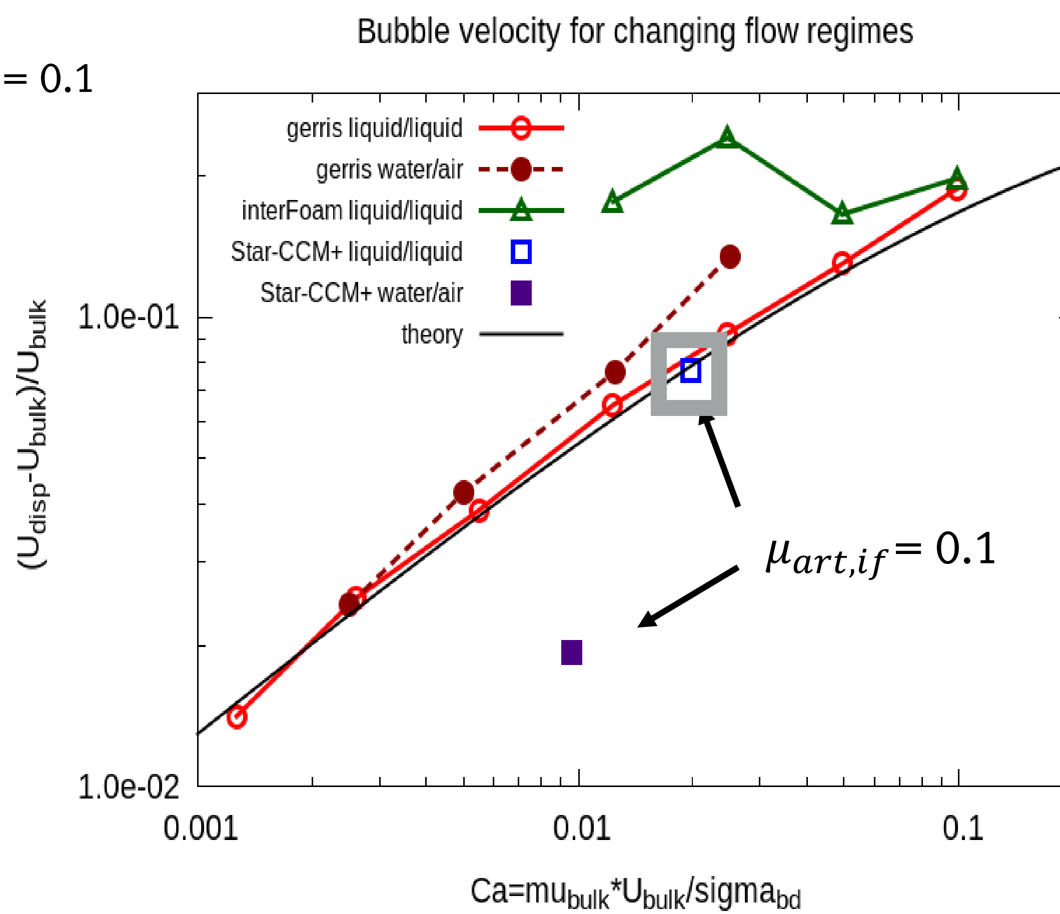
Taylor bubble – Bubble velocity over Ca

Star-CCM+

- Liquid/liquid: good agreement for $\mu_{art,if} = 0.1$

Liquid/liquid at $\mu_{art,if} = 0.1$





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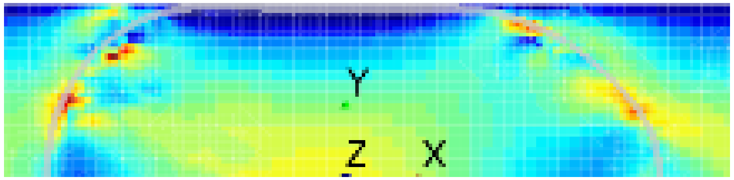
