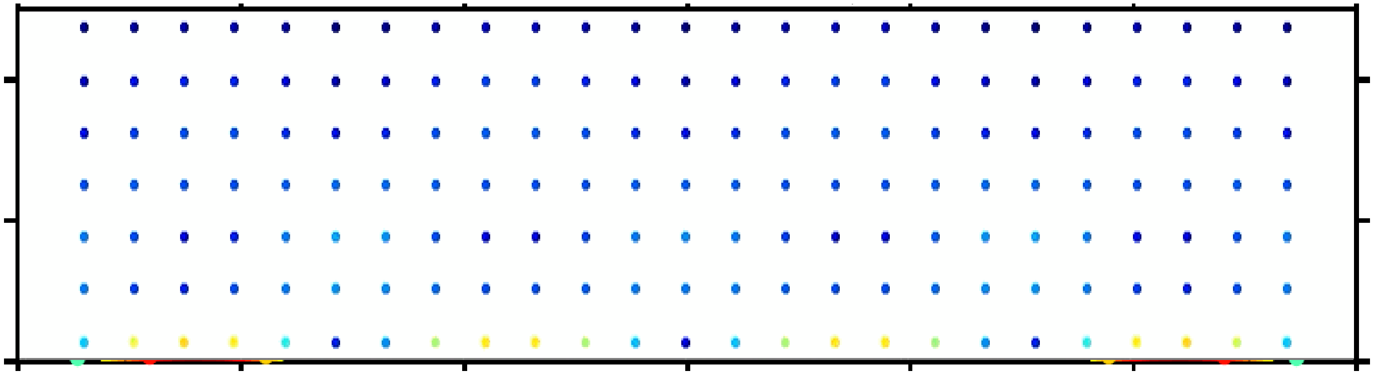
COMSOL
CONFERENCE
2015 BOSTON

Simulation of SAW-Driven Microparticle Acoustophoresis Using COMSOL Multiphysics®



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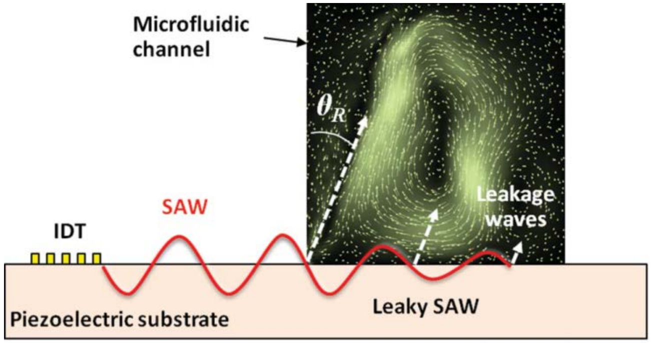
Outline

- Introduction
- Numerical scheme
- Model validation
- COMSOL Modeling and convergence
- Results
- Conclusion and Outlook

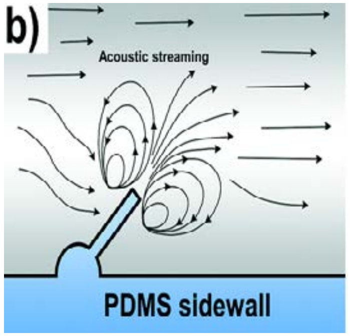
Acoustofluidics

Integration of acoustics with microfluidics

Acoustic Streaming



Ding et al, Lab on a Chip, 2012.



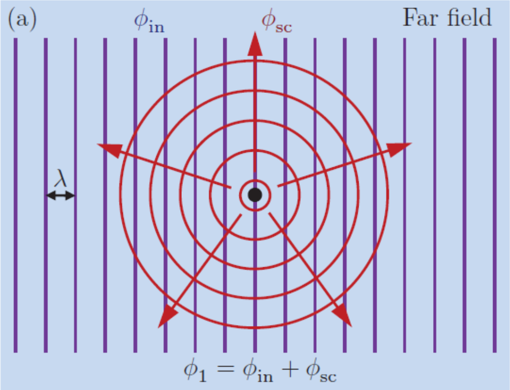
Tatsuno et al, Album Fluid Motion, 1982.

