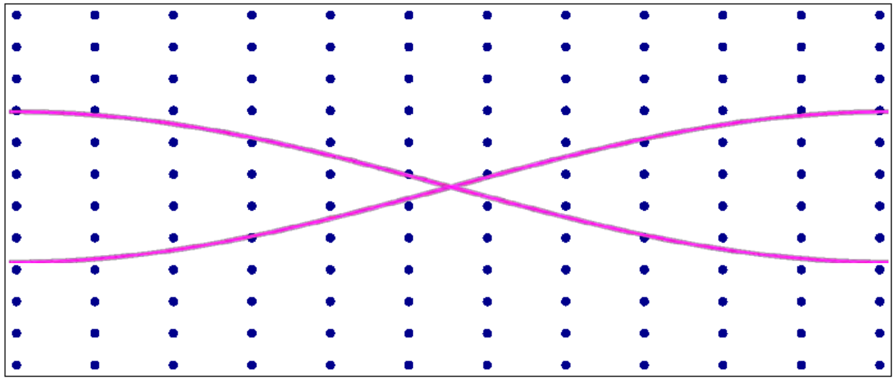
COMSOL analysis of acoustic streaming and microparticle acoustophoresis

COMSOL Conference, Milano Italy, 11 October 2012



Peter Barkholt Muller[a], Rune Barnkob[a],
Mads J. Herring Jensen[b], and Henrik Bruus[a]

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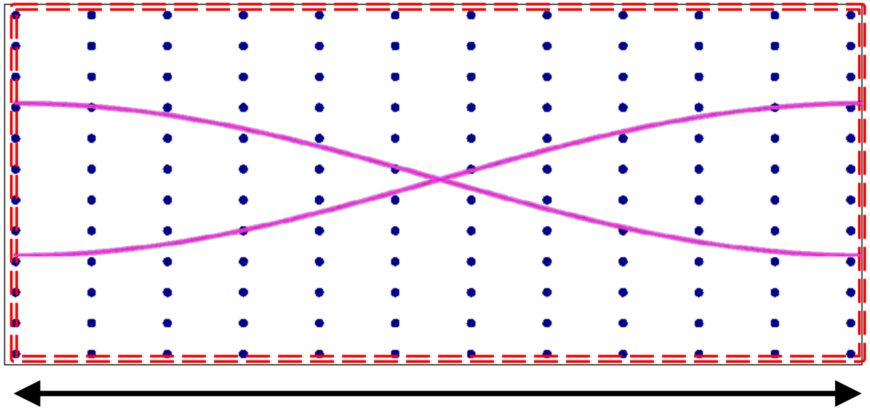
[b] COMSOL A/S, Kongens Lyngby, Denmark

Excerpt from the Proceedings of the 2012 COMSOL Conference in Milan

Introduction

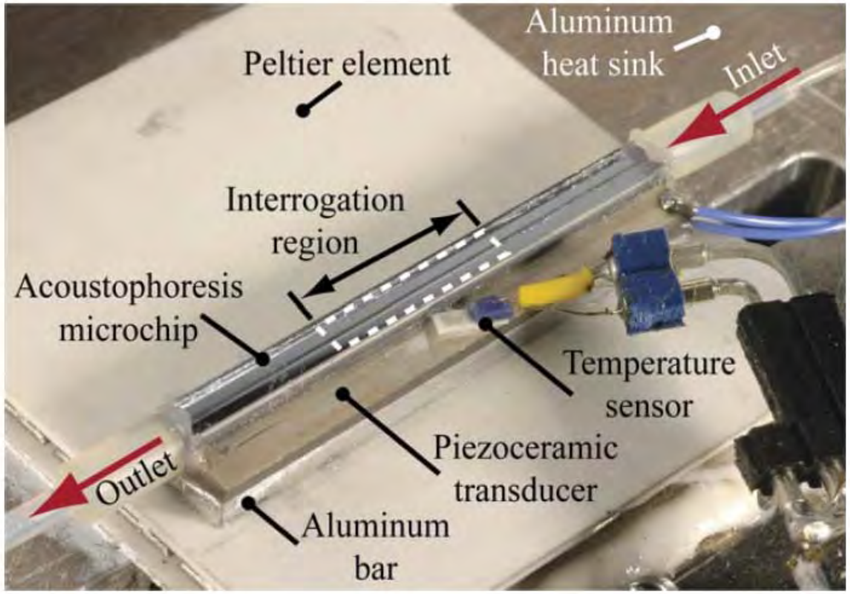
- **Acoustophoresis**
  - **Particle migration by sound**
  - Acoustic streaming (bulk flow driven at walls)
  - Acoustic radiation forces (sound scattering off particles)
- Applications
  - Ultrasound acoustofluidics
  - Non-invasive cell manipulation
  - Lab-on-a-chip
- Numerical simulations
  - Design and optimization
  - Acquire fundamental insight

Cross section



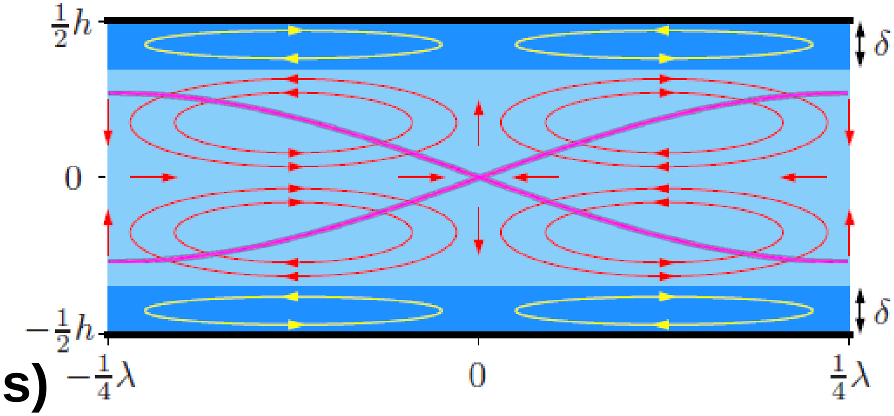
$\lambda/2 = 0.38$ mm

$c_s = 1495$ m/s $f = 1.95$ MHz



P. Augustsson, R. Barnkob,
S.T. Wereley, H. Bruus, and T. Laurell
Lab Chip **11**, 4152-4164 (2011)

Introduction



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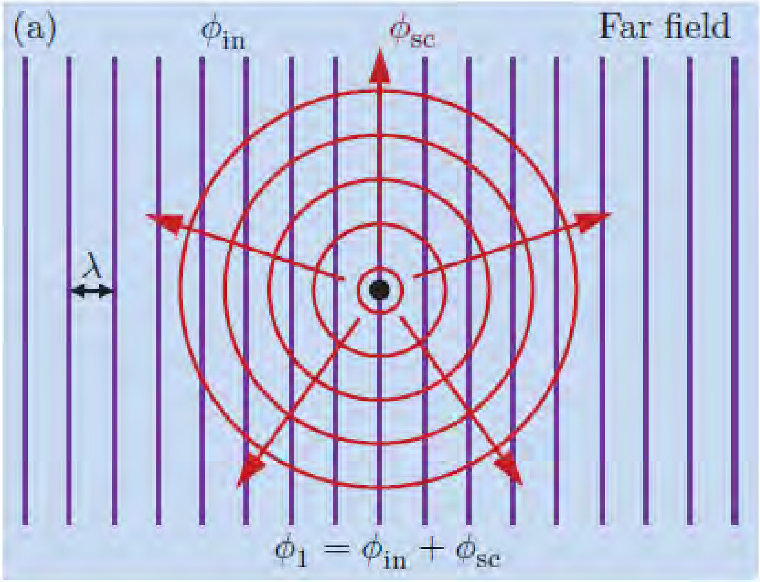

