# Application of high-performance computing for bubble simulations in sonochemistry

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MŰEGYETEM 1782

Nemzeti Kutatási, Fejlesztési és Innovációs Hivatal

Új Nemzeti Kiválóság Program

# Overview

# What is sonochemistry?

## Essence

Increasing the yield of chemical processes with ultrasound excitation

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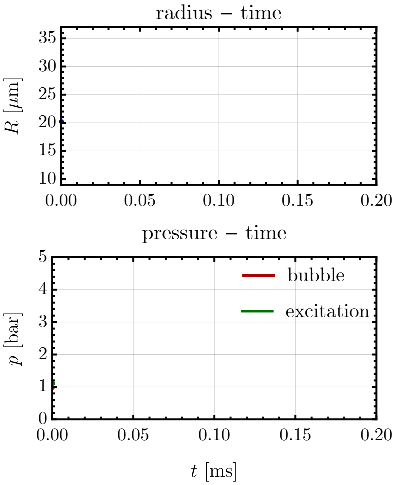
## Problems

- Achieving industrial size
- Simulating sonochemical reactors with millions of bubbles

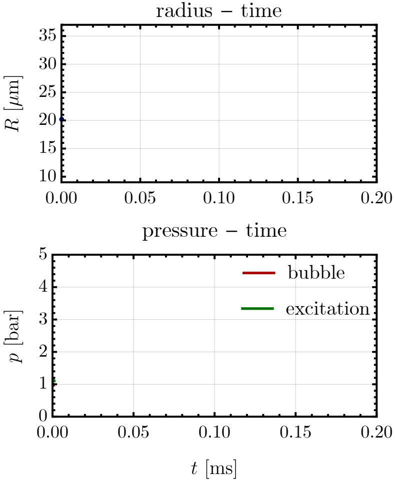
Goal: observing previously unmodeled phenomena using CFD (e.g. bubble break-up)

# Oscillation of a single bubble



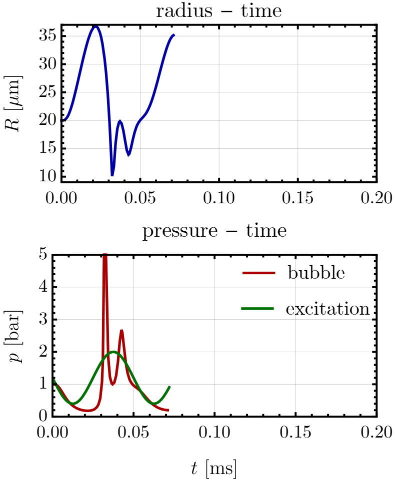

1. Bubbles in the liquid

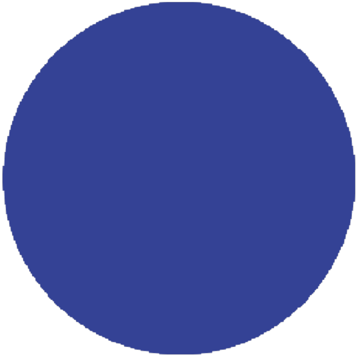
# Oscillation of a single bubble




1. Bubbles in the liquid
2. Oscillations due to excitation

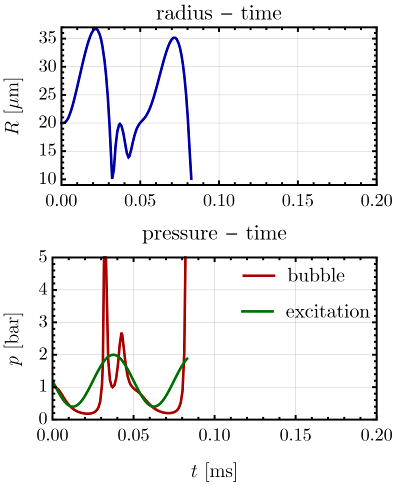
# Oscillation of a single bubble



1. Bubbles in the liquid
2. Oscillations due to excitation
3. Bubble collapse
   - Pressure and temp. increase
   - Inducing chemical reactions
   - Symmetry loss