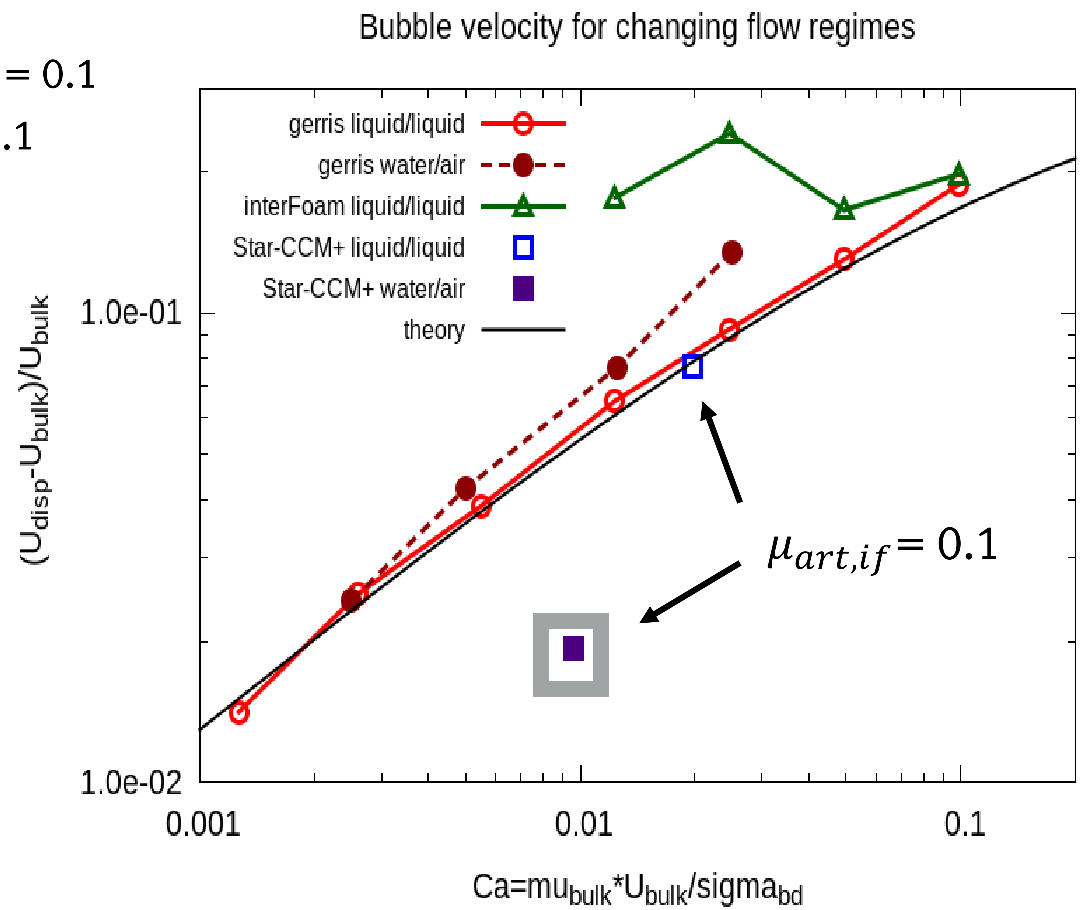
Taylor bubble – Bubble velocity over Ca

Star-CCM+

- Liquid/liquid: good agreement for $\mu_{art,if} = 0.1$
- Water/air: strong deviation for $\mu_{art,if} = 0.1$
  -> **Identifying optimal $\mu_{art,if}$ required**

