TU Clausthal

Modelling of acoustic cavitation on a large scale with OpenFOAM

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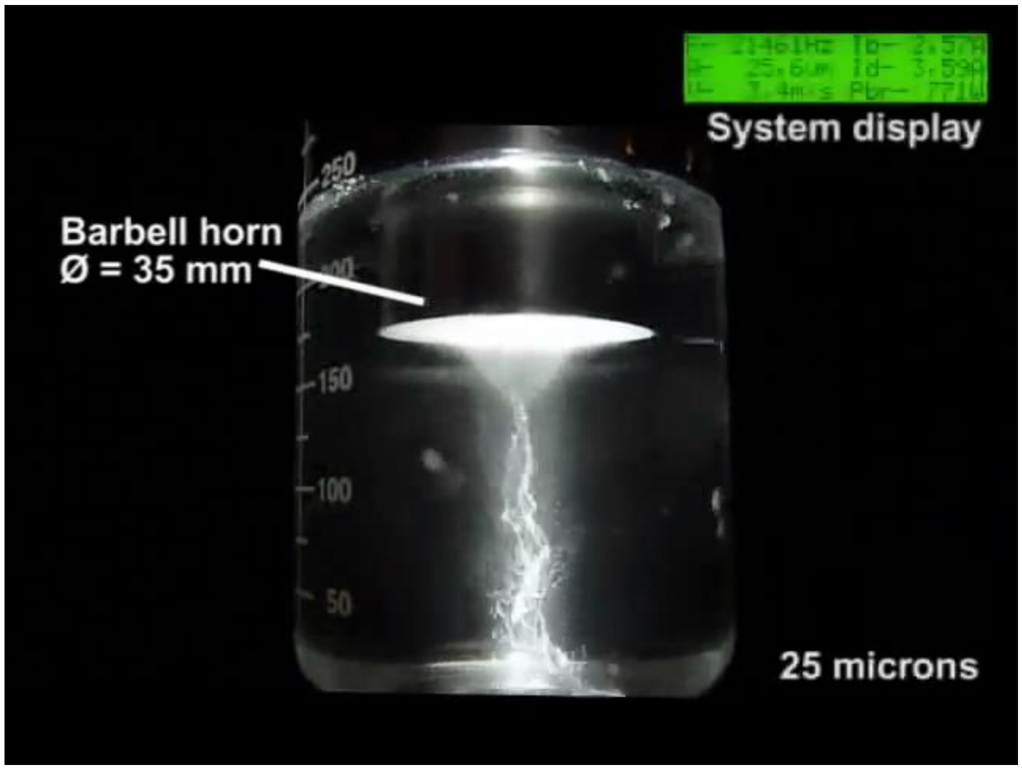
Institute of Applied Mechanics / TU Clausthal

in cooperation with University Göttingen

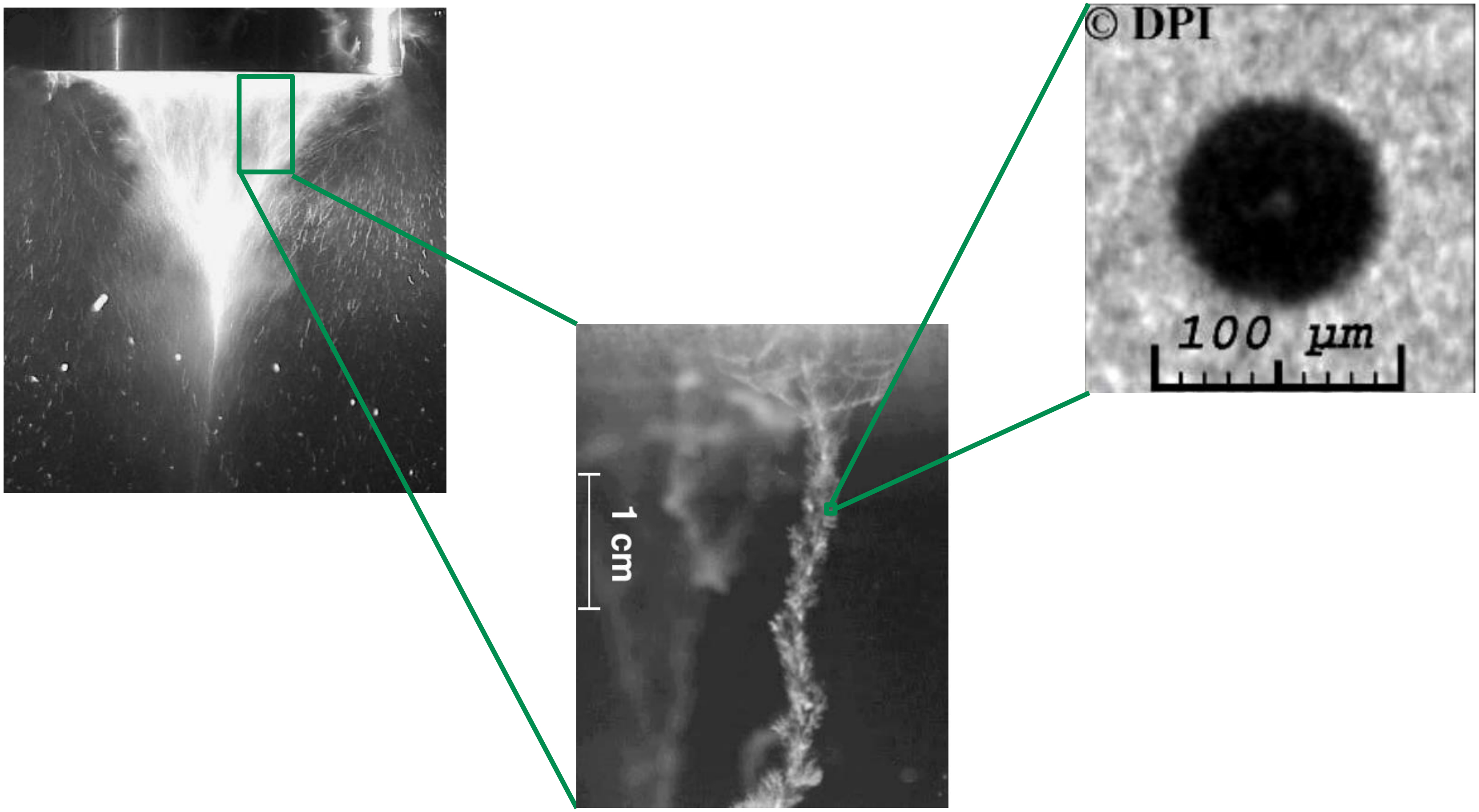
German OpenFoam User meetiNg, Online, 22.04.2020

Acoustic cavitation



Source: Industrial Sonomechanics, LLC

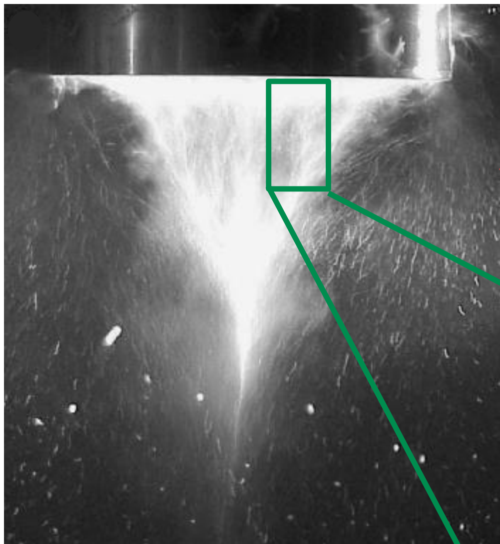
Acoustic cavitation: multiscale problem



Motivation

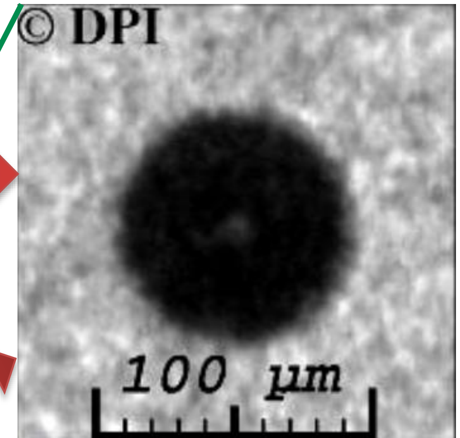
- State of the art
  - fundamental physics of microscopic phenomena well understood
  - macroscopic computations: only linear bubble oscillations with homogeneous distribution
- Current ansatz
  - non-linear cavitation bubble oscillations
  - spatially inhomogeneous bubble distribution
  - relatively large geometries (~1-10dm³)
  - prediction of
    - ultrasound field
    - location of cavitation bubble clustering