# Oscillation of a single bubble




1. Bubbles in the liquid
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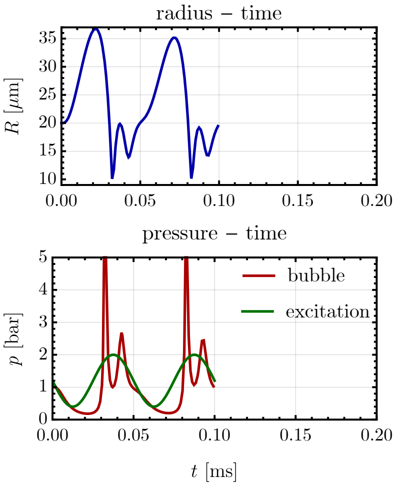


1. Bubbles in the liquid
2. Oscillations due to excitation
3. Bubble collapse
    - Pressure and temp. increase
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# Difficulties of the simulation

## Problems

- Two compressible phase
- Rapid change of the phase boundary
- Scale difference:
  - bubble $\approx 1 \times 10^{-5}\,\mathrm{m}$
  - domain $\approx 1 \times 10^{-2}\,\mathrm{m}$
- High pressure amplitudes $p_A = 0.5\,\mathrm{bar} - 2\,\mathrm{bar}$

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## ALPACA (CFD solver)

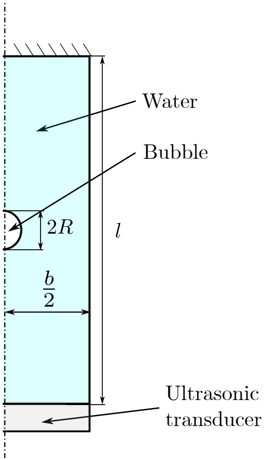
- Compressible multiphase flows
- *Level-set* method to track the phase boundary
- Adaptive meshing using *multiresolution*
- Large computational requirement $\rightarrow$ supercomputers
- MPI-parallelized C++ code
- Open-source

ALPACA available at `https://gitlab.lrz.de/nanoshock/ALPACA`
Developed by the Nanoshock research group (Technical University of Münich)

# Overview

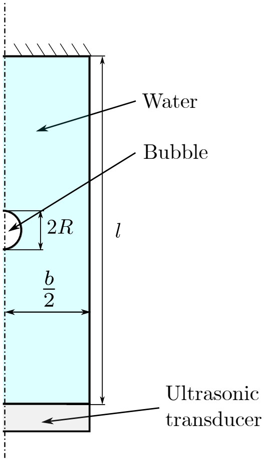
# Model

## Axisymmetric simulation



# Model

## Axisymmetric simulation



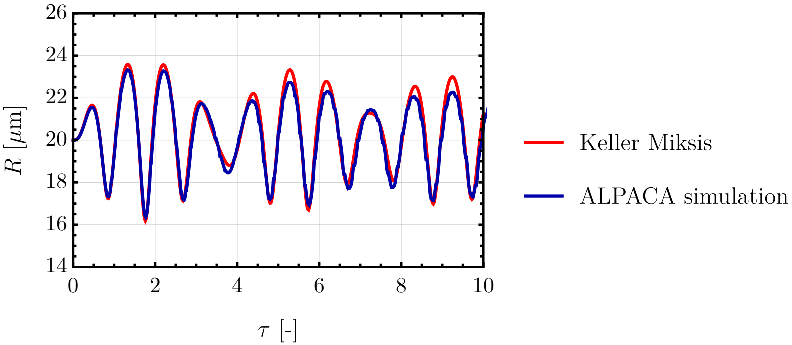

### Important parameters

- Equilibrium bubble radius $R_0$
- Excitation frequency $f$
- Excitation pressure amplitude $p_A$

### Keller-Miksis equation

- Describes a spherical bubble in acoustic field
- 2nd order ODE for the bubble radius $R(t)$
- Used for validation

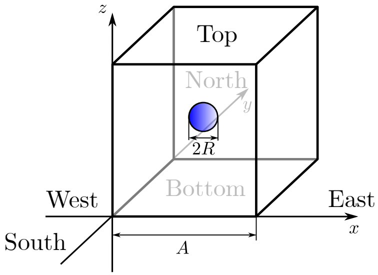
# Comparison with the Keller-Miksis equation




- Parameters: $R_0 = 20\,\mu\text{m}$, $p_A = 0.2\,\text{bar}$, $f = 130\,\text{kHz}$
- Dimensionless time $\tau = t \cdot f$
- Good agreement