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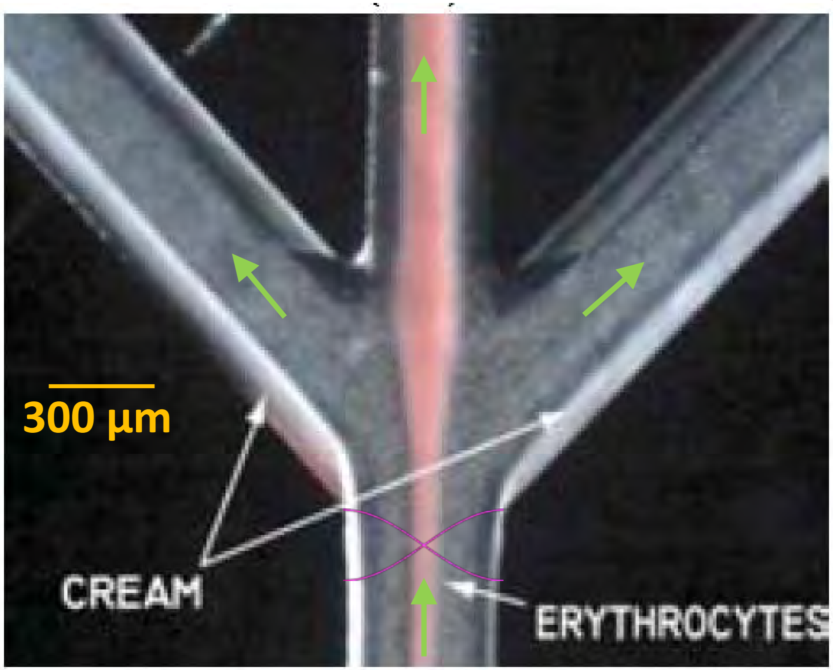
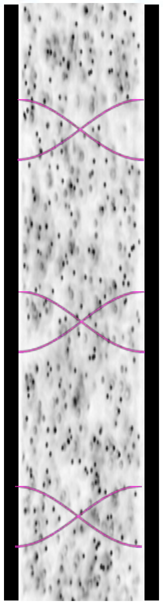
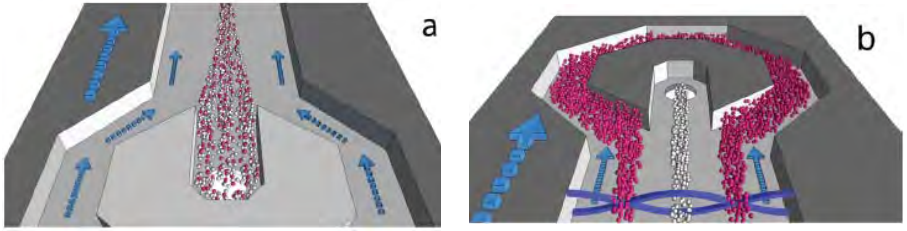


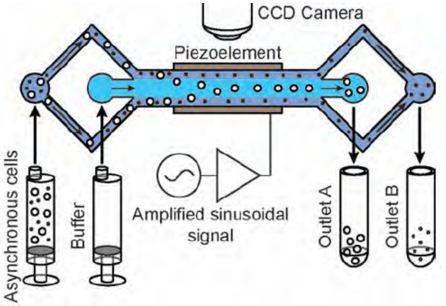


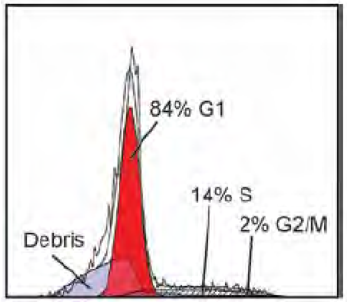
F. Petersson,
A. Nilsson,
C. Holm,
H. Jönsson &
T. Laurell
The Analyst
129, 938-943
(2004)

Introduction

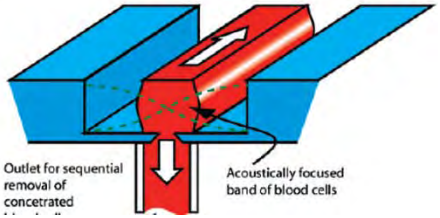


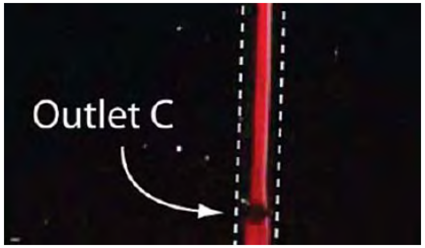
Grenvall, Augustsson, Folkenberg, and Laurell
Foss Analytics DK / Lund U
Raw milk quality control
Anal. Chem. **81**, 6195 (2009)





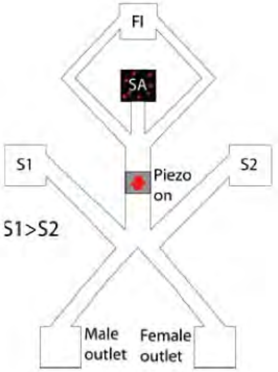
Thévoz, Adams, Shea, Bruus, and Soh
UCSB / DTU
Acoustophoretic synchronization of cells
Anal Chem **82**, 3094 (2010)



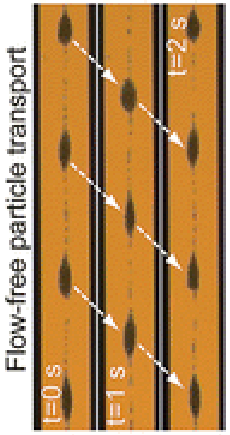


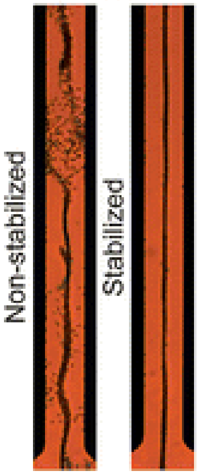
Lenshof, Lilja, Laurell *et al.*
Lund U / MSK Cancer Center NY
Whole blood plasmapheresis chip
Anal. Chem. **81**, 6030 (2009)

Barnkob, Augustsson, Laurell, and Bruus
Lund U / DTU
***In-situ* measurements of the local pressure**
Lab Chip **10**, 563 (2010)



Norris, Evander, Horsman-Hall, Nilsson, Laurell, and Landers
Univ Virginia / Lund U
Forensic analysis of sex assaults
Anal. Chem. **81**, 6089 (2009)





Manneberg, Wiklund *et al.*
KTH
Flow-free cell transport
Lab Chip **9**, 833 (2009)