Liquid/liquid at $\mu_{art,if} = 0.1$



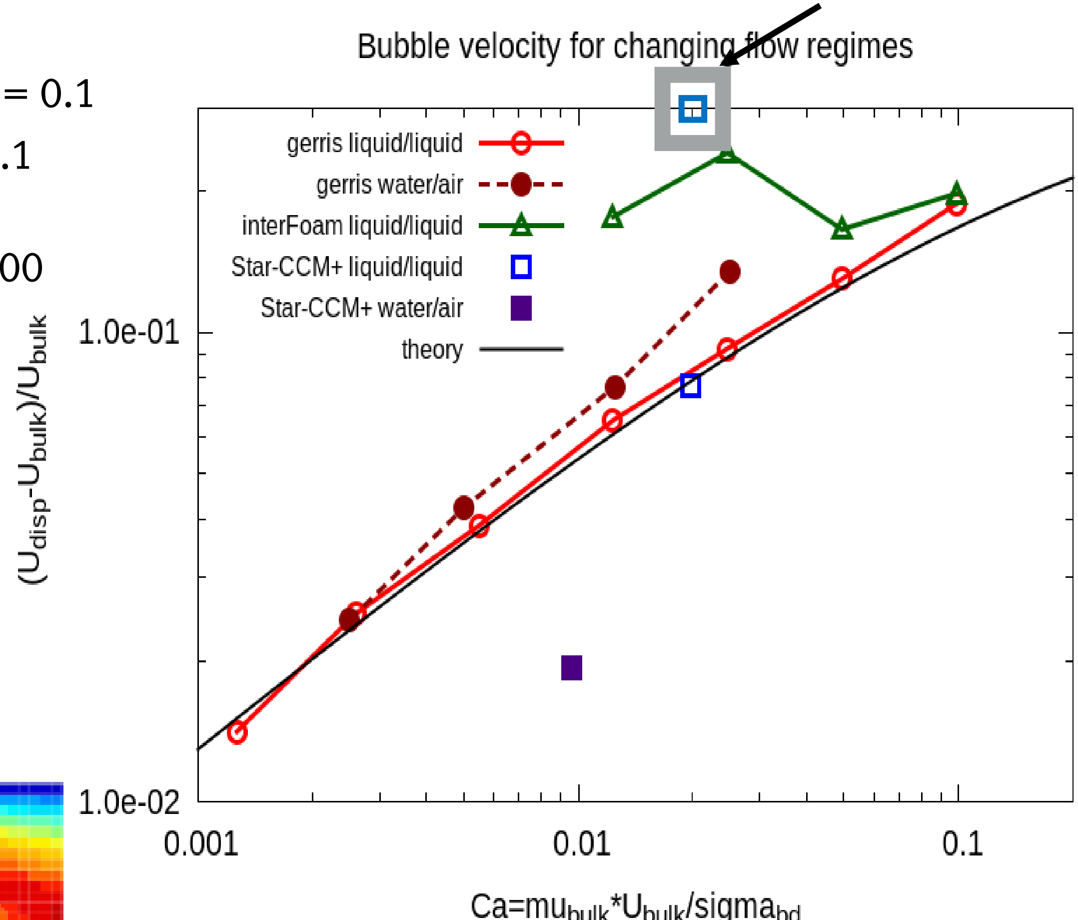


Taylor bubble – Bubble velocity over Ca

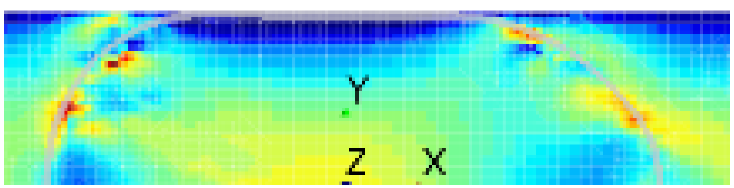
Star-CCM+

- Liquid/liquid: good agreement for $\mu_{art,if} = 0.1$
- Water/air: strong deviation for $\mu_{art,if} = 0.1$
  -> **Identifying optimal $\mu_{art,if}$ required**
- Strong distortion of bubble for $\mu_{art,if} = 100$
- **Predictive potential questionable**