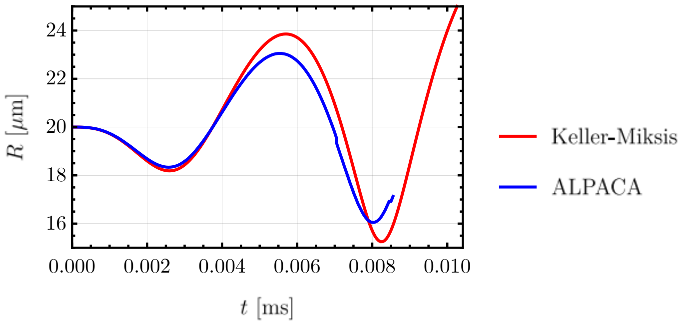
# Model and results

## Model in 3D




- West: Time-dependent pressure
- Only the bubble and the immediate neighbourhood

## Comparison with the Keller-Miksis equation



# Overview

# Computational problem

## 2D axisymmetric

- Number of cells: $10^4 - 10^5$
- Step size: $\approx 1 \times 10^{-10}$ s
- Number of steps: $\approx 10^6$
- Wall time per step: $50 - 500$ ms
- Runtime: $0.5 - 5$ days

# Computational problem

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### Full 3D

- Number of cells: $10^6 - 10^7$
- Step size: $\approx 1 \times 10^{-10}$ s
- Number of steps: $\approx 10^6$
- Wall time per step: $500 - 5000$ ms
- Runtime: $5 - 50$ days

Exact values depend on the parameters, resolution and compute configuration

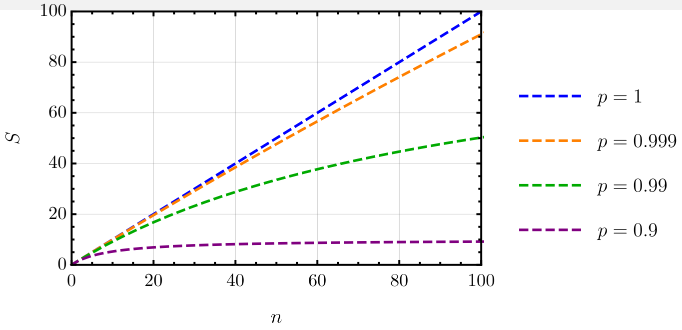
### The problem

- Number of cells is not too large (parallelization is not too efficient)
- More than a million time step is necessary

# Amdahl's law

$$S(n) = \frac{1}{(1-p) + \frac{p}{n}}$$

- $n$: number of CPU cores
- $S$: theoretical speedup
- $p$: parallel proportion



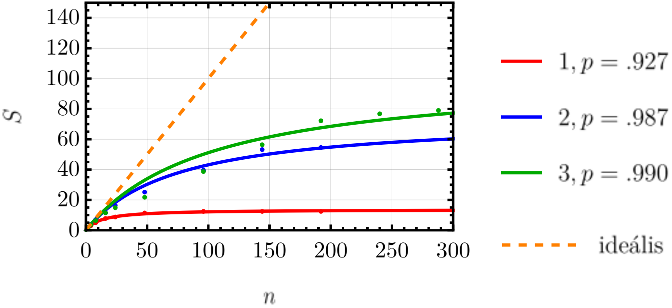

## SUPERMUC-NG (26.9 PFlop/s)

- Cores/node: 48
- Max. nodes (micro project): 16 ($n_{max} = 768$)
- Maximum run time of a single job: 48 h

# Strong scaling of ALPACA

## Strong scaling

- What is the speedup if the compute resources are increased?
- Described by Amdahl's law




Settings

| sim | $N_{cell}$ | $D_{cell}$ |
|---|---|---|
| 1 | $0.47 \cdot 10^6$ | 51 |
| 2 | $1.44 \cdot 10^6$ | 102 |
| 3 | $6.23 \cdot 10^6$ | 102 |

# The simulated bubble

- Parameters

  $p_A = 0.3\,\text{bar}, \quad f = 192\,\text{kHz}, R_0 = 20\,\mu\text{m}$

- Mesh

  $N_{\text{bubble}} = 0.56 \cdot 10^6, \quad N_{\text{cell}} = 6.23 \cdot 10^6$

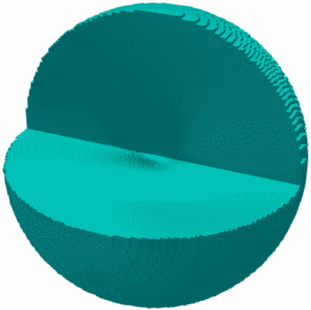
- Time step

  $\Delta t \approx 1 \times 10^{-10}\,\text{s}, \quad t_{\max} = 8.7 \times 10^{-6}\,\text{s}$