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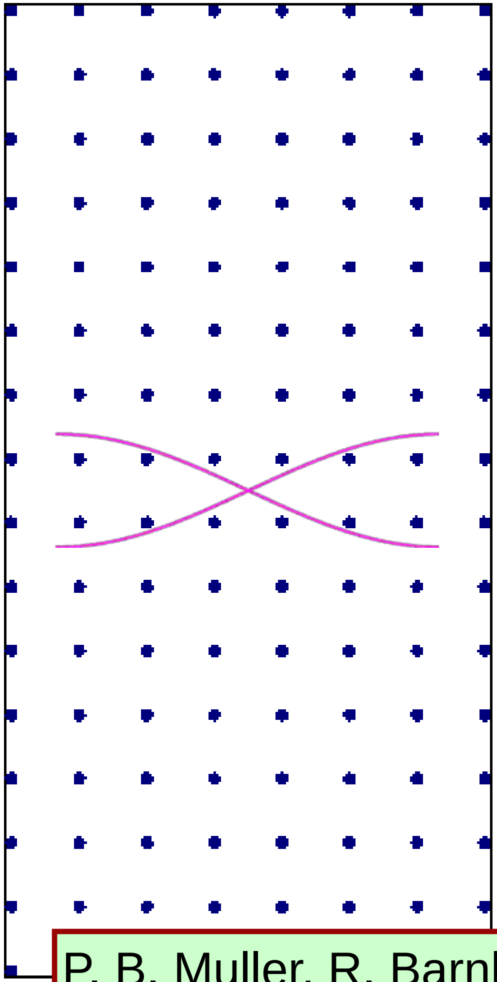

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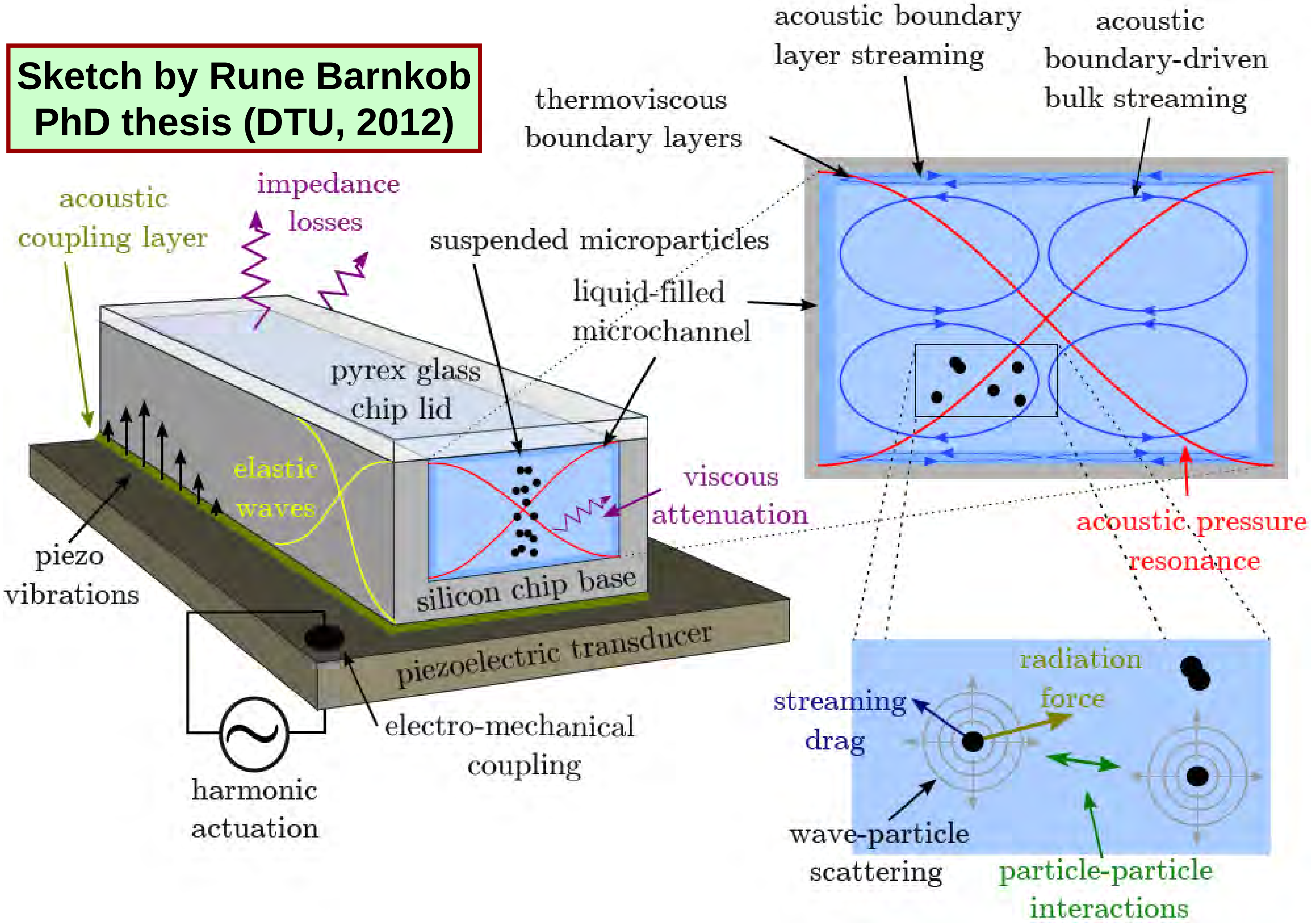
M. J. H. Jensen, and H. Bruus
Lab Chip **12**, online (2012)

Introduction

Sketch by Rune Barnkob PhD thesis (DTU, 2012)



Thermoacoustics
in first-order perturbation theory

- **Governing equations**

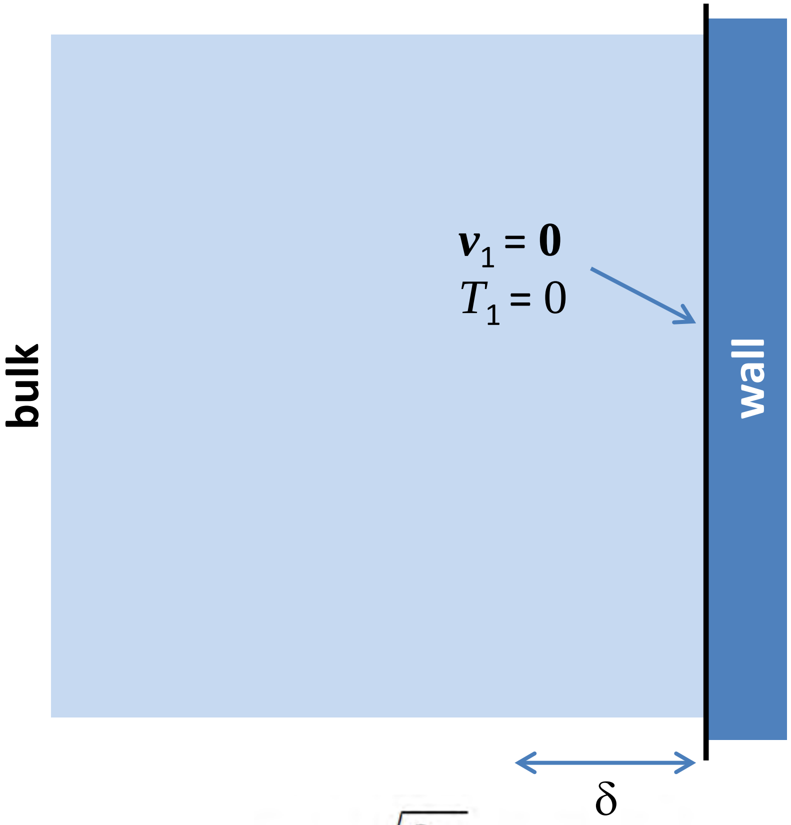
$$
\begin{aligned}
T &= T_0 + T_1 + \cancel{T_2},\\
p &= p_0 + p_1 + \cancel{p_2},\\
\boldsymbol{v} &= \mathbf{0} + \boldsymbol{v}_1 + \cancel{\boldsymbol{v}_2}.
\end{aligned}
$$