Outline

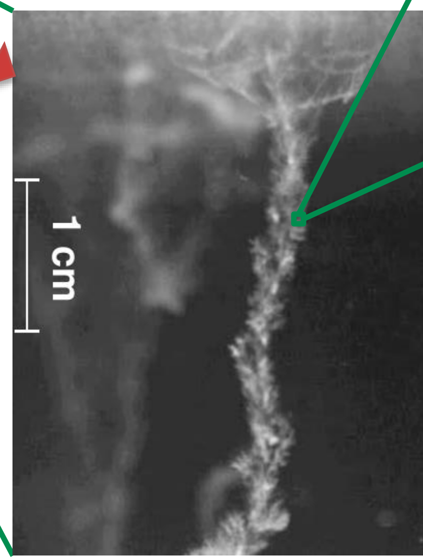


1. Ultrasound: Helmholtz Eqn.

Model Coupling



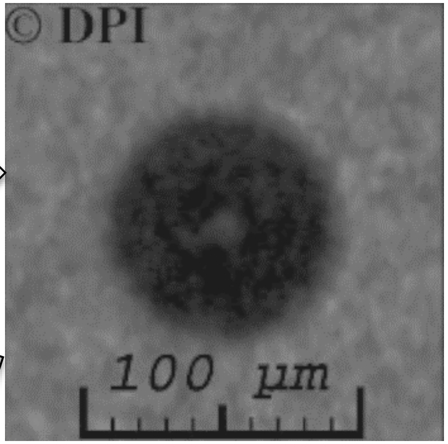
2. Radial Bubble Dynamics



3. Bubble Motion

Outline

1. **Ultrasound: Helmholtz Eqn.**



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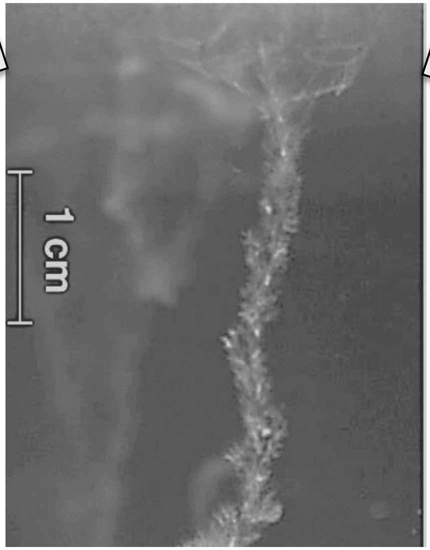


3. Bubble Motion

Helmholtz equation (HE)

- Wave equation in frequency domain
  - P_{ac} - complex sound pressure amplitude
  - k_{m} - complex wave number of the gas-liquid mixture
- Computation with OpenFOAM
  - no complex numbers
  - decompose HE in two equations
  - solving in segregated manner leads to divergence in most cases

$$\nabla^2 P_{\mathrm{ac}} + k_{\mathrm{m}}^2 P_{\mathrm{ac}} = 0$$

$$K_r = \mathrm{Re}(k_{\mathrm{m}}^2), K_i = \mathrm{Im}(k_{\mathrm{m}}^2)$$

$$P_r = \mathrm{Re}(P_{\mathrm{ac}}), P_i = \mathrm{Im}(P_{\mathrm{ac}})$$

$$\nabla^2 P_r + K_r P_r - K_i P_i = 0$$

$$\nabla^2 P_i + K_r P_i + K_i P_r = 0$$

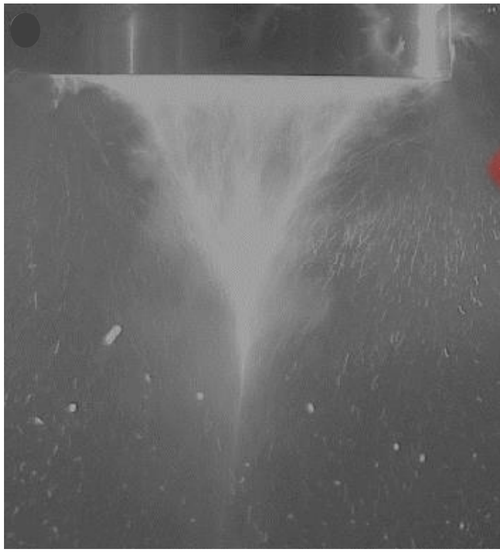
HE discretization and solution

- Discretized with **block-coupled matrix** to couple equations implicitly (foam-extend)

$$
\begin{bmatrix}
\begin{pmatrix} \nabla^2 + K_r & -K_i \\ K_i & \nabla^2 + K_r \end{pmatrix}_{d_0} & \begin{pmatrix} \nabla^2 & 0 \\ 0 & \nabla^2 \end{pmatrix}_{u_0} & \cdots \\
\begin{pmatrix} \nabla^2 & 0 \\ 0 & \nabla^2 \end{pmatrix}_{l_0} & \begin{pmatrix} \nabla^2 + K_r & -K_i \\ K_i & \nabla^2 + K_r \end{pmatrix}_{d_1} & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix}
\cdot
\begin{bmatrix}
\begin{pmatrix} P_r \\ P_i \end{pmatrix}_0 \\
\begin{pmatrix} P_r \\ P_i \end{pmatrix}_1 \\
\vdots
\end{bmatrix}
=
\begin{bmatrix}
\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}_0 \\
\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}_1 \\
\vdots
\end{bmatrix}
$$

- The matrix of discretized HE is highly indefinite
  - iterative solvers diverge
- => Interface implemented to a **direct solver (MUMPS)**
  - **MU**ltifrontal **M**assively **P**arallel sparse direct **S**olver

Outline



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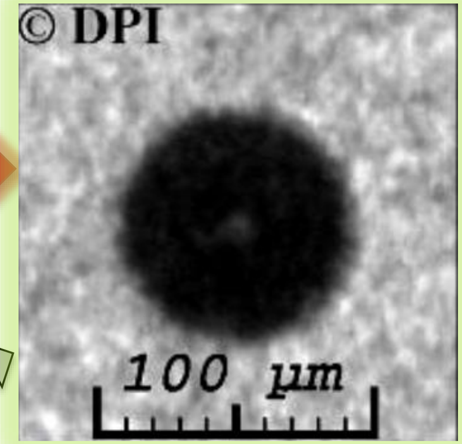