- Execution

  $$n = 192, \quad T_{\text{run}} = 36\,\text{h}$$

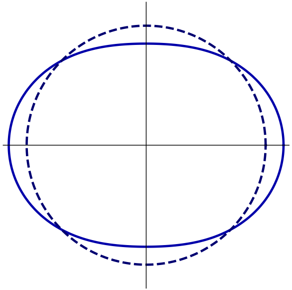
  $$T_{CPU} = n \cdot T_{\text{run}} \approx 7000\,\text{h}$$



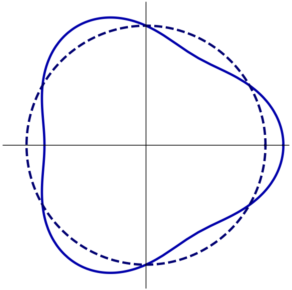
# Overview

# Surface modes

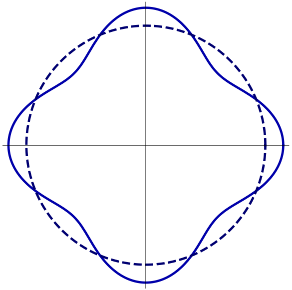
Depending on the parameters different axisymmetric shapes are stable. Example for a $R_E = 20\,\mu m$ bubble:



$M_2$ at $f = 105\,kHz$



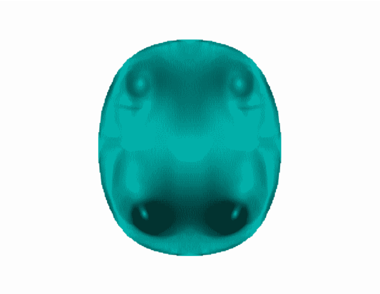
$M_3$ at $f = 192\,kHz$



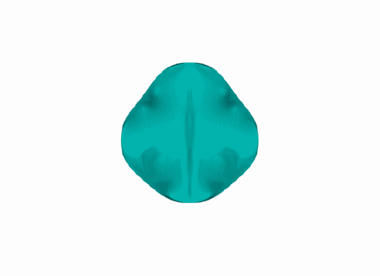
$M_4$ at $f = 288\,kHz$

# Simulation results

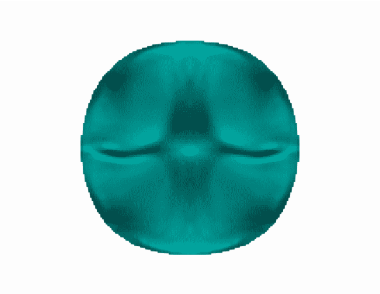
- At least 100 cells along the diameter
- Mode 3 is initialized with a horizontal asymmetry



$M_2$ at $f = 105\,\text{kHz}$



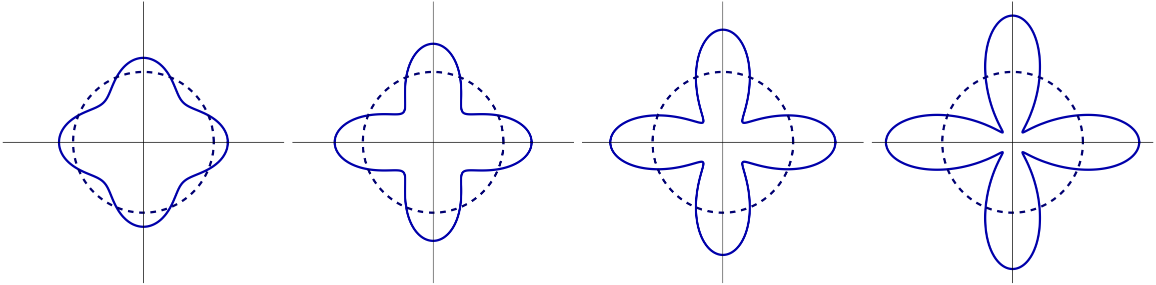
$M_3$ at $f = 192\,\text{kHz}$



$M_4$ at $f = 288\,\text{kHz}$

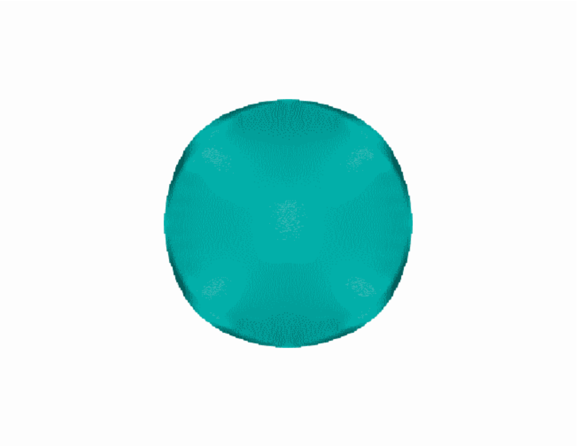
# Break-up of bubbles

- Amplitude of a surface oscillation becomes to large
- Requires high enough pressure amplitude