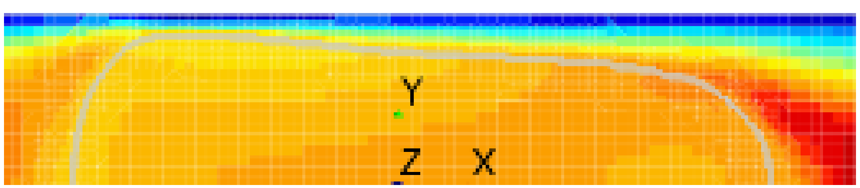
$\mu_{art,if} = 100$



Liquid/liquid at $\mu_{art,if} = 0.1$



Liquid/liquid at $\mu_{art,if} = 100$

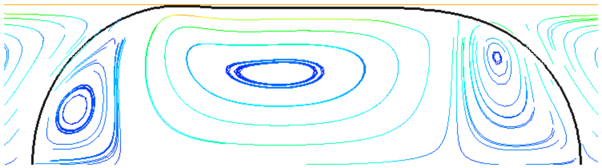


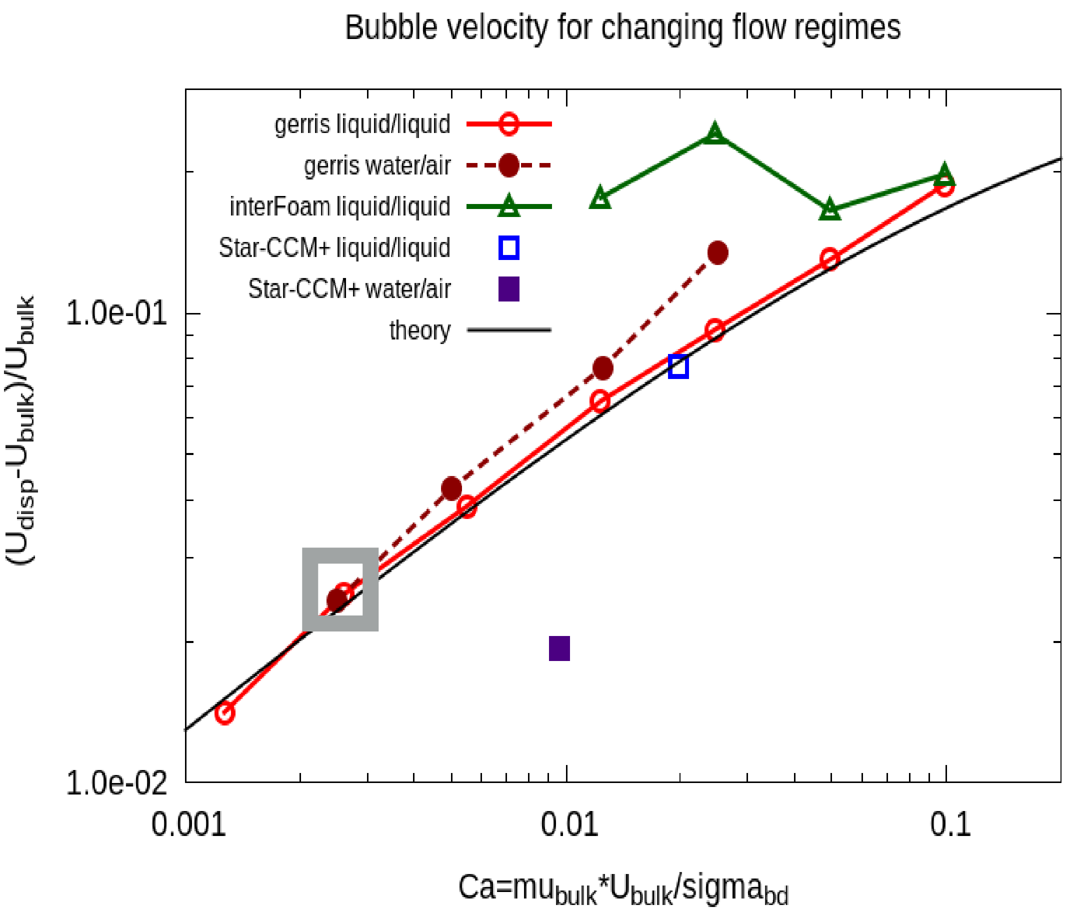
Taylor bubble – Bubble velocity over Ca

Gerris

- Liquid/liquid: Very accurate prediction

Water/air at $Ca = 0.003$



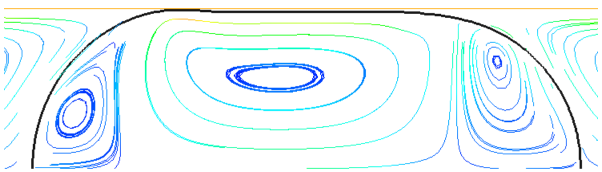


Taylor bubble – Bubble velocity over Ca

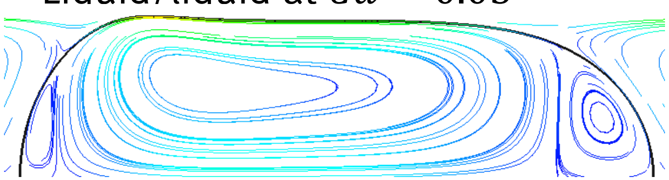
Gerris

- Liquid/liquid: Very accurate prediction
- Water/air: similarity lost for $Ca \geq 0.03$
- **In total good accuracy**