$$
\boxed{
\begin{aligned}
\partial_t T_1 &= D_{\mathrm{th}} \nabla^2 T_1 + \frac{\alpha T_0}{\rho_0 c_p}\, \partial_t p_1,\\
\partial_t p_1 &= \frac{1}{\gamma\kappa}\Big[\alpha \partial_t T_1 - \boldsymbol{\nabla}\cdot \boldsymbol{v}_1\Big],\\
\rho_0 \partial_t \boldsymbol{v}_1 &= -\boldsymbol{\nabla} p_1 + \eta \nabla^2 \boldsymbol{v}_1 + \beta\eta\, \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot \boldsymbol{v}_1).
\end{aligned}
}
$$

$$\partial_t p_1 = -\mathrm{i}\omega p_1$$

$$\nabla^2 p_1 + k_0^2 p_1 = 0$$

$$k_0 = \omega / c_0$$



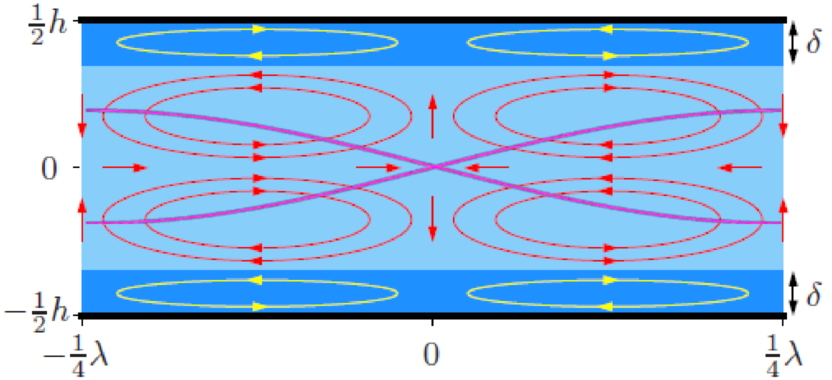
$$\delta = \sqrt{\frac{2\nu}{\omega}} = 0.38\ \mu\mathrm{m}$$

for water at 20 ºC and *f* = 2 MHz

Acoustic streaming in second-order perturbation theory

- **Governing equations**

$$\begin{aligned}\partial_t\rho_2 &= -\rho_0\boldsymbol{\nabla}\cdot\boldsymbol{v}_2 - \boldsymbol{\nabla}\cdot(\rho_1\boldsymbol{v}_1),\\ \rho_0\partial_t\boldsymbol{v}_2 &= -\boldsymbol{\nabla}p_2 + \eta\nabla^2\boldsymbol{v}_2 + \beta\eta\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}_2)\\ &\quad - \rho_1\partial_t\boldsymbol{v}_1 - \rho_0(\boldsymbol{v}_1\cdot\boldsymbol{\nabla})\boldsymbol{v}_1,\end{aligned}$$



Sketch of the classical Rayleigh-Schlichting streaming pattern in a parallel-plate geometry

- **Time averaging over one period**

µs time scale of the ultrasound is not resolved

$$\begin{aligned}\rho_0\langle\boldsymbol{\nabla}\cdot\boldsymbol{v}_2\rangle &\boxed{= -\langle\boldsymbol{\nabla}\cdot(\rho_1\boldsymbol{v}_1)\rangle,}\\ \eta\nabla^2\langle\boldsymbol{v}_2\rangle + \beta\eta\boldsymbol{\nabla}\Big(\boldsymbol{\nabla}\cdot\langle\boldsymbol{v}_2\rangle\Big) - \langle\boldsymbol{\nabla}p_2\rangle &\\ \boxed{= \langle\rho_1\partial_t\boldsymbol{v}_1\rangle + \rho_0\langle(\boldsymbol{v}_1\cdot\boldsymbol{\nabla})\boldsymbol{v}_1\rangle.}&\end{aligned}$$

Thermal second-order effects ignored but see
Rednikov and Sadhal, JFM **667**, 426 (2011)

The acoustic radiation and drag force on a small particle in a viscous fluid for $\boxed{a,\delta << \lambda}$

- **Radiation force:**

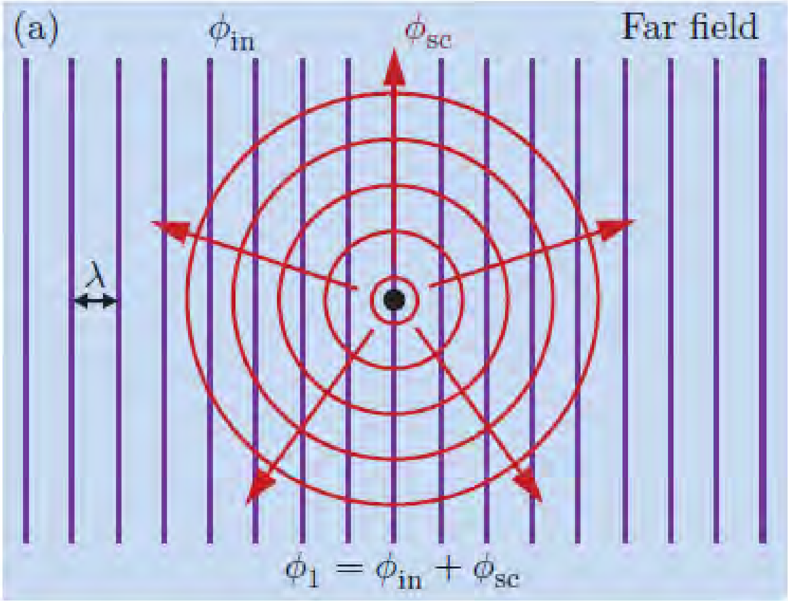
$$\boldsymbol{F}^{\mathrm{rad}} = -\pi a^3 \left[\frac{2\kappa_0}{3} \mathrm{Re}\left[f_1^* p_1^* \boldsymbol{\nabla} p_1\right] - \rho_0 \mathrm{Re}\left[f_2^* \boldsymbol{v}_1^* \cdot \boldsymbol{\nabla} \boldsymbol{v}_1\right] \right]$$

$$f_1(\tilde{\kappa}) = 1 - \tilde{\kappa}, \qquad \text{with } \tilde{\kappa} = \frac{\kappa_\mathrm{p}}{\kappa_0},$$

$$f_2(\tilde{\rho}, \tilde{\delta}) = \frac{2\left[1-\gamma(\tilde{\delta})\right](\tilde{\rho}-1)}{2\tilde{\rho} + 1 - 3\gamma(\tilde{\delta})}, \qquad \text{with } \tilde{\rho} = \frac{\rho_\mathrm{p}}{\rho_0},$$

$$\gamma(\tilde{\delta}) = -\frac{3}{2}\left[1 + \mathrm{i}(1+\tilde{\delta})\right]\tilde{\delta}, \qquad \text{with } \tilde{\delta} = \frac{\delta}{a}.$$

M. Settnes and H. Bruus
Phys. Rev. E **85**, 016327 (2012)



- **Drag force:** $\boldsymbol{F}^{\mathrm{drag}} = 6\pi\eta a\left(\langle \boldsymbol{v}_2 \rangle - \boldsymbol{u}\right)$

- **Coefficients:**

$$\Phi(\tilde{\kappa}, \tilde{\rho}, \tilde{\delta}) = \frac{1}{3} f_1(\tilde{\kappa}) + \frac{1}{2} \mathrm{Re}\left[f_2(\tilde{\rho}, \tilde{\delta})\right]$$