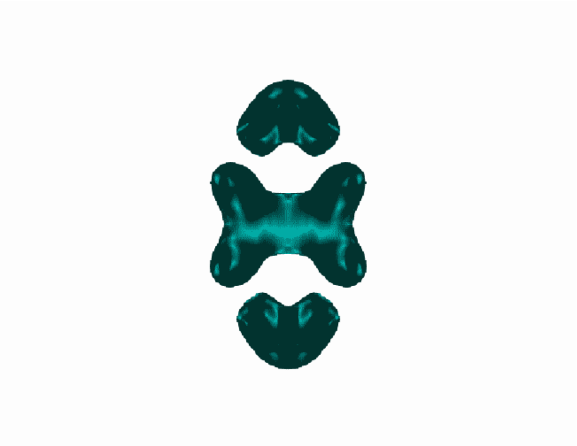
Bubble break-up initiating from Mode 4

# Simulation of bubble break-ups

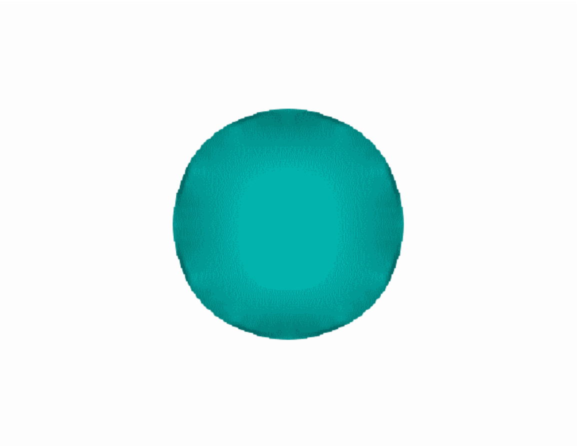


$R_E = 20\,\mu\text{m}$, $p_A = 0.9\,\text{bar}$, $f = 192\,\text{kHz}$

# Simulation of bubble break-ups



$R_E = 20\,\mu m$, $p_A = 0.9\,bar$, $f = 192\,kHz$



$R_E = 30\,\mu m$, $p_A = 0.7\,bar$, $f = 130\,kHz$

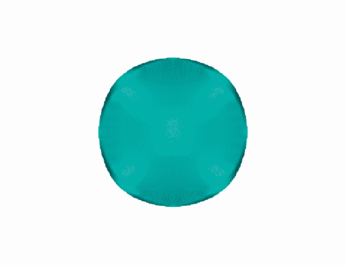
# Important references


- Kaiser, Jakob WJ et al. "An adaptive local time-stepping scheme for multiresolution simulations of hyperbolic conservation laws". In: *Journal of Computational Physics: X* 4 (2019), p. 100038.
- Lauterborn, Werner and Thomas Kurz. "Physics of bubble oscillations". In: *Reports on progress in physics* 73.10 (2010), p. 106501.
- Mason, TJ, AP Newman, and SS Phull. "Sonochemistry in water treatment". In: *Division of Chemistry, Coventry University, Convetry CVI 5FB* (1994), pp. 3927–3933.
- Mason, Timothy J. "Sonochemistry and the environment–Providing a "green" link between chemistry, physics and engineering". In: *Ultrasonics sonochemistry* 14.4 (2007), pp. 476–483.

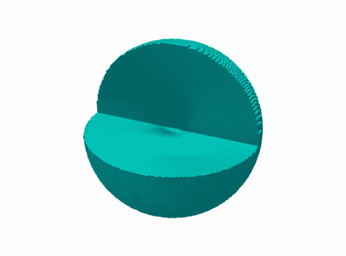
# Thank you for your attention!