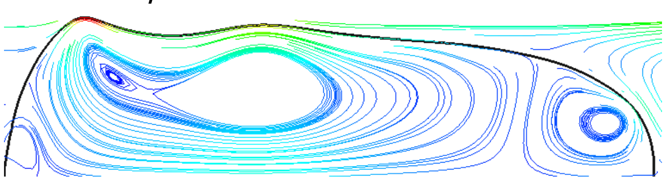
Water/air at $Ca = 0.003$

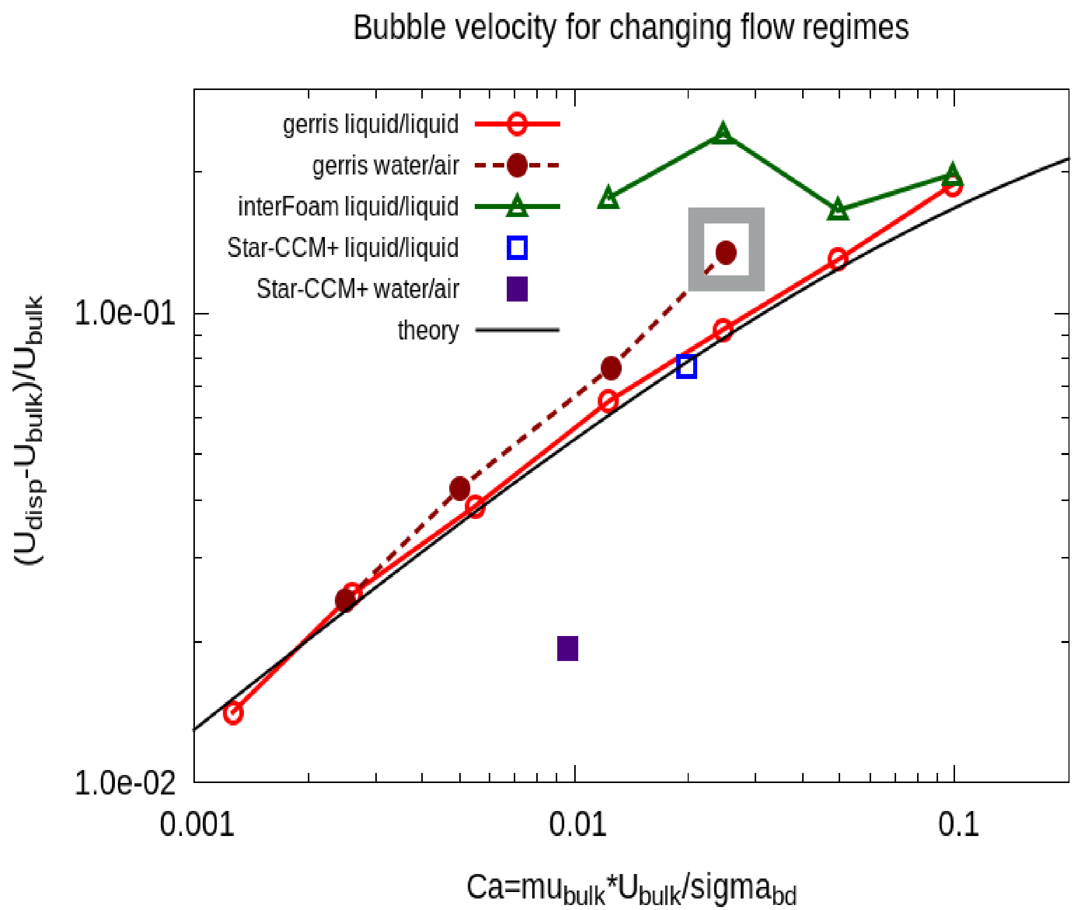


Liquid/liquid at $Ca = 0.03$

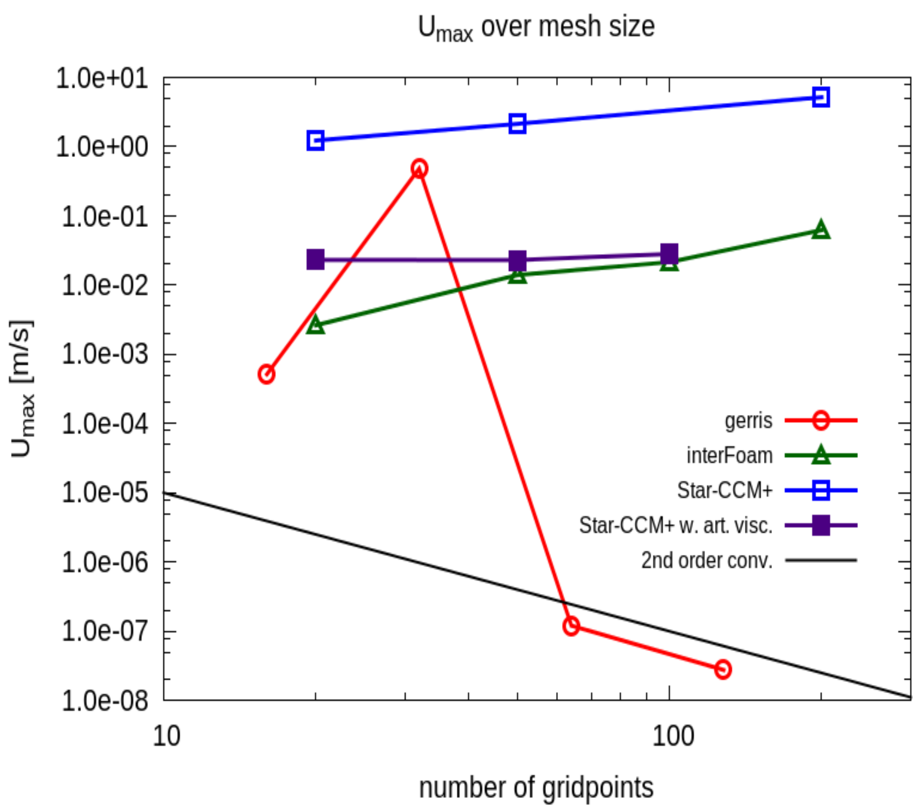


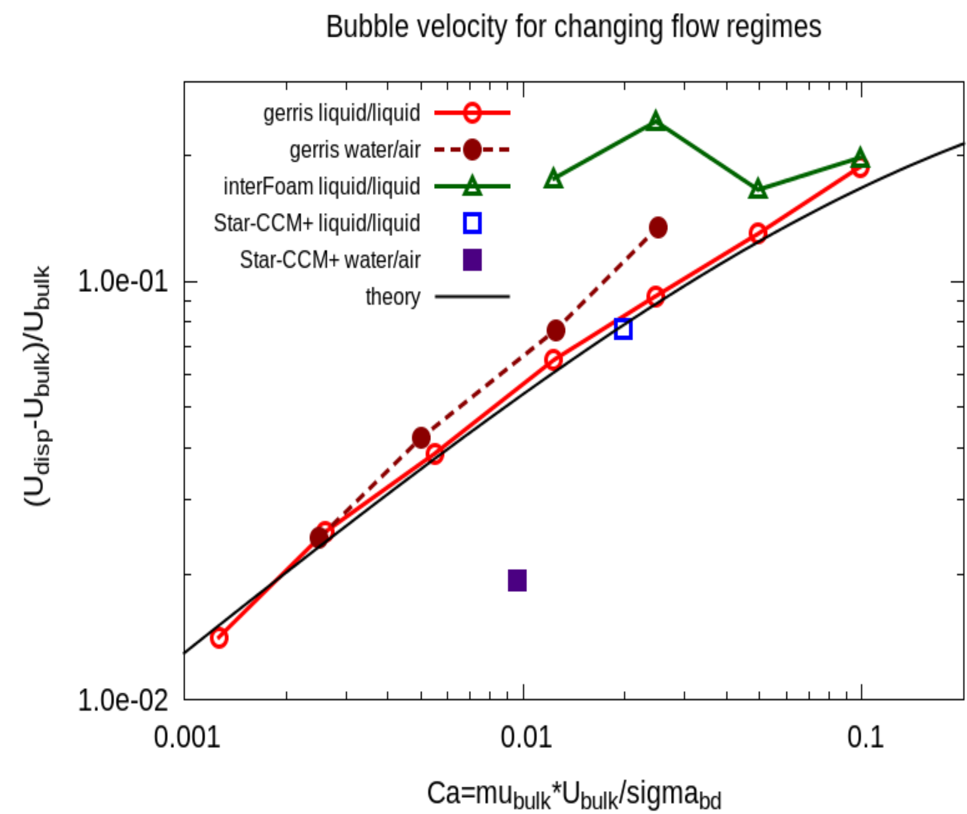
Water/air at $Ca = 0.03$





Summary – Test cases





- $O\left(U_{pc}\right)$ & $\epsilon(\Delta p \cdot R)$ determined for Gerris, interFoam and StarCCM+ for bubble at rest