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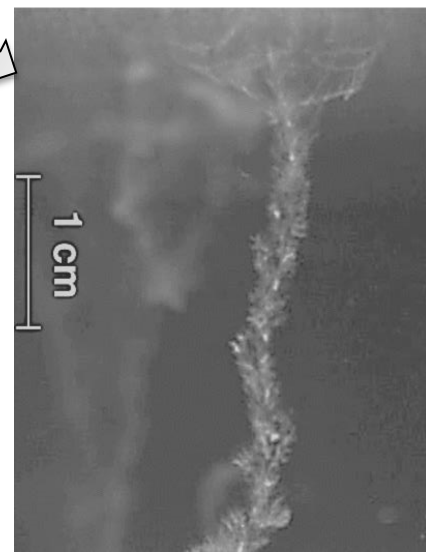
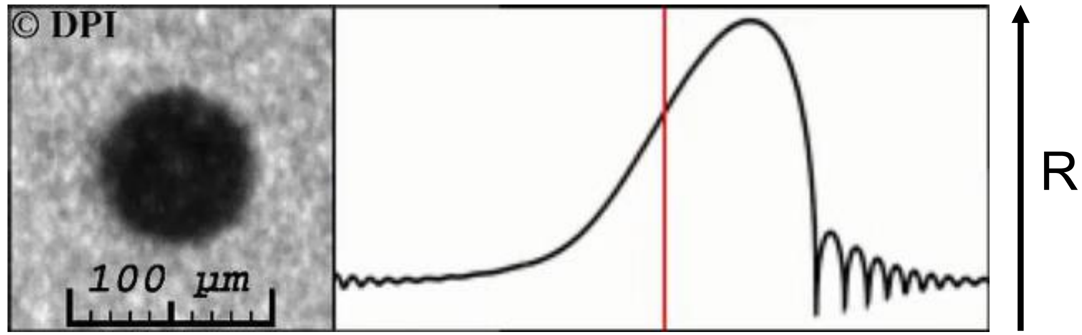


3. Bubble Motion

Radial bubble dynamics (RBD)

Time period
$T = 50\mu\text{s}$
$(f = 20\text{kHz})$



Source: University of Göttingen, Drittes Physikalisches Institut

- Toegel model: 3 ODEs
  - Keller-Miksis eqn. (R – bubble radius)

$$\left(1-\frac{\dot{R}}{c}\right)R\ddot{R}+\left(1-\frac{\dot{R}}{3c}\right)\frac{3}{2}\dot{R}^2=\frac{1}{\rho}\left[\left(1+\frac{\dot{R}}{c}\right)\left(p_\mathrm{g}-|P_\mathrm{ac}|\sin(\omega t)-p_0\right)+\frac{R\dot{p}_\mathrm{g}}{c}-\frac{4\mu\dot{R}}{R}-\frac{2\sigma}{R}\right]$$

  - energy transfer (θ – temperature)

$$\dot{\theta}=\frac{-p_g\frac{\mathrm{d}V}{\mathrm{d}t}+\dot{Q}+\frac{\mathrm{d}n_\mathrm{vap}}{\mathrm{d}t}\left(h_\mathrm{vap}(\theta_0)-u_\mathrm{vap}(\theta)\right)}{n_\mathrm{vap}c_{V,\mathrm{vap}}(\theta)+n_\mathrm{ncg}c_{V,\mathrm{ncg}}(\theta)}$$

  - mass (vapor) transfer (n – amount of substance)

$$\dot{n}_\mathrm{vap}=SD(\theta_0)\frac{c_\mathrm{vap}(R)-c_\mathrm{vap}}{l_\mathrm{m,nl}}$$

Coupling non-linear RBD and sound field

- Coupling via k_m (Louisnard model)
  - β – void fraction / bubble density
  - $\Pi_{\mathrm{Vi,Th}}$ – integrals over one oscillation period; physically: energy dissipated per bubble;

$$\nabla^2 P_\mathrm{ac} + k_\mathrm{m}^2 P_\mathrm{ac} = 0$$

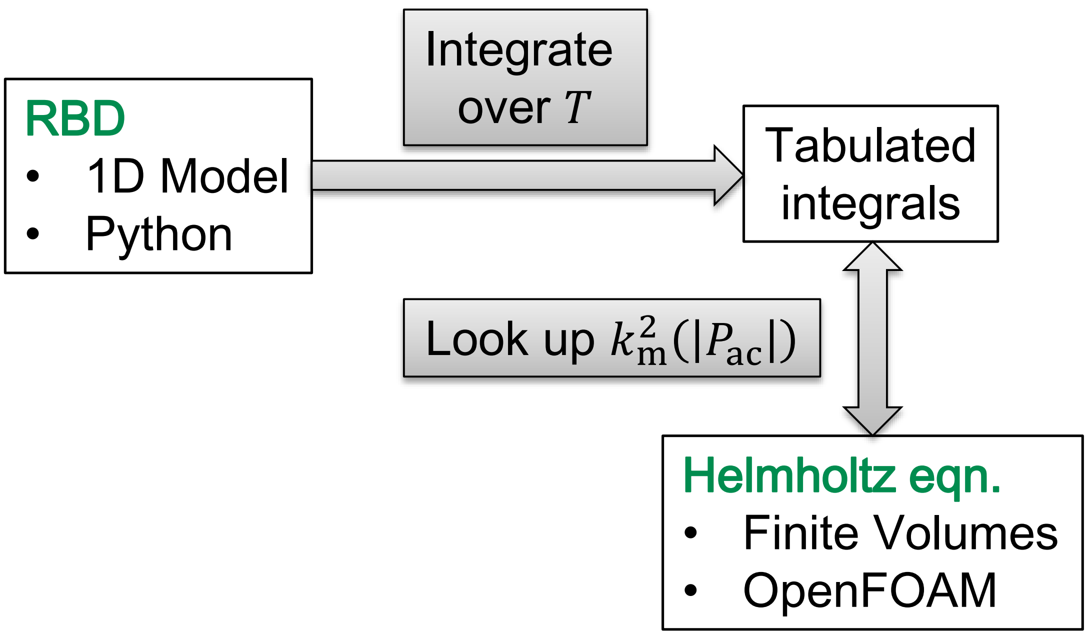
$$\mathrm{Im}(k_\mathrm{m}^2) = -\frac{3\rho\omega\beta}{2\pi R_0^3}\frac{\Pi_\mathrm{Vi} + \Pi_\mathrm{Th}}{|P_\mathrm{ac}|^2}$$

$$\Pi_\mathrm{Vi} = \frac{1}{T}\int_0^T 16\pi\mu R\dot{R}^2\,\mathrm{d}t$$

- $\Pi_{\mathrm{Vi,Th}}$ indirectly dependent on P_ac
- 100cm³ reactor and $\beta = 10^{-5}$ => 2.3e+6 bubbles