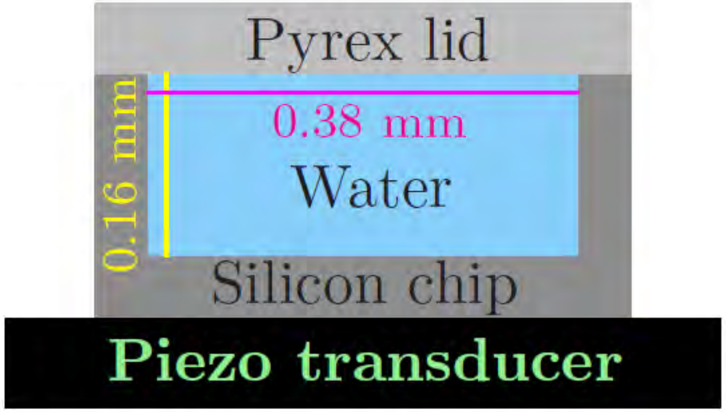
Critical particle size is given by $F^{\mathrm{rad}} = F^{\mathrm{drag}}$

or

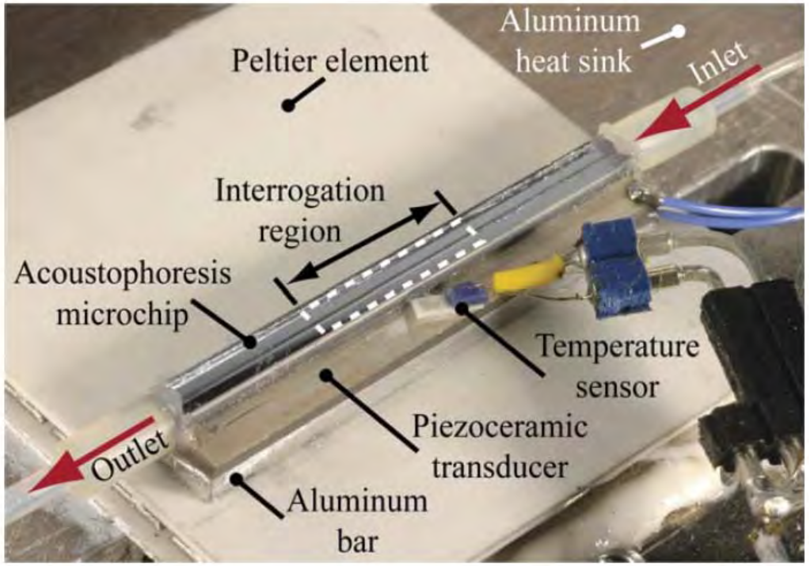
$$2a_c = \sqrt{12 \frac{\Psi}{\Phi} \delta} \approx 2.0\ \mu\mathrm{m}$$

The model system:
a straight rectangular channel in silicon/glass

End view



2D cross section of a long, straight rectangular channel



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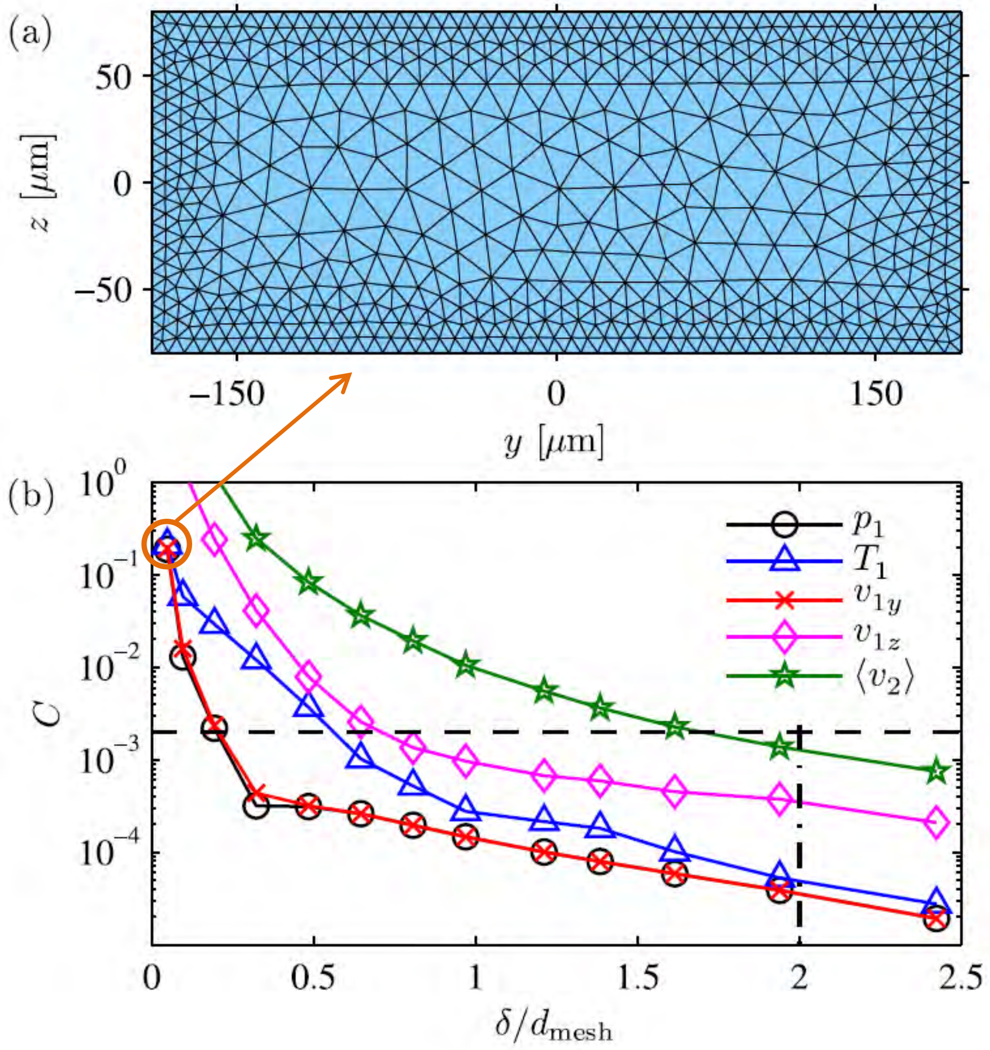
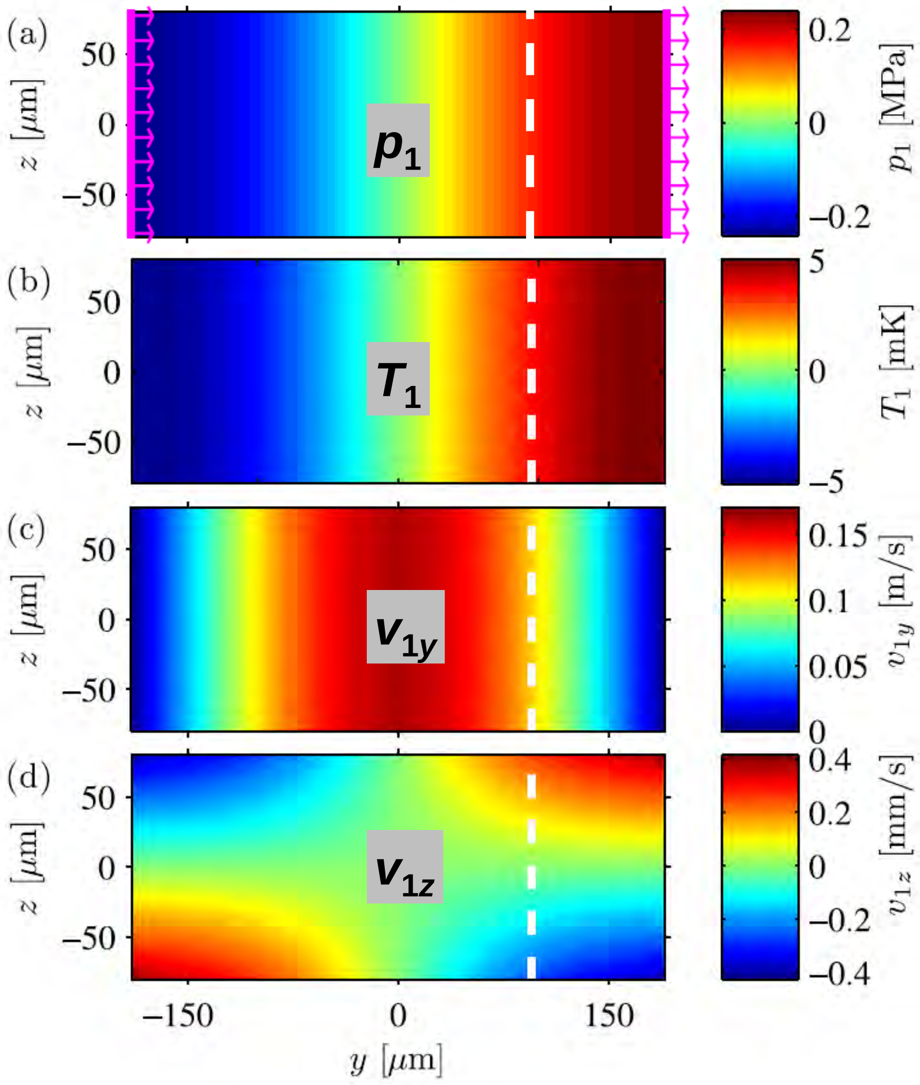
H. Bruus, and T. Laurell,
Lab Chip **11**, 4152-4164 (2011)