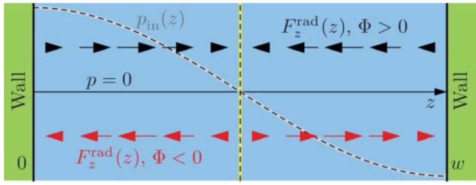
Huang et al, Lab on a Chip, 2014.

- Oscillating boundaries
- Time-averaged motion of the fluid

Useful for fluid and particle manipulation

Acoustic Radiation Force





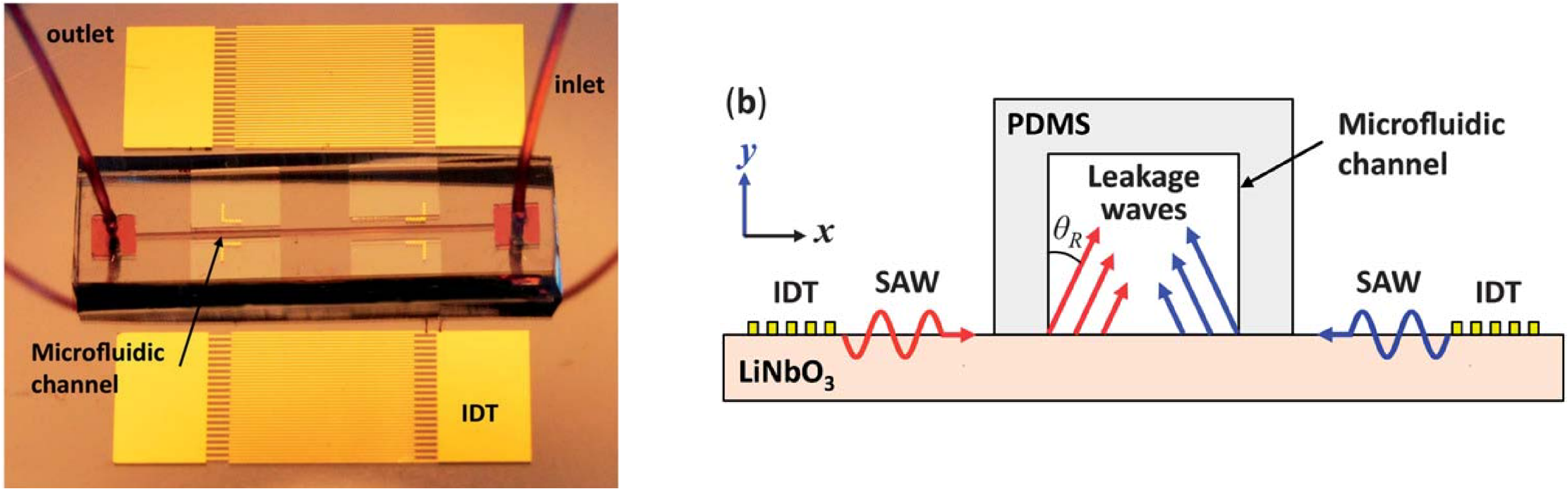
$$\boldsymbol{F}^{\mathrm{rad}} = -\pi a^3 \left[\frac{2\kappa_0}{3} \mathrm{Re}[f_1^* p_{\mathrm{in}}^* \boldsymbol{\nabla} p_{\mathrm{in}}] - \rho_0 \mathrm{Re}[f_2^* \boldsymbol{v}_{\mathrm{in}}^* \cdot \boldsymbol{\nabla} \boldsymbol{v}_{\mathrm{in}}] \right]$$

M. Settnes and H. Bruus, Phys Rev E, 2012.

- Scattering of incident acoustic waves from the particles
- ARF acting towards pressure node or antinode

Surface Acoustic Wave (SAW)

- Surface Acoustic Wave (SAW) systems have gained prominence for various lab-on-a-chip applications.

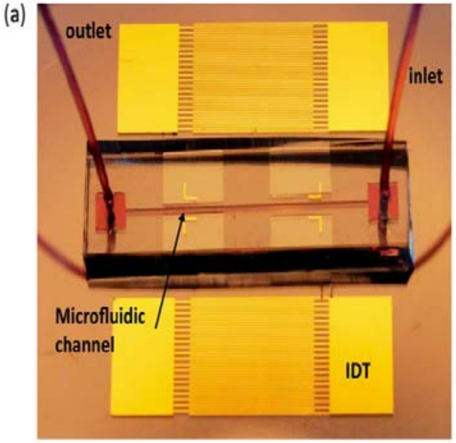


Typical SAW device

Questions:

- Type of acoustic fields setup inside the channel?
- Effect of PDMS walls as opposed to harder materials (e.g. silicon)
- Critical transition size for particle motion inside the microchannel?