## The problem

- Number of cells is not too large (parallelization is not too efficient, max. 80× speedup)
- More than a million time step is necessary



Axisymmetric simulations (bubble breakup)



Full 3D simulation

# Index

# Index Postprocessing in *paraview*

*i* goes through cells inside the bubble

- Area of the bubble

$$A_B = \sum_i A_i$$

- Average pressure of the bubble

$$p_B = \frac{1}{A_B} \sum_i A_i \cdot p_i$$

- Average density of the bubble

$$\rho_B = \frac{1}{A_B} \sum_i A_i \cdot \rho_i$$

- Mass of the bubble

$$m = \rho_B \cdot A_B \cdot h \quad \text{or} \quad m = h \sum_i A_i \rho_i$$

- Radius of the bubble I

$$R = \sqrt{\frac{A_B}{\pi}}$$

- Radius of the bubble II

$$R_y = \frac{y_{north} - y_{south}}{2} \quad \text{or} \quad R_x = \frac{x_{east} - x_{west}}{2}$$

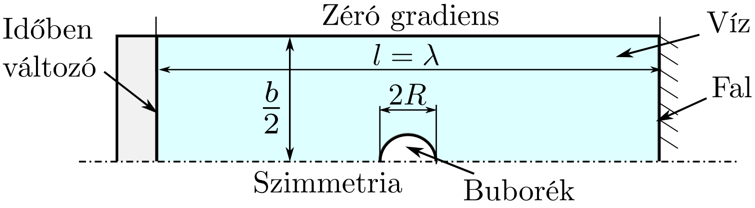
# ◂ Index Boundary and initial conditions

- Initial conditions (standing wave in water)

$$\text{Water:} \quad p(0,x) = p_0, \quad \rho(0,x) = \rho_{0,v}, \quad u(0,x) = -\frac{p_A}{c\rho_0}\sin\left(2\pi\frac{f}{c}x\right)$$

$$\text{Gas bubble:} \quad p(0,x) = p_0, \quad \rho(0,x) = \rho_{0,l}, \quad u(0,x) = 0$$

- Utilizing the symmetry
- boundary conditions



◂ Index

# Convergence study settings

- Standing wave

$$f = 20\,\mathrm{kHz}, \quad p_A = 0.1\,\mathrm{bar}$$

- Bubble

$$p_0 = 1\,\mathrm{bar}, \quad R_0 = 20\,\mu\mathrm{m}$$

- Domain

$$\lambda \times \lambda \Leftrightarrow 81.25\,\mathrm{mm} \times 81.25\,\mathrm{mm}$$

- Meshing with different minimum sized cells ($a_{min}$)

Starting from 64 × 64 cells

| $l_{max}$ | $a_{min}$ | bubble/all cell |
|---|---|---|
| 9 | 2.48 µm | 208 / 40960 |
| 10 | 1.24 µm | 812 / 50176 |
| 11 | 0.62 µm | 3268 / 62462 |
| 12 | 0.31 µm | 13076 / 87040 |
| 13 | 0.15 µm | 33908 / 136192 |

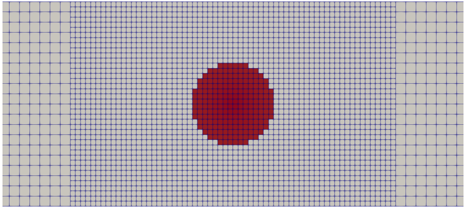
Starting from 96 × 96 cells

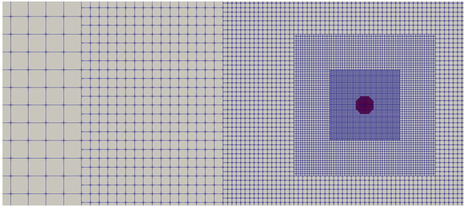
| | | |
|---|---|---|
| 9 | 1.65 µm | 460 / 61440 |
| 10 | 0.83 µm | 1844 / 73728 |