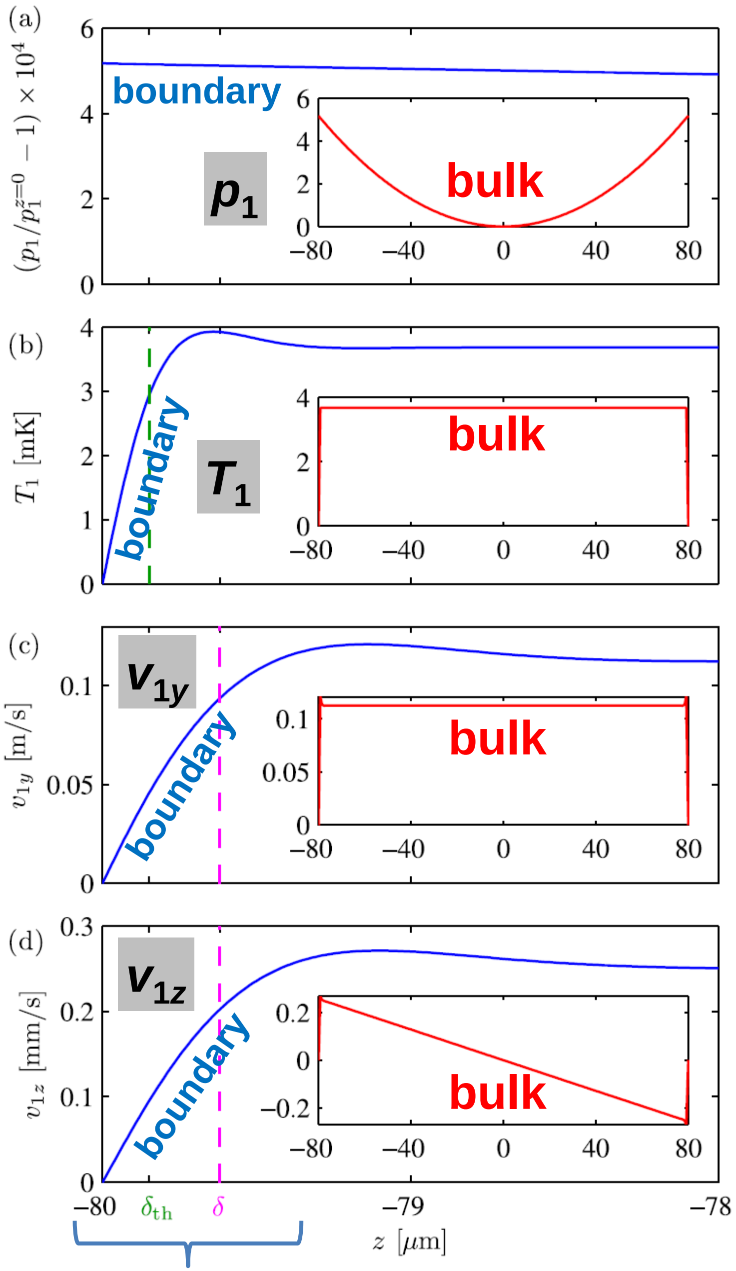
Numerical procedure using COMSOL

- **COMSOL Multiphysics**
  - **Finite element program**
  - **User defined equations and expressions**
- **First order fields**
  - **Thermoacoustics**
- **Second order fields**
  - **Flow with sources**
- **Forces on particles**
  - **Radiation force**
  - **Stokes drag force**
- **Transient particle tracing**
- **Mesh**
  - **Several length scales**
  - **Acoustic boundary layer**
  - **Mesh convergence test!!**