Governing equations



Balance of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

Balance of linear momentum

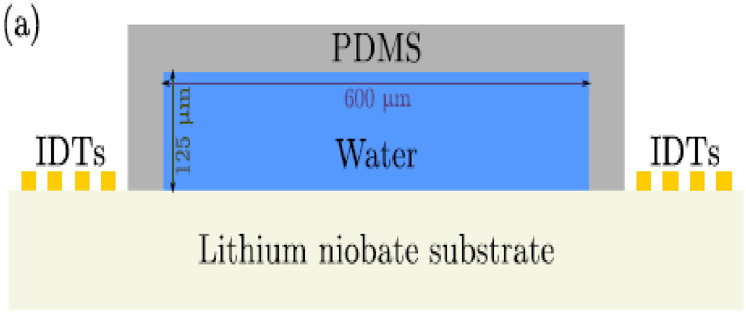
$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla p + \mu \nabla^2 \mathbf{v} + \left(\mu_b + \frac{1}{3}\mu\right)\nabla(\nabla \cdot \mathbf{v})$$

Constitutive relation

$$p = c_0{}^2 \rho$$

Numerical Challenges:

- Widely separated time scales – Characteristic oscillation period (10^{-7} s) vs. characteristic times dictated by streaming speeds (10^{-1} s)



Numerical Model

Perturbation expansion

$$\mathbf{v} = \mathbf{v}_0 + \varepsilon \tilde{\mathbf{v}}_1 + \varepsilon^2 \tilde{\mathbf{v}}_2 + O(\varepsilon^3) + \cdots$$

$$p = p_0 + \varepsilon \tilde{p}_1 + \varepsilon^2 \tilde{p}_2 + O(\varepsilon^3) + \cdots$$

$$\rho = \rho_0 + \varepsilon \tilde{\rho}_1 + \varepsilon^2 \tilde{\rho}_2 + O(\varepsilon^3) + \cdots$$

Isentropic, compressible Newtonian fluid

First-order equations

$$\frac{\partial \rho_1}{\partial t} + \rho_0 (\nabla \cdot \mathbf{v}_1) = 0,$$

$$\rho_0 \frac{\partial \mathbf{v}_1}{\partial t} = -\nabla p_1 + \mu \nabla^2 \mathbf{v}_1 + (\mu_b + \tfrac{1}{3}\mu) \nabla (\nabla \cdot \mathbf{v}_1)$$

No background flow

Second-order equations

$$\left\langle \frac{\partial \rho_2}{\partial t} \right\rangle + \rho_0 \nabla \cdot \langle \mathbf{v}_2 \rangle = -\nabla \cdot \langle \rho_1 \mathbf{v}_1 \rangle$$

$$\rho_0 \left\langle \frac{\partial \mathbf{v}_2}{\partial t} \right\rangle + \left\langle \rho_1 \frac{\partial \mathbf{v}_1}{\partial t} \right\rangle + \rho_0 \langle \mathbf{v}_1 \cdot \nabla \mathbf{v}_1 \rangle = -\nabla \langle p_2 \rangle + \mu \nabla^2 \langle \mathbf{v}_2 \rangle + (\mu_b + \tfrac{1}{3}\mu) \nabla \nabla \cdot \langle \mathbf{v}_2 \rangle$$