◂ Index

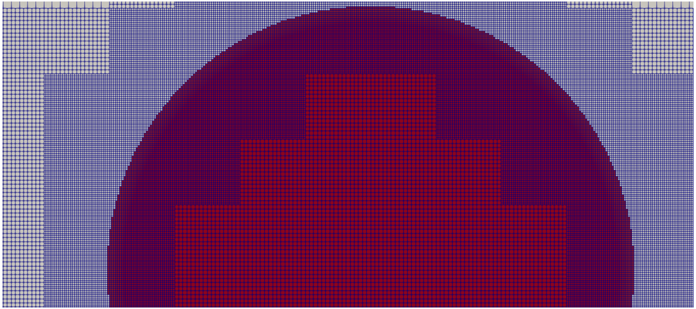
# Created mesh

Coarse resolution $a_{\min} = 2.48\,\mu\text{m}$



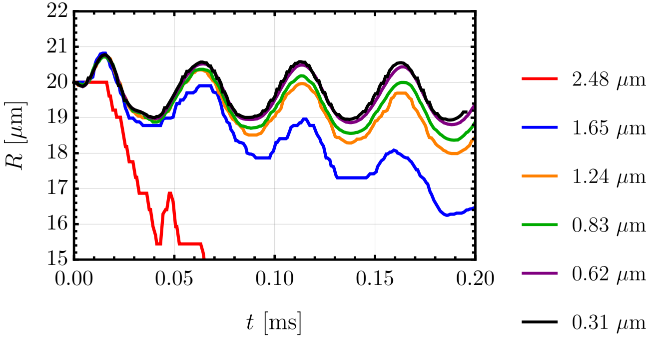


Fine resolution $a_{\min} = 0.15\,\mu\text{m}$

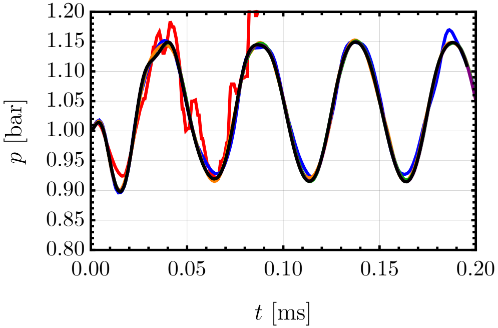


# Convergence study plots

Index

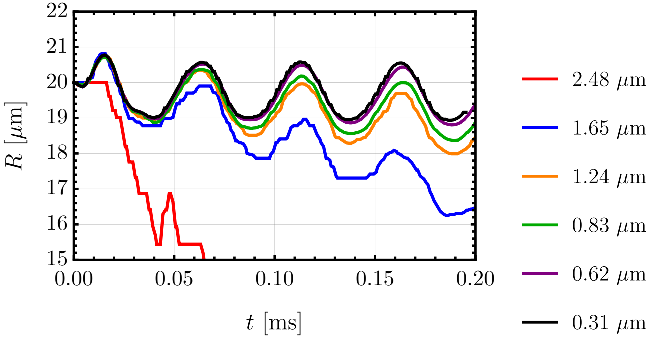



radius – time

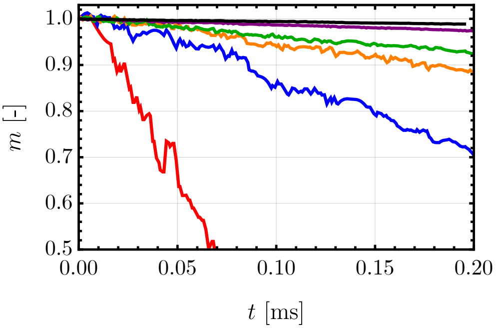



pressure – time

# Index Convergence study plots




radius – time




mass – time

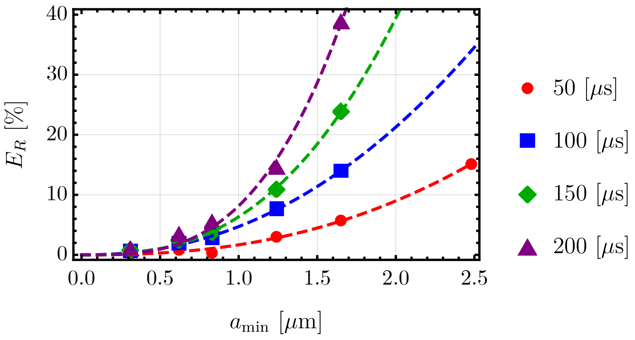
# Index Convergence order

- Finest simulation: reference
- Relative derivation from the bubble radius

$$E_R(t) = \left| \frac{R_{ref}(t) - R(t)}{R_{ref}(t)} \right| \cdot 100 \quad [\%]$$

- Fitting a curve on the relative errors $E_R = b \cdot a_{min}^r$

  $r$ is the convergence order, $b$ is a constant




relative deviation – minimum cell size

## Measured convergence

$r_{50\,\mu s} = 2.43$, $r_{100\,\mu s} = 2.18$, $r_{150\,\mu s} = 2.64$, $r_{200\,\mu s} = 3.10$ $\Rightarrow$ at least 2nd order