Results: First-order field amplitudes

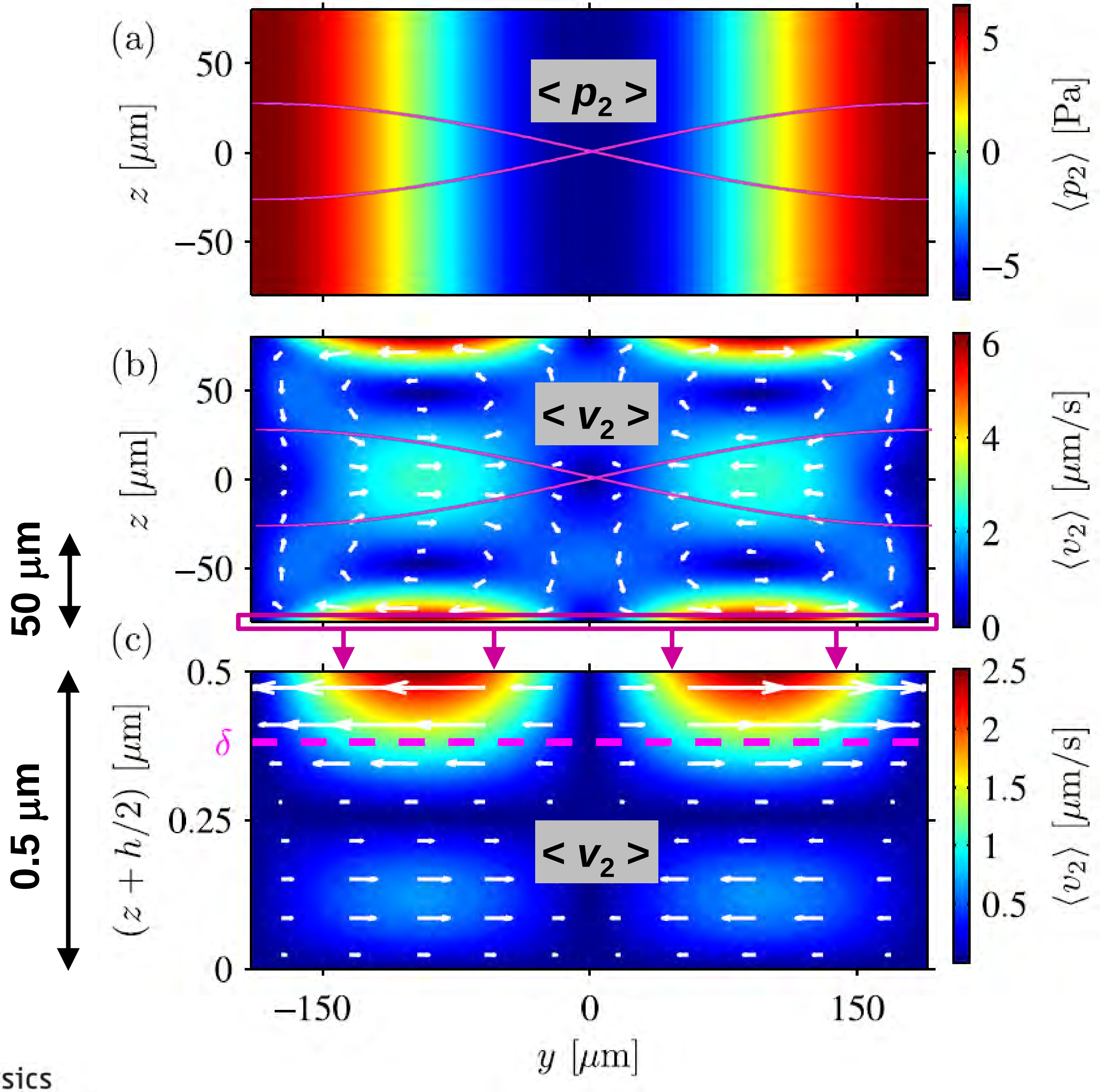




boundary layer

$$\delta_{\mathrm{th}} = \sqrt{\frac{2D_{\mathrm{th}}}{\omega}} = 0.15\ \mu\mathrm{m}, \quad \text{and} \quad \delta = \sqrt{\frac{2\nu}{\omega}} = 0.38\ \mu\mathrm{m}$$