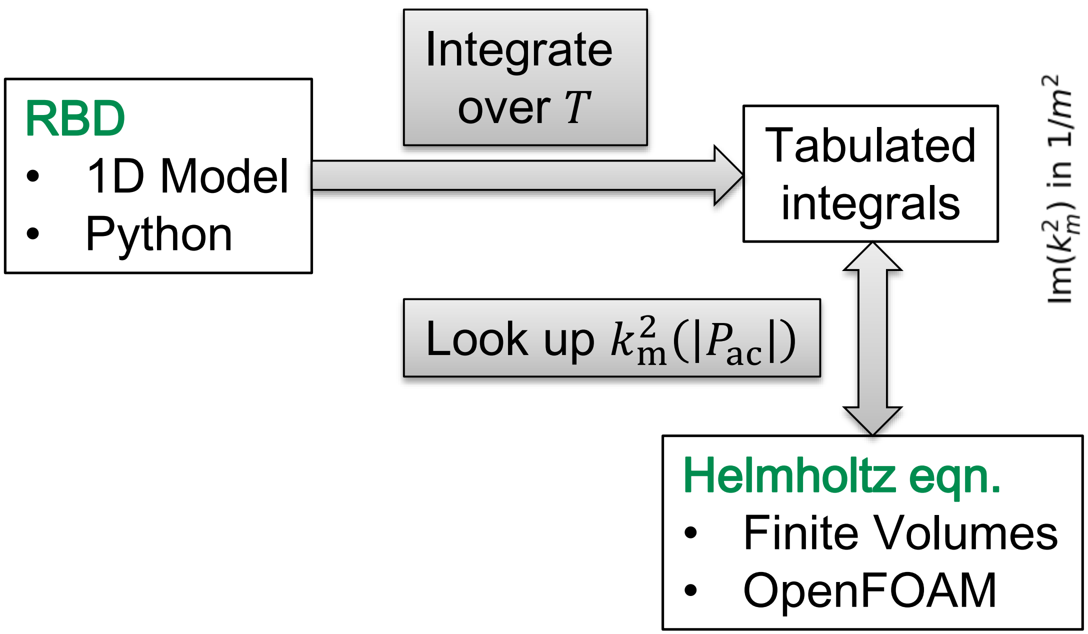
Coupling non-linear RBD and sound field

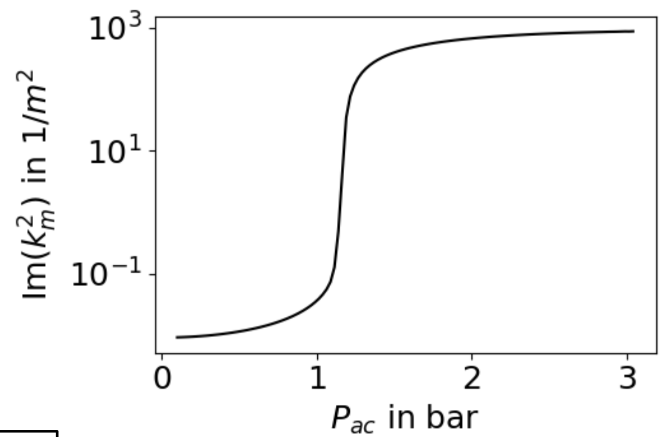
- Approach as **pre-processing step**:
  1. choose parameter range for $|P_{\mathrm{ac}}|$
  2. solve RBD (implemented in python)
  3. compute integral values and save as interpolation tables



Coupling non-linear RBD and sound field

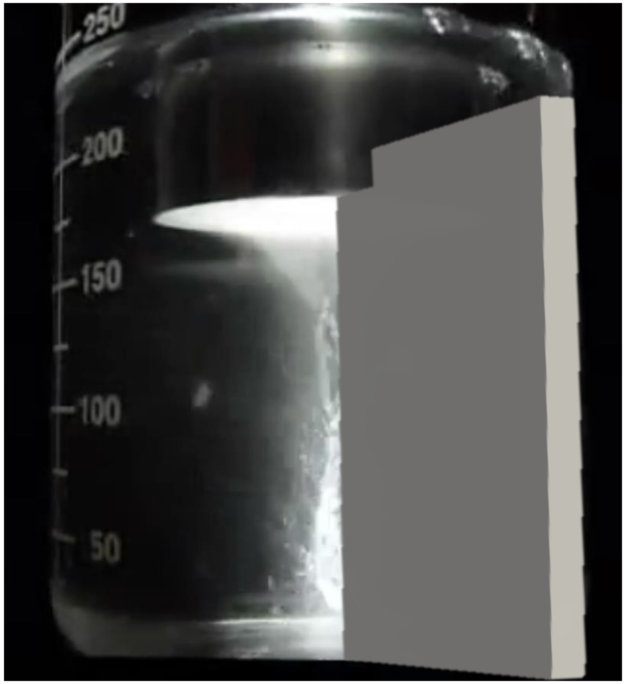
- Iterative process
  - highly non-linear, under-relaxation not sufficient
  - **damped Newton-Raphson method** implemented
    - jacobian with numeric differentiation





Boundary conditions

- Sonotrode immersed in a cylindrical geometry
  - typical setup also for large scale reactors
  - axisymmetric



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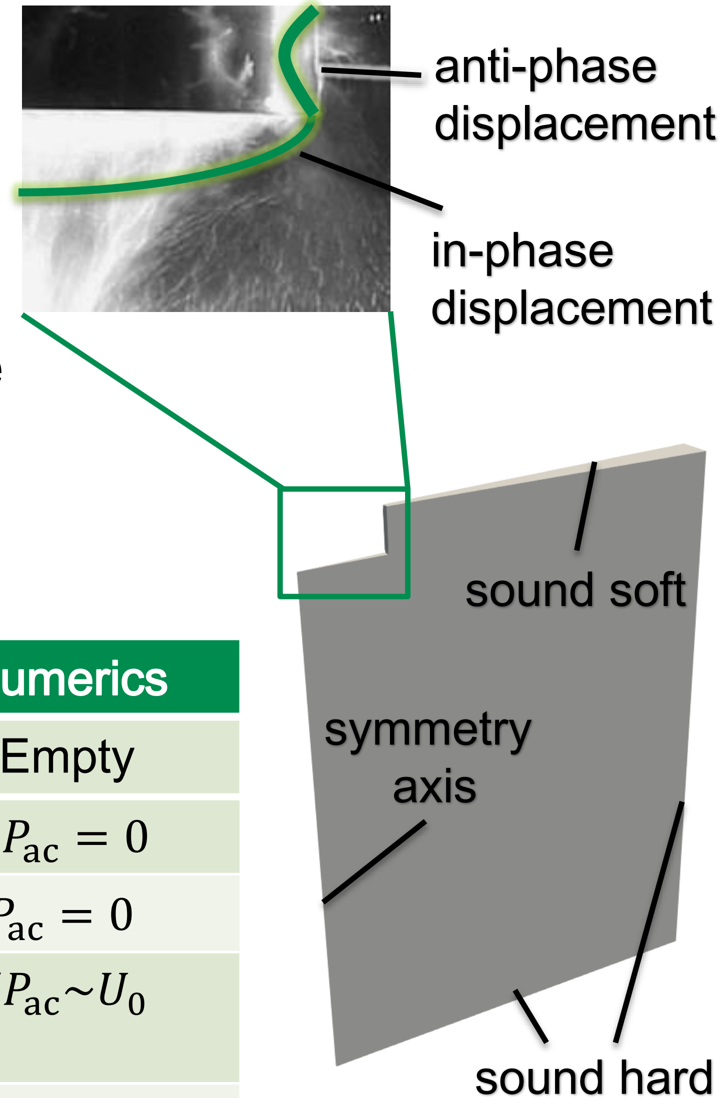
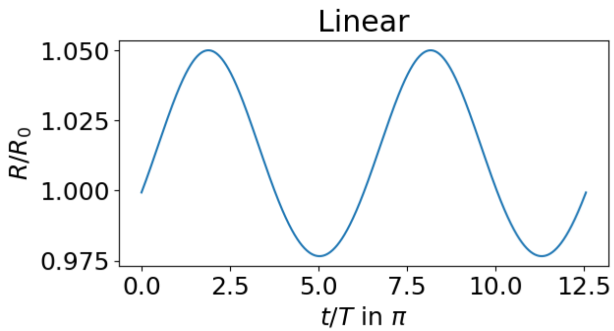
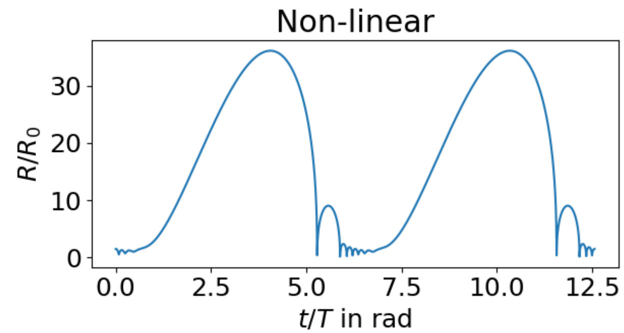