- U_{bub} compared to theory for lubricated Taylor bubble

Outline

Introduction

- Festo
- Motivation
- Simulative challenges
- Simulative approach

Bubble at rest

- Case description
- Results

Taylor bubble

- Case description
- Results

Conclusions & Outlook

Conclusions

Evaluated CFD solver potential for microfluidic multiphase simulation

- interFoam 2.31: unsuited / StarCCM+ 10.4: mediocre / Gerris: good results
- Comp. costs generally very high

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FESTO

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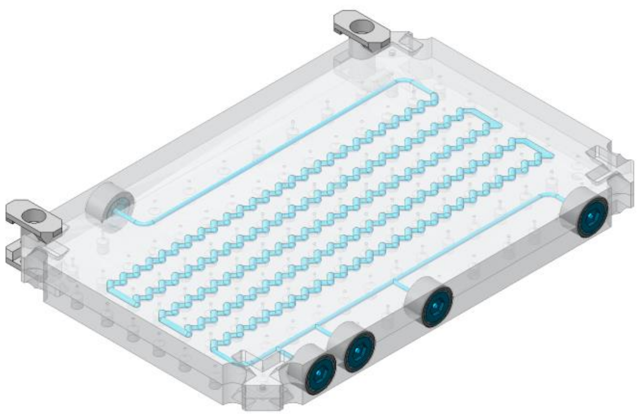
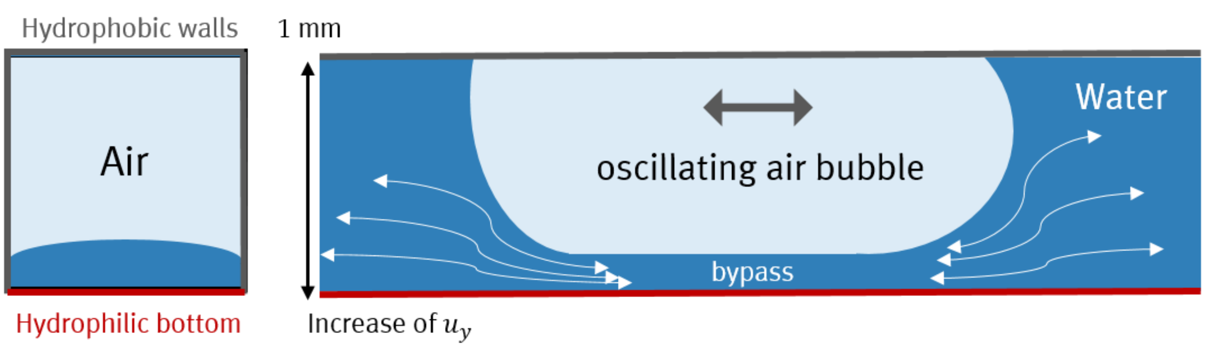
- Semi-implicit surface tension implementation
- Artificial viscosity option
- Combination of balanced forces and momentum conservation
- Advanced schemes for contact angle dynamics and hysteresis