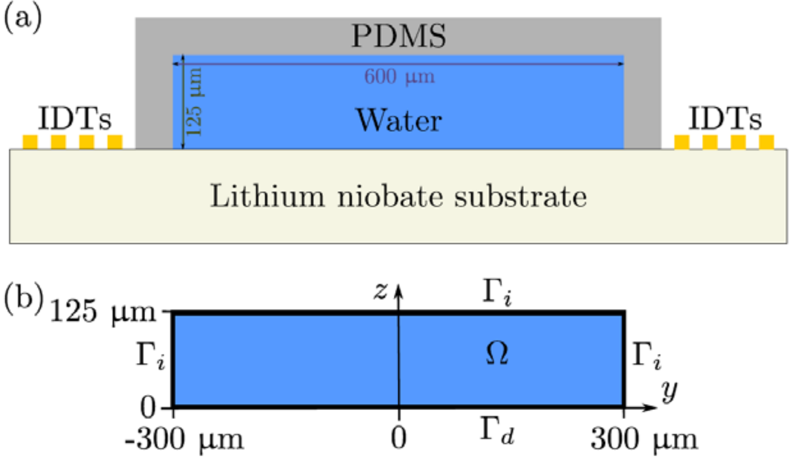
- The nonlinear problem is divided into two sets to linear equations which can be solved successively.
- Numerical Scheme: COMSOL Multiphysics 5.1 with P2-P1 elements for velocity and pressure.

Model System and Boundary conditions

Impedance condition on the channel walls (PDMS)

$$\mathbf{n}\cdot\nabla p_1 = i\frac{\omega\rho_0}{\rho_m c_m}p_1$$

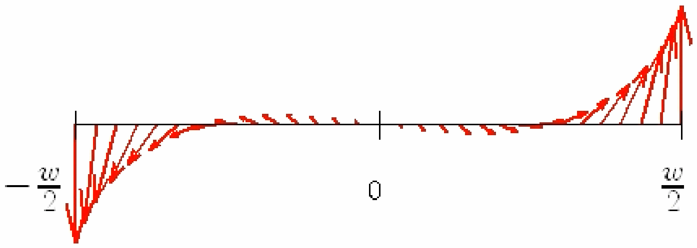
Cross-sectional View



Standing SAW displacement on the bottom wall

$$u_y(t,y) = 0.6u_0\, e^{-C_d y}\left[\sin\left(\frac{-2\pi(y-w/2)}{\lambda}+\omega t-\Delta\phi\right)\right.$$
$$\left.+\sin\left(\frac{-2\pi(w/2-y)}{\lambda}+\omega t\right)\right],$$

$$u_z(t,y) = -u_0\, e^{-C_d y}\left[\cos\left(\frac{-2\pi(y-w/2)}{\lambda}+\omega t-\Delta\phi\right)\right.$$
$$\left.+\cos\left(\frac{-2\pi(w/2-y)}{\lambda}+\omega t\right)\right],$$



The displacement on the bottom wall was adopted from the results of numerical simulations by Gantner.

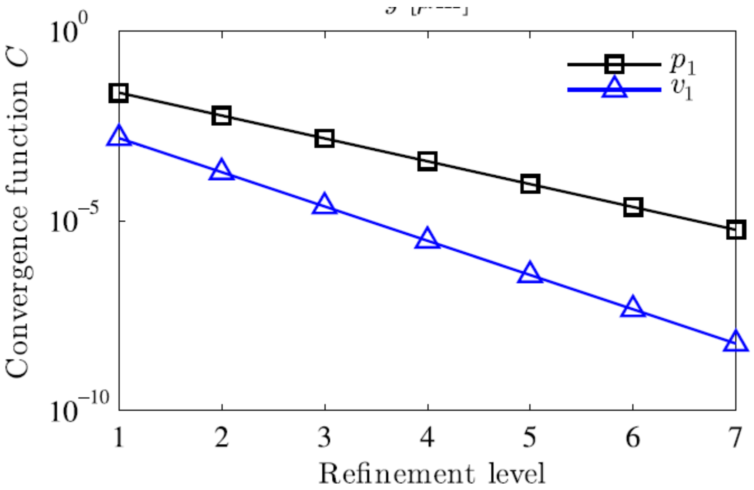
A. Gantner, Mathematical Modeling and Numerical Simulation of Piezoelectrical Agitated Surface Acoustic Waves. PhD thesis, Universitat Augsburg, Germany, 2005.

Model Validation
Method of Manufactured Solution

Step 1: Assume a solution for both pressure and velocity.