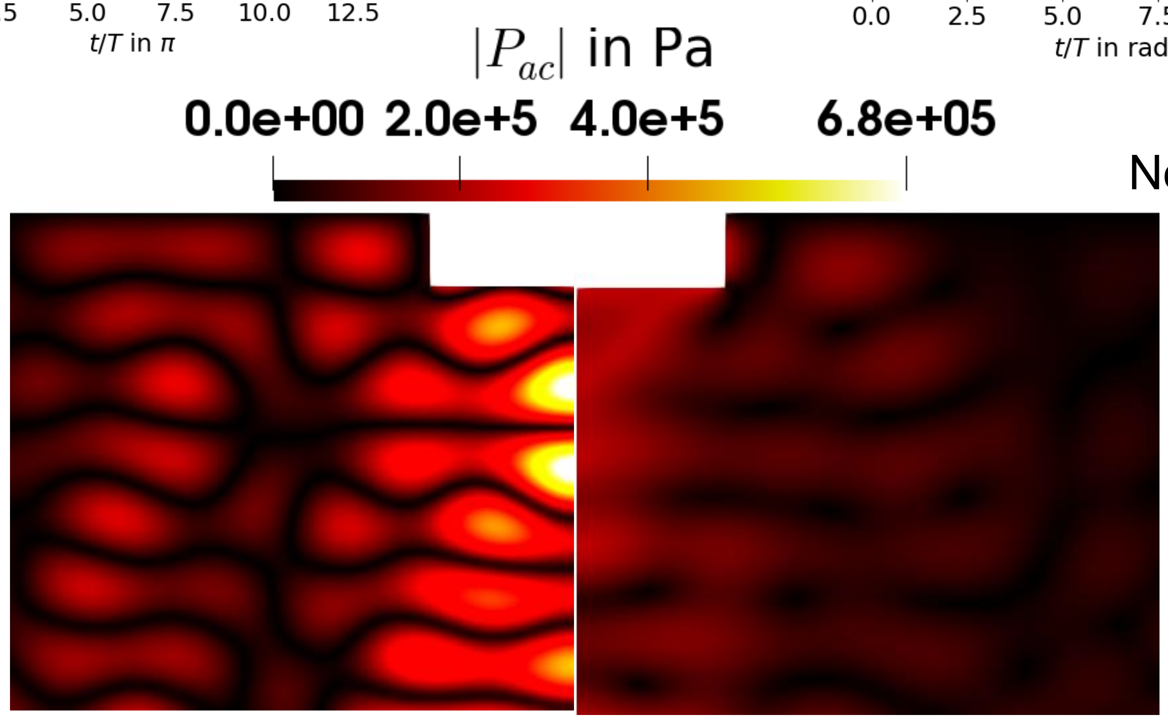
Geometry	Acoustics	Numerics
Symmetry axis	Symmetry axis	Empty
Walls	Sound hard	$\nabla P_{\mathrm{ac}} = 0$
Free surface	Sound soft	$P_{\mathrm{ac}} = 0$
Sonotrode surface	In-phase displacement U_0	$\nabla P_{\mathrm{ac}} \sim U_0$
Sonotrode wall	Anti-phase displacement U_0	$\nabla P_{\mathrm{ac}} \sim (U_0, \phi_0)$

