Modelling of acoustic cavitation on a large scale with OpenFOAM

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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.

2. Radial Bubble Dynamics

3. Bubble Motion

Model Coupling

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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

\[
\nabla^2 P_{ac} + k_m^2 P_{ac} = 0
\]

\[
K_r = \text{Re}(k_m^2), \quad K_i = \text{Im}(k_m^2)
\]

\[
P_r = \text{Re}(P_{ac}), \quad P_i = \text{Im}(P_{ac})
\]

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

\[
\nabla^2 P_i + K_r P_i + K_i P_r = 0
\]
HE discretization and solution

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

\[
\begin{bmatrix}
(\nabla^2 + K_r & -K_i \\
K_i & \nabla^2 + K_r)
\end{bmatrix}_{d_0}
\begin{bmatrix}
(\nabla^2 & 0) \\
0 & \nabla^2
\end{bmatrix}_{u_0}
\begin{bmatrix}
(\nabla^2 + K_r & -K_i \\
K_i & \nabla^2 + K_r)
\end{bmatrix}_{d_1}
\ldots
\ldots
\ldots
\begin{bmatrix}
(P_r) \\
P_i
\end{bmatrix}_0
=
\begin{bmatrix}
(b_1) \\
b_2
\end{bmatrix}_0
\]

- The matrix of discretized HE is highly indefinite
  - iterative solvers diverge
  - \(=>\) Interface implemented to a **direct solver (MUMPS)**
    - **MUltifrontal Massively P**arallel sparse direct **Solver**
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Radial bubble dynamics (RBD)

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

- Toegel model: 3 ODEs
  - Keller-Miksis eqn. \((R – \text{bubble radius})\)
  \[
  \left(1 - \frac{\dot{R}}{c}\right) R \ddot{R} + \left(1 - \frac{\dot{R}}{3c}\right) \frac{3}{2} \dot{R}^2 = \frac{1}{\rho} \left[ \left(1 + \frac{\dot{R}}{c}\right) \left(p_g - |P_{ac}| \sin(\omega t) - p_0\right) + \frac{R \ddot{p}_g}{c} - \frac{4 \mu \dot{R}}{R} - \frac{2 \sigma}{R} \right]
  \]
  - energy transfer \((\theta – \text{temperature})\)
  \[
  \dot{\theta} = \frac{-p_g \frac{dV}{dt} + Q + \frac{dn_{vap}}{dt} (h_{vap}(\theta_0) - u_{vap}(\theta))}{n_{vap} c_{V,vap}(\theta) + n_{ncg} c_{V,ncg}(\theta)}
  \]
  - mass (vapor) transfer \((n – \text{amount of substance})\)
  \[
  \dot{n}_{vap} = SD(\theta_0) \frac{c_{vap}(R) - c_{vap}}{l_{m,ml}}
  \]
Coupling non-linear RBD and sound field

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

$$\nabla^2 P_{ac} + k_m^2 P_{ac} = 0$$

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

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

- $\Pi_{Vi, Th}$ indirectly dependent on $P_{ac}$
- 100 cm$^3$ 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 $|P_{ac}|$
  2. solve RBD (implemented in python)
  3. compute integral values and save as interpolation tables

- **RBD**
  - 1D Model
  - Python

- Integrate over $T$

- Tabulated integrals

- Look up $k_m^2(|P_{ac}|)$

- **Helmholtz eqn.**
  - Finite Volumes
  - OpenFOAM
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

RBD
- 1D Model
- Python

Integrate over $T$

Tabulated integrals

Look up $k_m^2(|P_{ac}|)$

Helmholtz eqn.
- Finite Volumes
- OpenFOAM

Graph

$\text{Im}(k_m^2)$ in $1/m^2$

$P_{ac}$ in bar

$0 \quad 1 \quad 2 \quad 3$

$10^{-1} \quad 10^1 \quad 10^3$
Boundary conditions

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

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

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Acoustics</th>
<th>Numerics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetry axis</td>
<td>Symmetry axis</td>
<td>Empty</td>
</tr>
<tr>
<td>Walls</td>
<td>Sound hard</td>
<td>( \nabla P_{ac} = 0 )</td>
</tr>
<tr>
<td>Free surface</td>
<td>Sound soft</td>
<td>( P_{ac} = 0 )</td>
</tr>
<tr>
<td>Sonotrode surface</td>
<td>In-phase displacement ( U_0 )</td>
<td>( \nabla P_{ac} \sim U_0 )</td>
</tr>
<tr>
<td>Sonotrode wall</td>
<td>Anti-phase displacement ( U_0 )</td>
<td>( \nabla P_{ac} \sim (U_0, \phi_0) )</td>
</tr>
</tbody>
</table>
Linear vs. non-linear bubble oscillations

\[ |P_{ac}| \text{ in Pa} \]

Linear: 0.0e+00 2.0e+5 4.0e+5

Non-linear: 6.8e+05
Linear vs. non-linear bubble oscillations

Linear

Non-linear

$P_{ac}$ in Pa

Linear  0.0e+00  5.0e+4  1.0e+5  1.4e+05  Non-linear
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Model Coupling
Bubble motion

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

\[ m_b \frac{dU_b}{dt} = F_G + F_{Am} + F_D + F_{Bj} \]

- \( m_b, U_b \)- 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 $T$

$$F_{Bj} = \langle V_b \rangle_T \nabla P_{ac}$$

**RBD**
- 1D Model
- Python

- **Integrate over $T$**
- **Tabulated integrals**

- **Look up** \( k_m^2(|P_{ac}|) \)
- **Look up** \( <V_b>_T(|P_{ac}|) \)

**OpenFOAM**
- Helmholtz eqn.
  - Euler-Euler
- Bubble Motion
  - Euler-Lagrange

- **Interpolate** \( \nabla P_{ac} \)
1D case

- **Bjerkes force**

- **Stagnation locations**

\[ \text{displacement} = 5\mu m \]
1D case inhomogeneous void fraction

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

OpenFOAM

- RBD
  - 1D Model
  - Python

- Tabulated integrals

- Helmholtz eqn.
  - Euler-Euler

- Liquid Motion
  - Euler-Euler
  - URANS

- Bubble Motion
  - Euler-Lagrange

- Momentum transfer

- Interpolate $\nabla P_{ac}$
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?