Step 2: Plug into PDEs to get the forcing and boundary conditions.

$$
\begin{aligned}
\mu_v \frac{\partial v}{\partial t} - \nu_1 \Delta v - \nu_2 \nabla(\nabla \cdot v) + \nabla p &= f_v && \text{in } \Omega,\ t > 0 \\
\mu_p \frac{\partial p}{\partial t} + \nabla \cdot v &= f_p && \text{in } \Omega,\ t > 0 \\
v &= g && \text{on } \partial\Omega,\ t > 0
\end{aligned}
$$



Step 3: Use the computed forcing and boundary conditions in the numerical model to obtain a solution.

Step 4: Compare the obtained solution with the assumed solution.

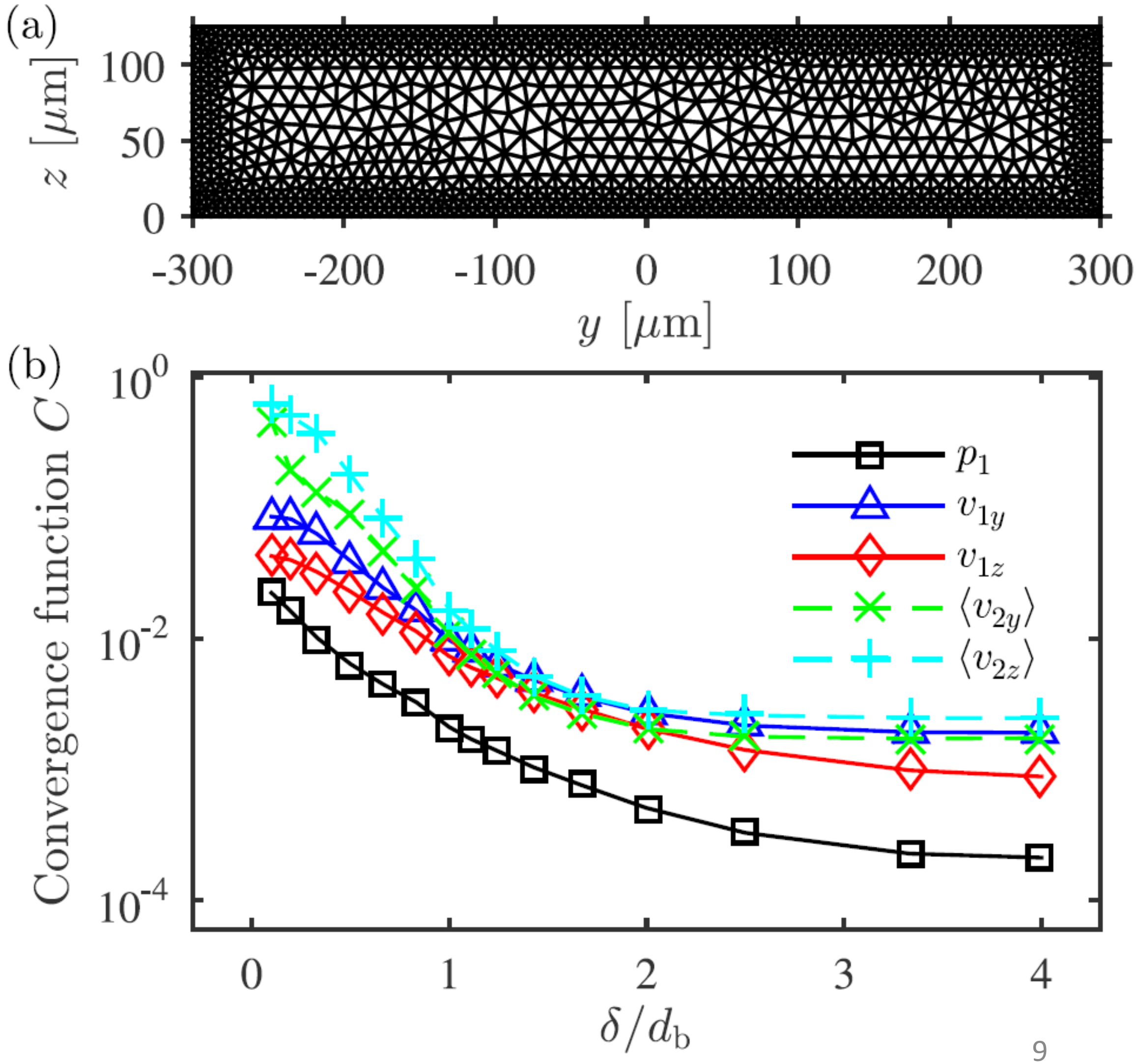
COMSOL Modeling and convergence

- *Weak PDE* interface
- Parametric sweep over mesh size.
- Finer mesh near the boundaries to resolve the boundary layers.