Thank you for your attention!

Outlook – Motivation: Microfluidic Mixing

- Microfluidic flows are laminar
  - Mixing only via diffusion -> **slow process**
- State of the art
  - Introduction of a mixing section
  - Disadvantages:
    - **High volume**
    - **Clogging of sharp turns** by gas bubbles
- Proposed solution
  - **Mix with oscillating Taylor bubble**
  - **Optimize by simulation**
  - **Validate with experiment**



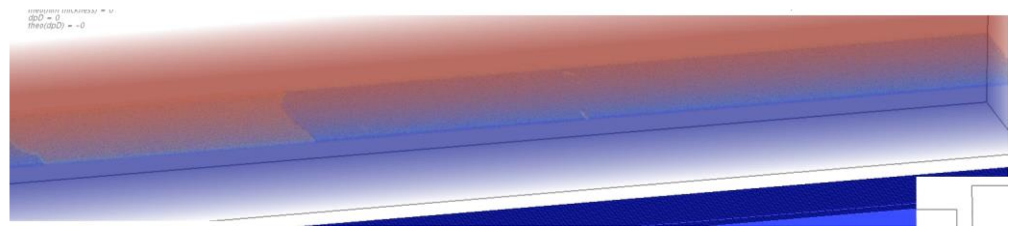


Outlook – Concept of the bubble mixer

- Comparison of mixing behavior with oscillating water in microchannel
- inhomogeneous initialized passive scalar for visualization ($c_{top} = 1,\ c_{bottom} = 0$)
- Hydrophobic walls + hydrophilic bottom

Plain Fluid

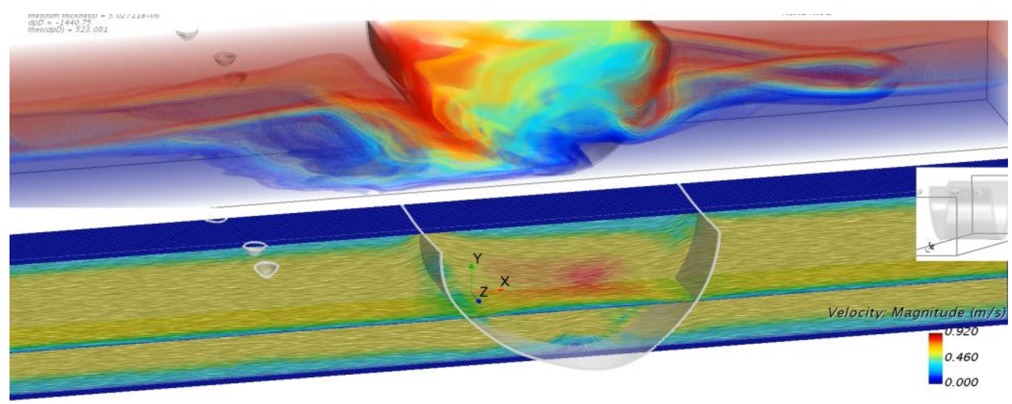
Diffusion-dominated
very slow mixing



19 cycles

With Air Bubble

Diffusion + forced convection
fast mixing
especially near hydrophilic bottom



1.5 cycles