Linear vs. non-linear bubble oscillations



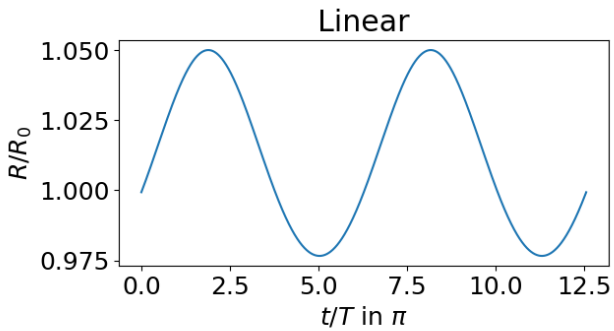


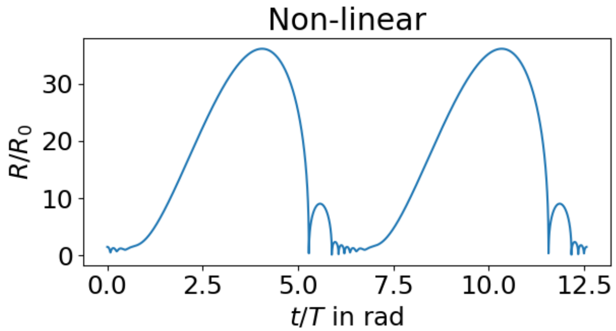
Linear

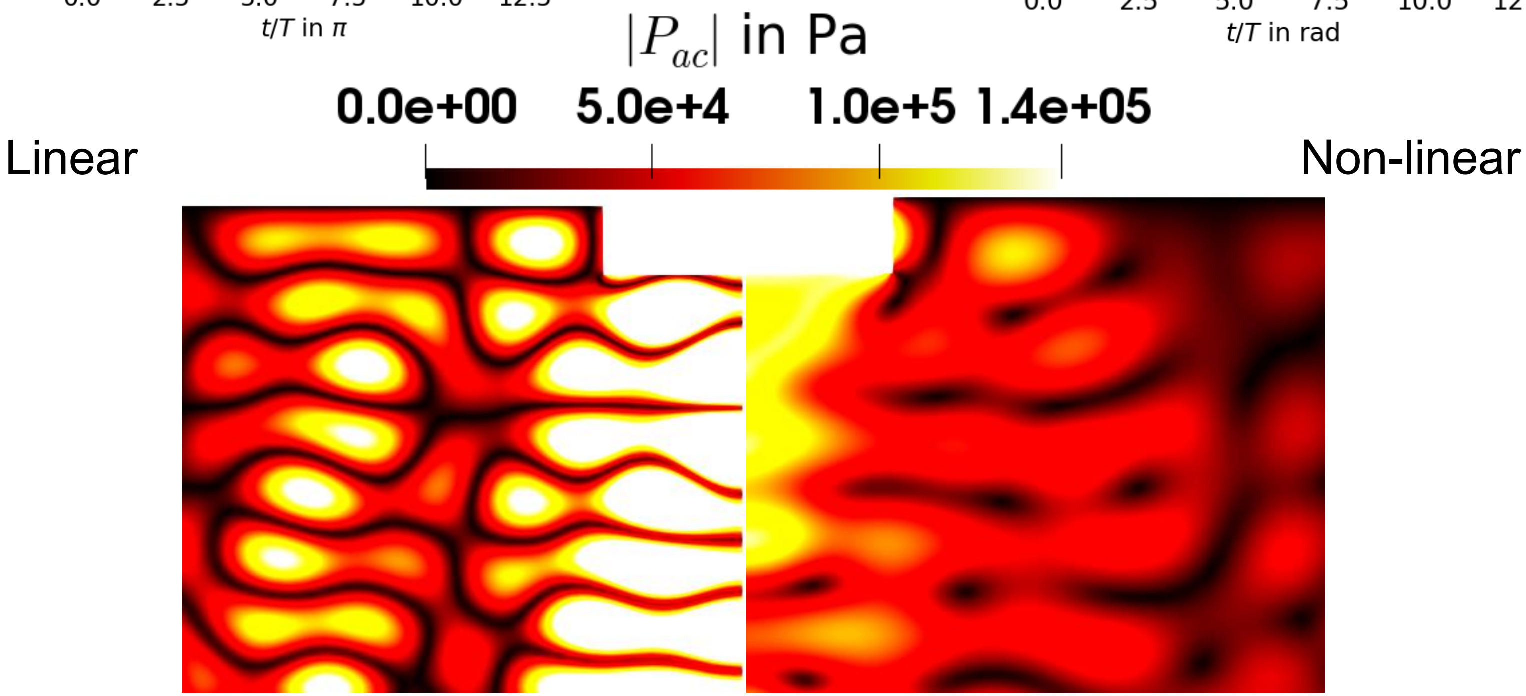


Non-linear

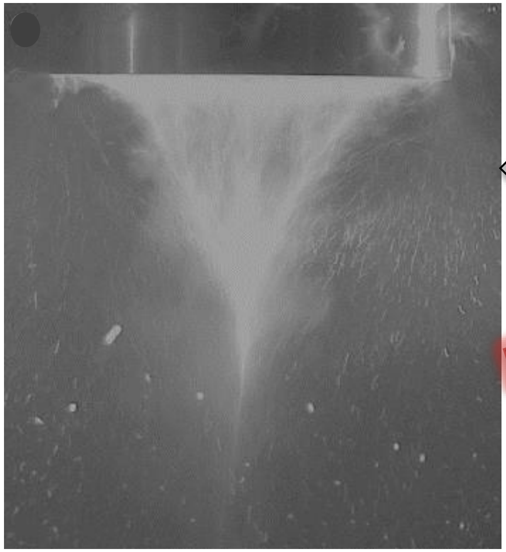
Linear vs. non-linear bubble oscillations

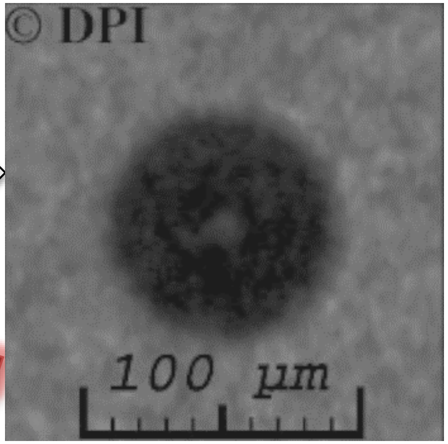




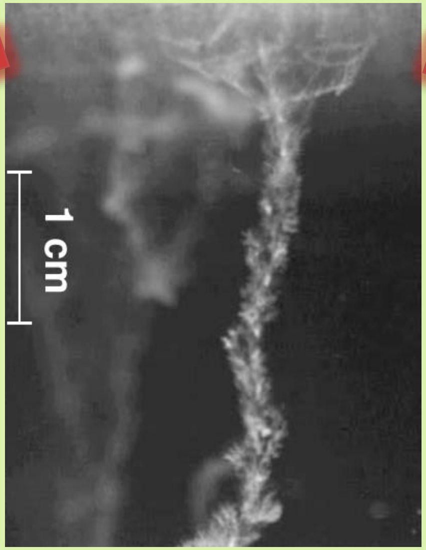


Outline





Model Coupling



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Bubble motion

- Euler-Lagrange (foam-extend)
- Force balance

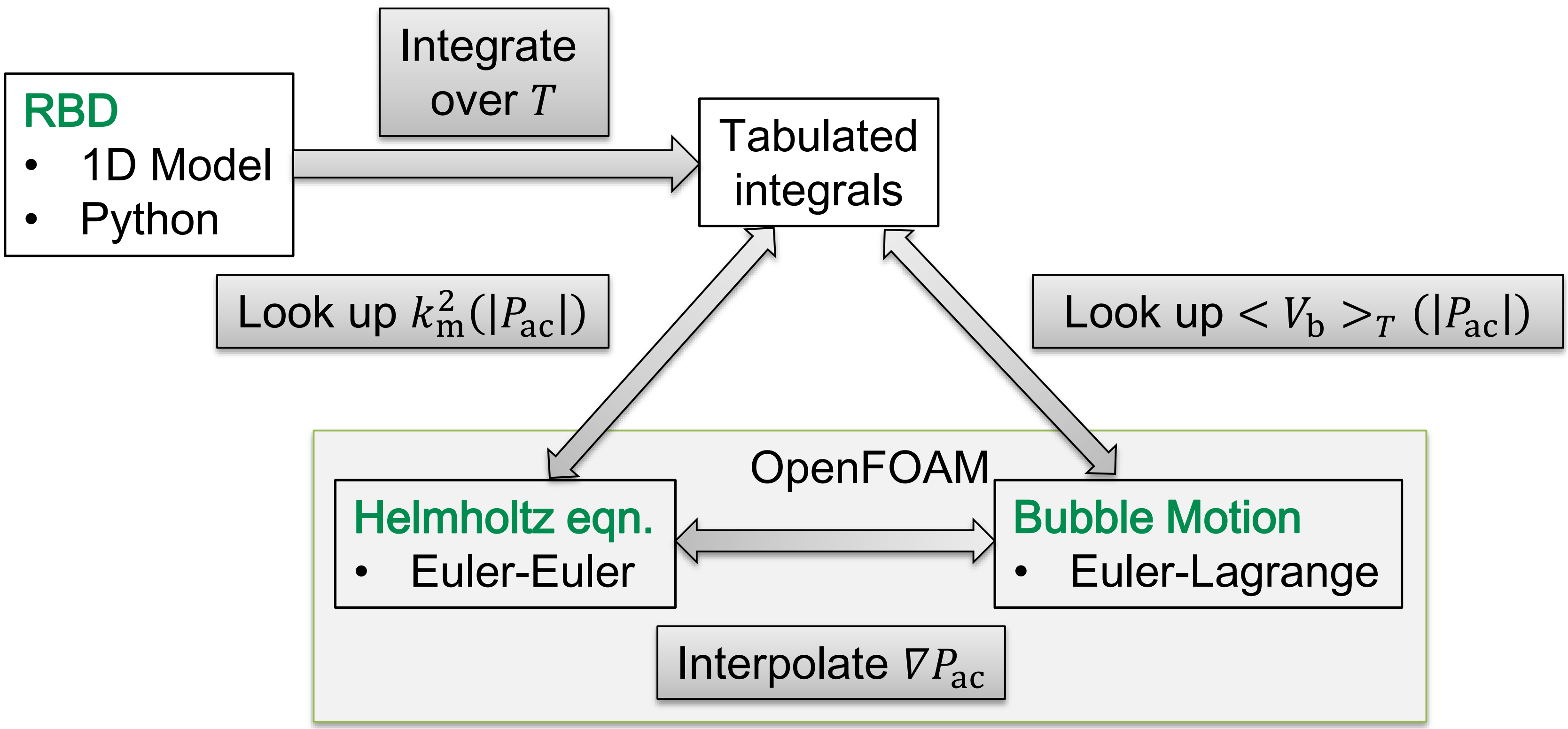
$$m_{\mathrm{b}} \frac{\mathrm{d}U_{\mathrm{b}}}{\mathrm{d}t} = F_{\mathrm{G}} + F_{\mathrm{Am}} + F_{\mathrm{D}} + F_{\mathrm{Bj}}$$

- $m_{\mathrm{b}}, U_{\mathrm{b}}$- bubble mass and velocity
- Forces:
  - F_{G} - gravitation
  - F_{Am} - added mass
  - F_{D} - drag
  - F_{Bj} - Bjerknes, due to interaction of non-linear oscillation and acoustic pressure gradient