# Index The *level-set* method

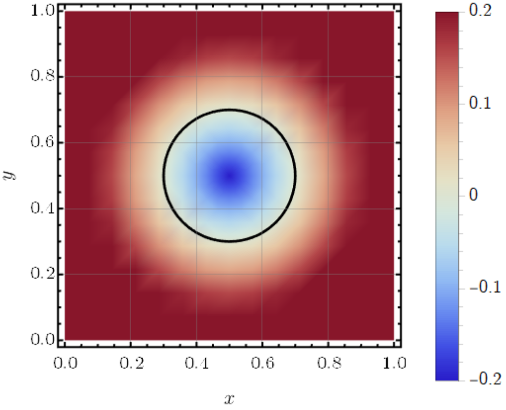
1. Implicit description of the phase-boundary

$$\phi(x, y) = 0 = \sqrt{(x - x_0)^2 + (y - y_0)^2} - R_0$$

2. Phase-boundary tracking

$$\frac{\partial \phi}{\partial t} + \mathbf{u}_\phi \cdot \nabla \phi = 0,$$

3. Phase boundary velocity ($\mathbf{u}_\phi$)




A bubble described using the *level-set* method

# Index The *multiresolution* algorithm

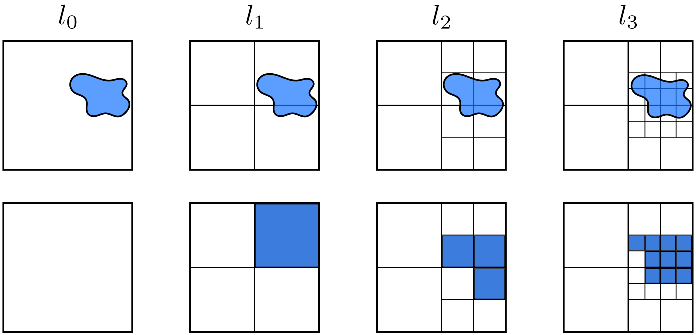
Adaptive meshing in space and time using a combination of different resolution levels.

- $l_i$ – $i$th level
- $l_0$ level: Square based mesh
- Vanishing detail

$$||u_{l_{m+1}} - u_{l_m}|| < \varepsilon_{l_m}$$

$u_{l_i}$ is the representation of a conserved quantity on the $l_i$ level

- Every non-vanishing detail is resolved




Parameters: $l_{\max}$ max. level, $\varepsilon_{l_m}$ level-wise threshold

# Index Multiresolution – wavelet analysis

Any function can be written as the sum of an infinite number of increasingly fine-resolution wavelets. A function $u(x)$ can be expressed with wavelets as

$$u(x) = \sum_{m\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} d_k^{l_m} \Psi_k^{l_m}(x)$$

where $d_k^{l_m}$ is the detail and $\Psi_k^{l_m}(x)$ is a wavelet formed as,

$$\Psi_k^{l_m}(x) = 2^{-l_m/2}\Psi(2^{l_m}x - k)$$

where $\Psi(x)$ is the mother wavelet. The detail $d_k^{l_m}$ can be calculated as

$$d_k^{l_m} = \int_{\mathbb{R}} u(x)\Psi_k^{l_m}(x)\mathrm{d}x.$$

The essence of the adaptive MR algorithm is that in places where the detail $d_k^{l_m}$ is negligible, i.e. less than the specified threshold, the terms can be completely neglected.

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# Keller-Miksis equation

Usual form:

$$\left(1-\frac{\dot{R}}{c_L}\right)R\ddot{R}+\left(1-\frac{\dot{R}}{3c_L}\right)\frac{3}{2}\dot{R}^2=\left(1+\frac{\dot{R}}{c_L}+\frac{R}{c_L}\frac{d}{dt}\right)\frac{(p_L-p_\infty(t))}{\rho_L},$$

$R(t)$ is the bubble radius, $c_L$ is the speed of sound and $\rho_L$ is the density of the liquid. The pressure $p_\infty$ includes the excitation:

$$p_\infty(t)=1+P_{A1}\sin(\omega_1 t)+P_{A2}\sin(\omega_2 t+\theta).$$

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# Equation of state

Tait equation of state

$$p = B\left(\frac{\rho}{\rho_0}\right)^{\gamma} - B + A, \qquad \gamma = 7.15, \quad A = 1 \times 10^5\,\text{Pa}, \quad B = 3.31 \times 10^8\,\text{Pa}$$

Stiffened gas equation of state

$$p = (\gamma - 1)\rho e - p_\infty$$

- Water: $\gamma = 4.4$ and $p_\infty = 6 \times 10^8\,\text{Pa}$
- Air: $\gamma = 1.4$ and $p_\infty = 0\,\text{Pa}$

# Spam

1[1]

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