Results: Second-order time-averaged fields

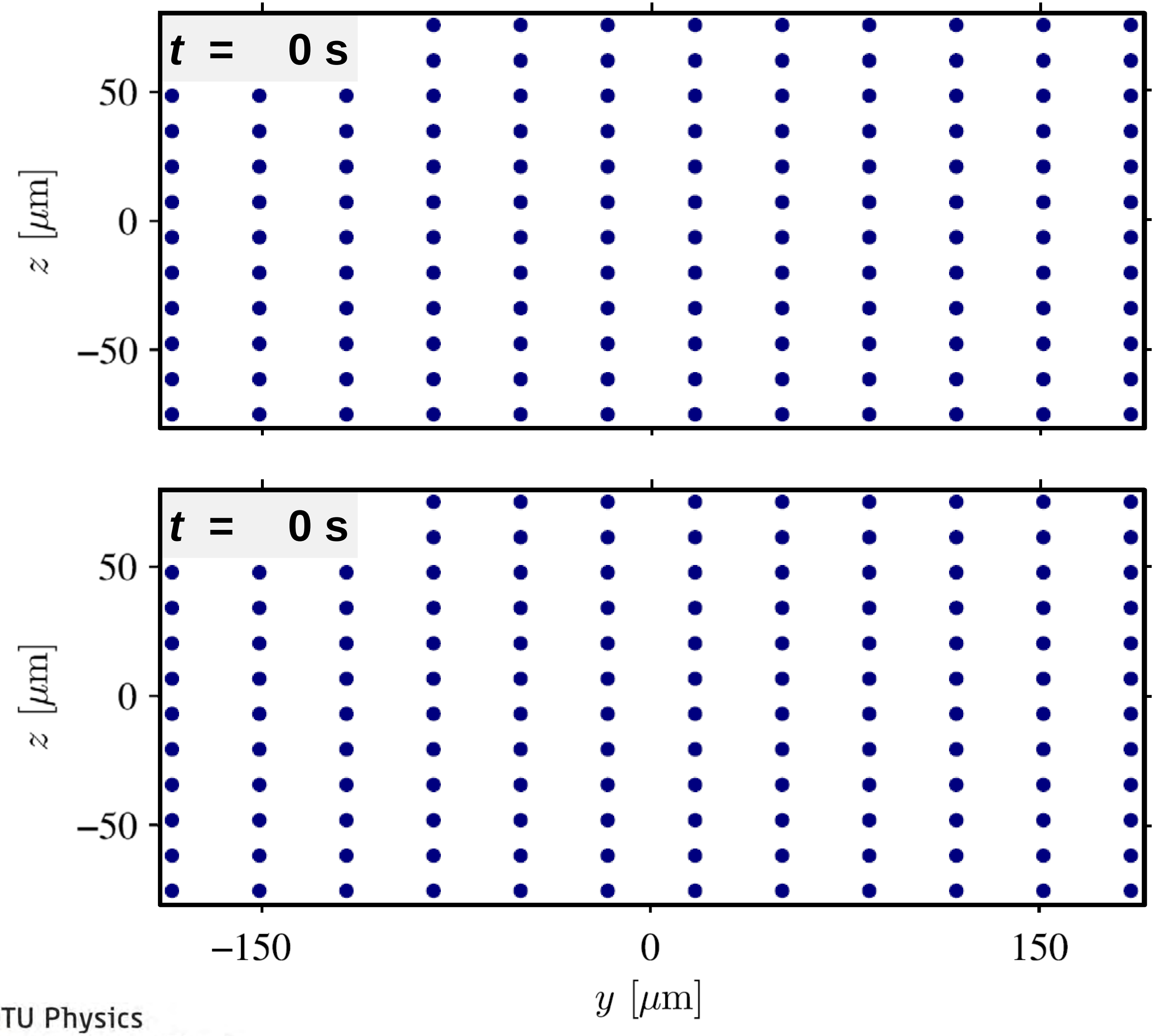


Bulk field:
no stretching

Bulk field:
no stretching

Boundary field:
***z*-axis stretched**
by a factor 1000

Results: Particle tracing animations



***2a* = 0.5 µm**

Critical particle size is given by

$$F^{\text{rad}} = F^{\text{drag}}$$

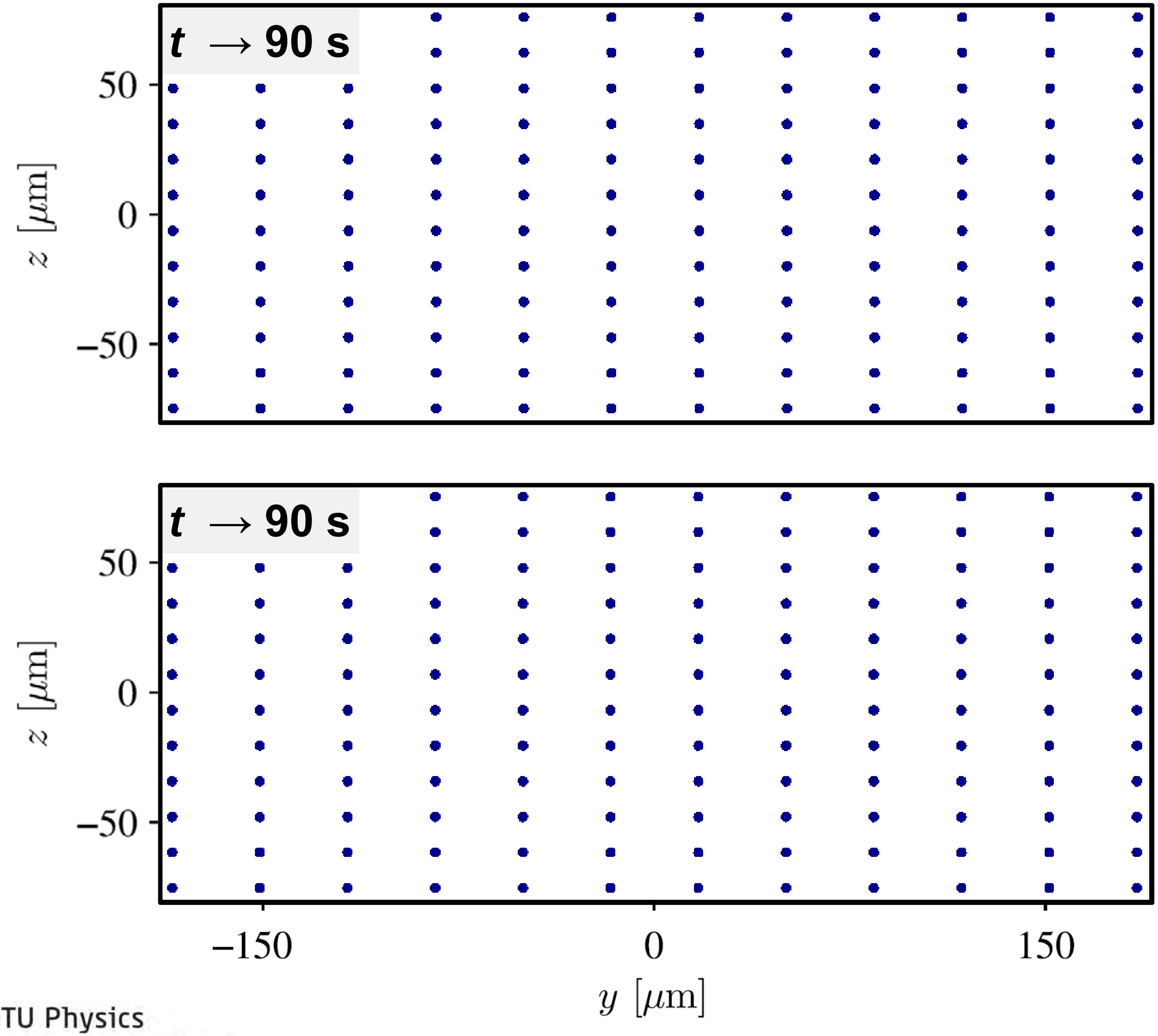
or

$$2a_c = \sqrt{12\frac{\Psi}{\Phi}\,\delta}$$

$$\approx 2.0\ \mu\text{m}$$

***2a* = 5.0 µm**

Results: Particle tracing animations



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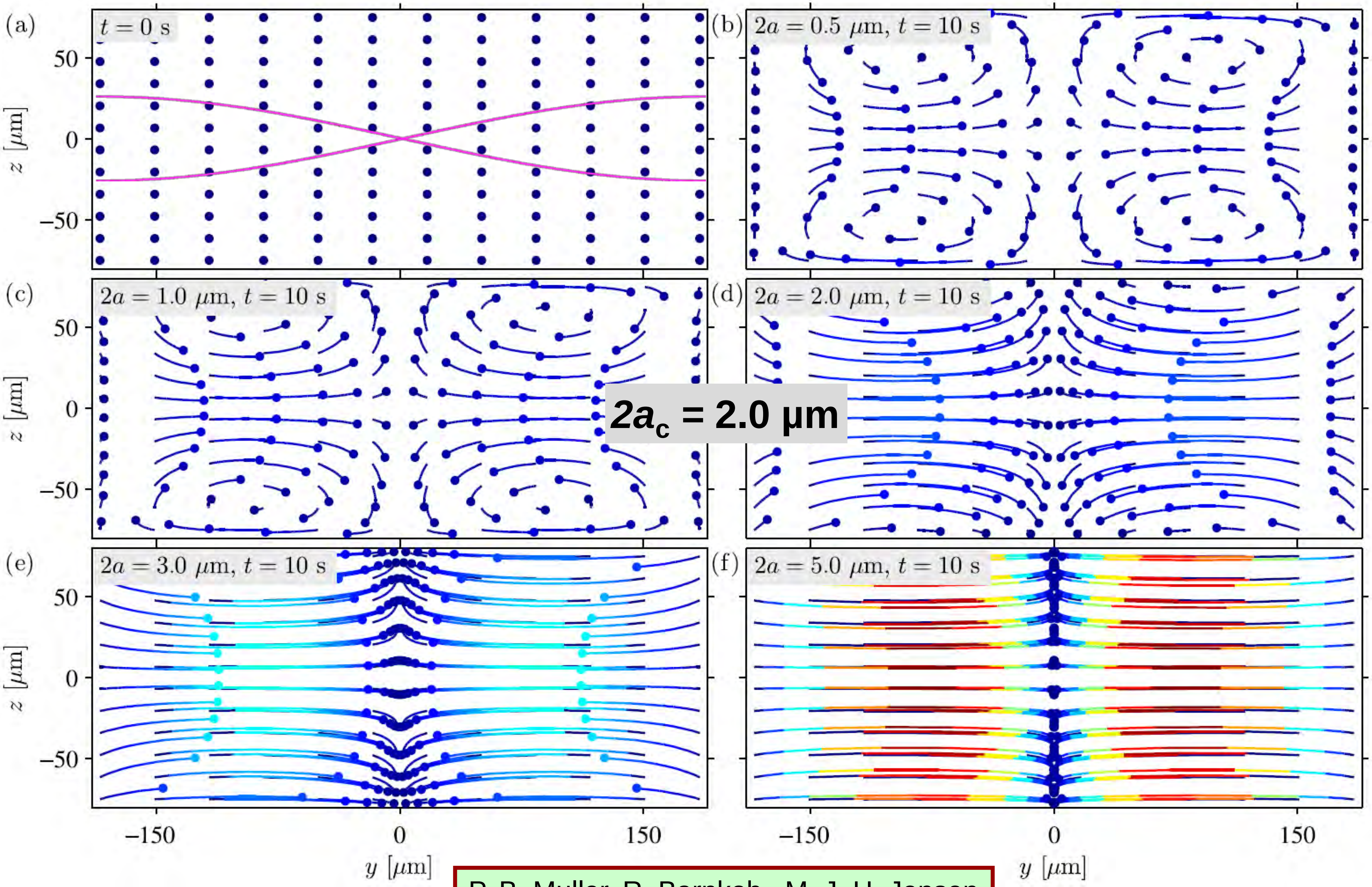
$$\approx 2.0\ \mu\text{m}$$

***2a* = 5.0 µm**

Results: Particle tracing gallery



$2a_c$ = 2.0 µm

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Conclusion

- **Implementation and numerical solution of:**
  - **Acoustophoretic motion of particles**
  - **Second-order acoustic phenomena**
  - **Streaming**
  - **Radiation forces**
  - **Second-order thermal effects need to be incorporated**

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Lab Chip **12**, online (2012)

- **Application to a relevant geometry**
  - **Motion dependent on particle size**
  - **Development and design of lab-on-a-chip systems**
  - **Elasticity of the walls needs to be incorporated**

- **3D measurements of acoustophoresis needed**
  - **New collaboration between the groups of**
    Laurell (Lund University, Sweden)
    Kähler (Universität der Bundeswehr, Germany)
    Bruus (Technical University of Denmark, Denmark)