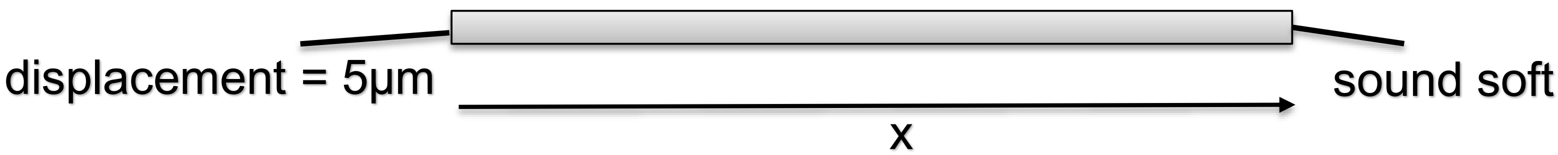
Coupling bubble motion

- Bjerknes force contains bubble volume term averaged over T

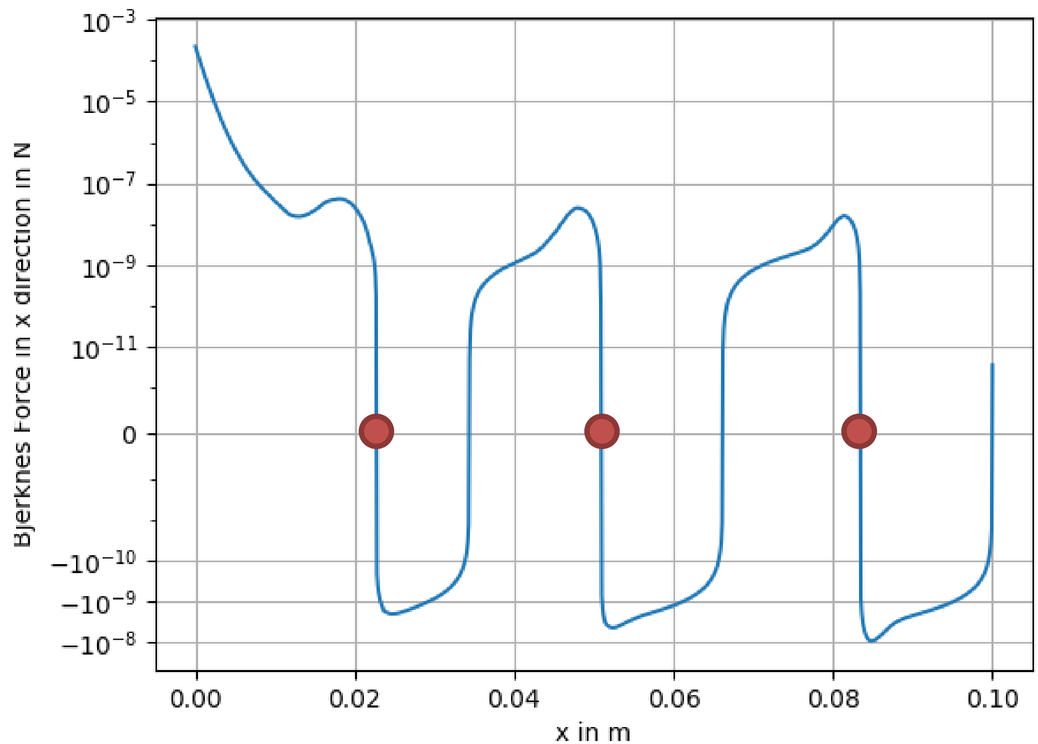
$$F_{\mathrm{Bj}} = \langle V_{\mathrm{b}} \rangle_T \, \nabla P_{\mathrm{ac}}$$



1D case



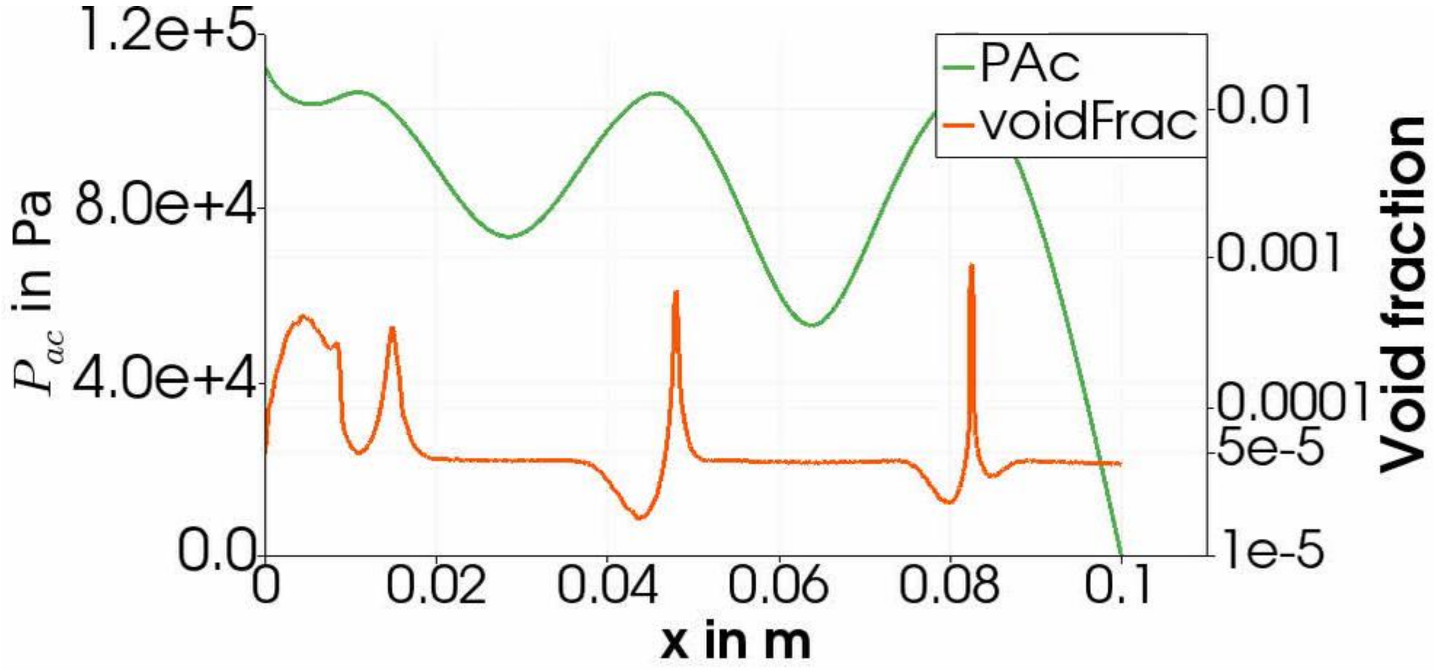
- Bjerknes force



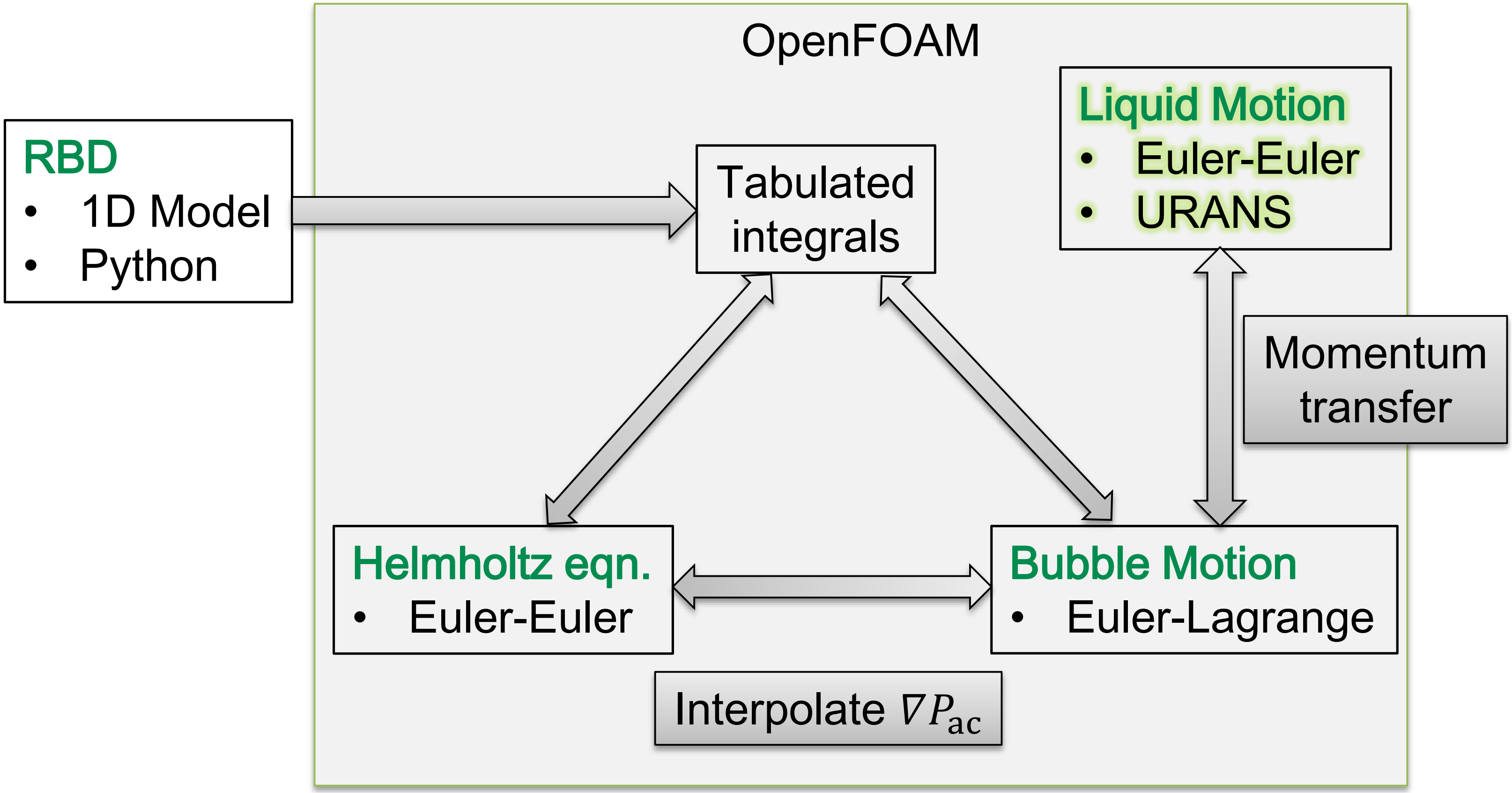
- Stagnation locations

1D case inhomogeneous void fraction

- Void fraction kept constant at transducer (on the right)

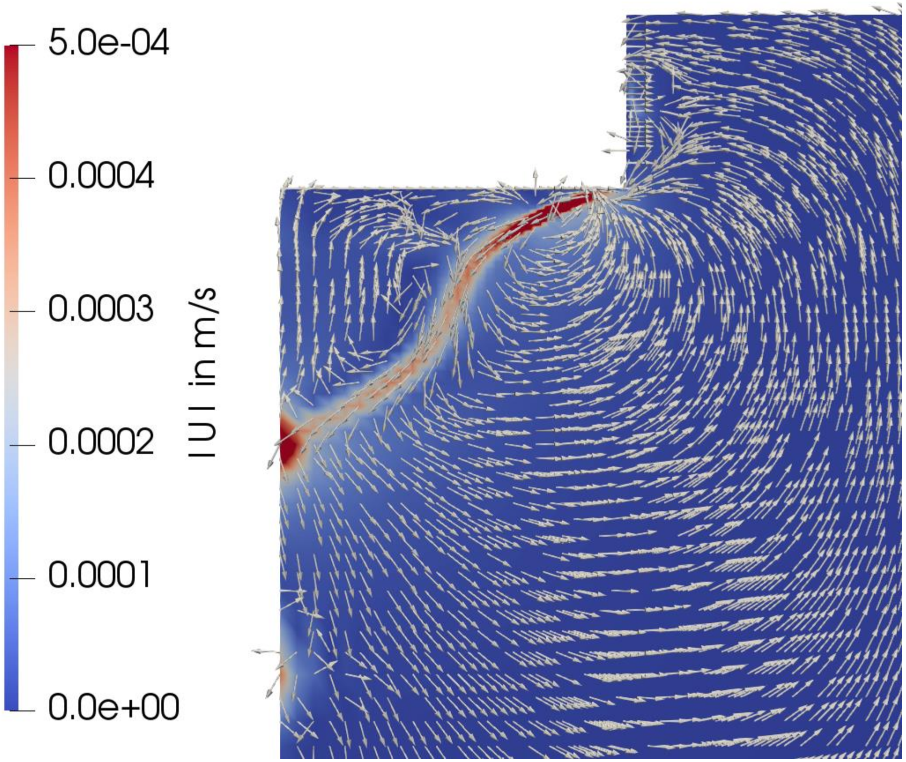


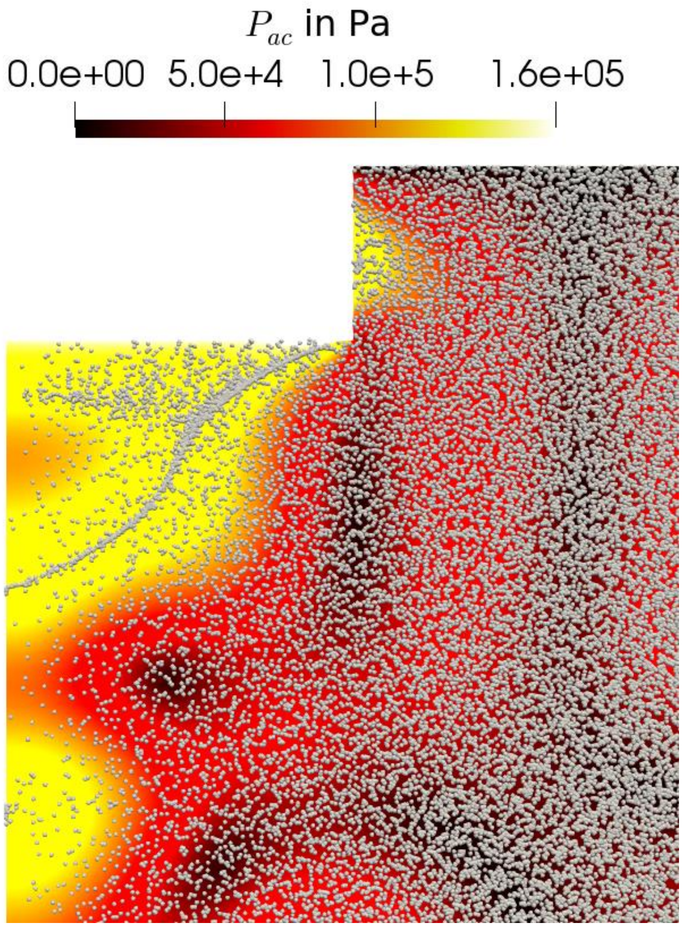
Coupling Liquid motion



2D axisymmetric wedge case

- Liquid and bubble motion





Summary

- Computation of cavitation flows in large scale reactors
  - apply different models to different scales
  - coupling needs caution
- Validation of sub-models with the data from experiments
- Nucleation process needs more consideration
  - where do bubbles nucleate and dissolve?

Source code for Helmholtz solver (MUMPS interface):

https://github.com/technoC0re

Questions?

DFG Deutsche Forschungsgemeinschaft

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