$$C(g) = \sqrt{\frac{\int (g - g_{\mathrm{ref}})^2 \, \mathrm{d}y \, \mathrm{d}z}{\int (g_{\mathrm{ref}})^2 \, \mathrm{d}y \, \mathrm{d}z}}$$

Here, g_{ref} = most refined solution

- Slower convergence of second-order fields since they depend on the gradients of first-order fields.

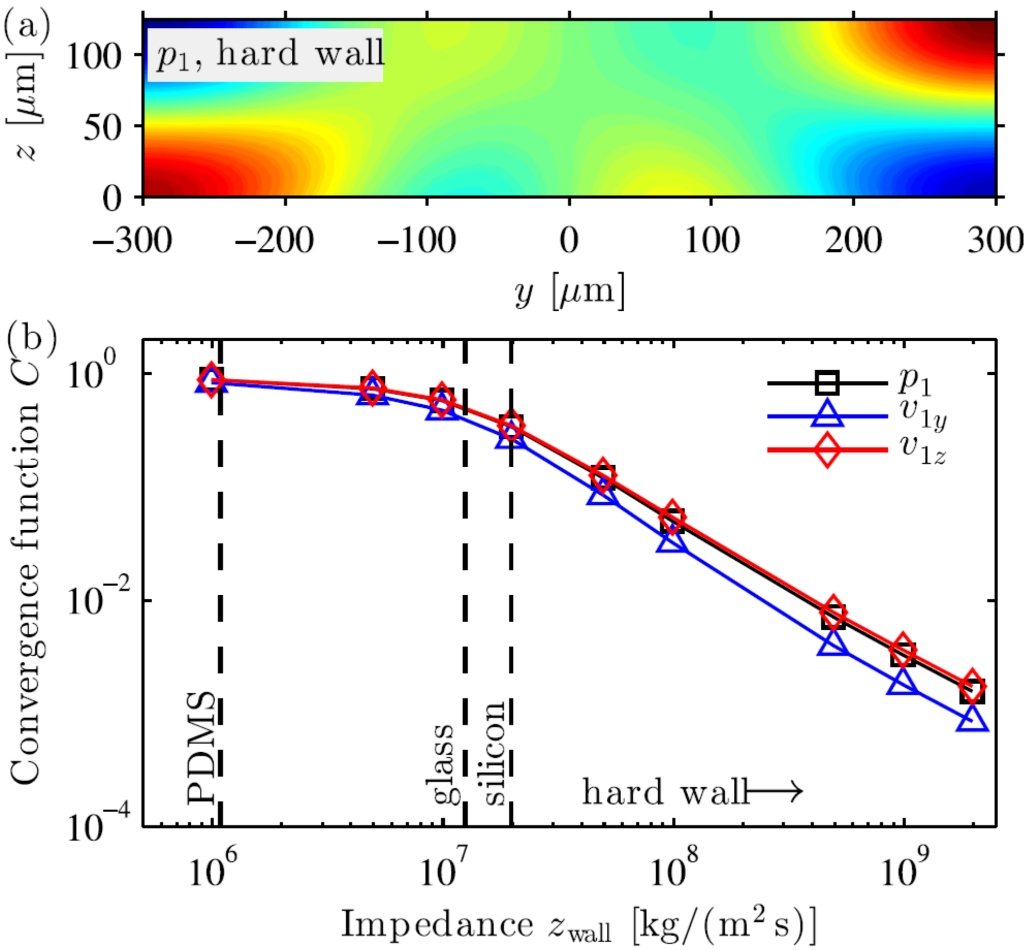


Impedance Sweep

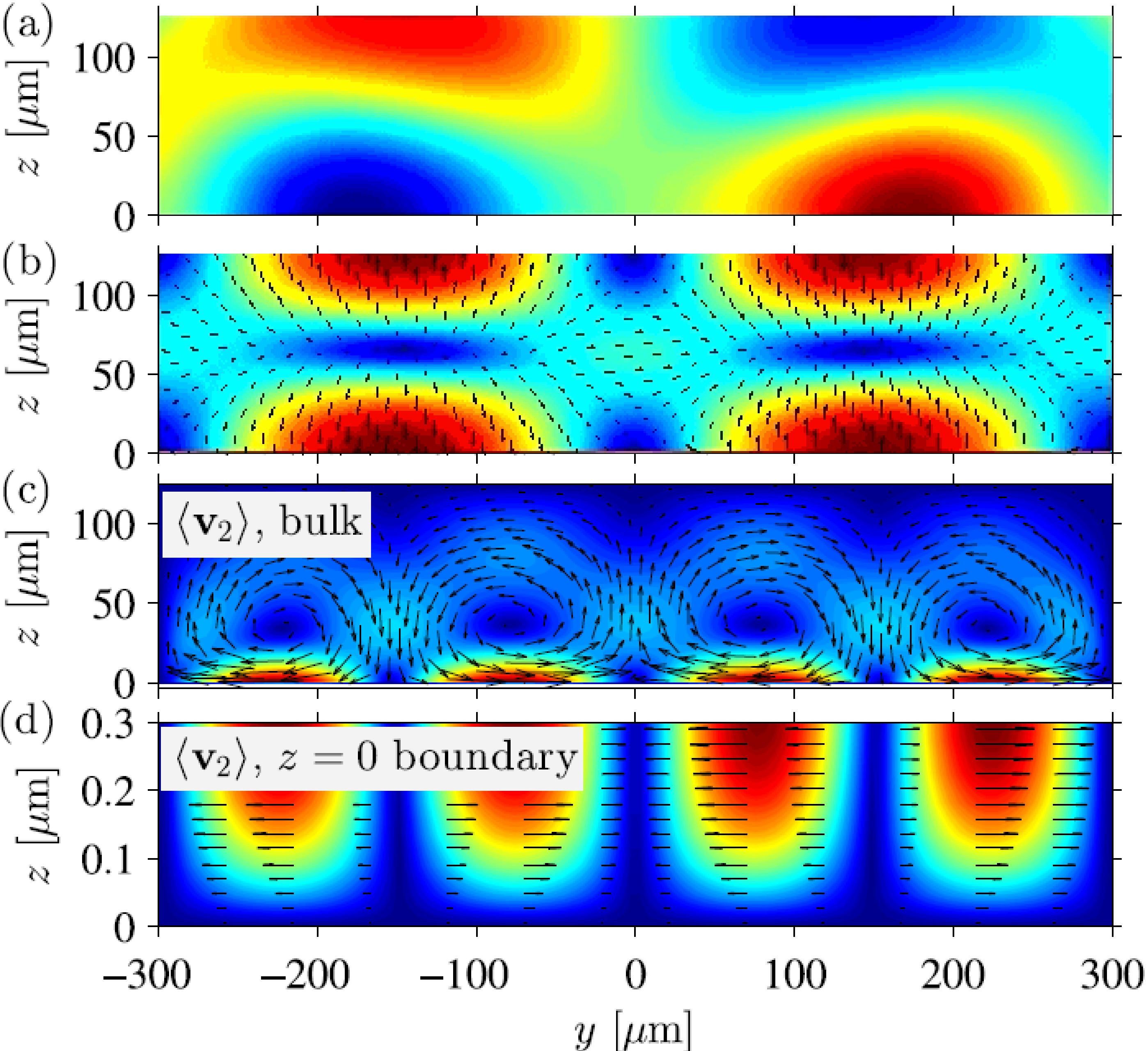
- Convergence to hard wall solution on increasing impedance of the wall.
- Resonances similar to hard wall system were observed for high values of impedances.
- Hard wall conditions suitable for bulk acoustic wave (BAW) systems but not SAW systems.

$$C(g) = \sqrt{\frac{\int (g - g_{\mathrm{ref}})^2 \,\mathrm{d}y\,\mathrm{d}z}{\int (g_{\mathrm{ref}})^2 \,\mathrm{d}y\,\mathrm{d}z}}$$

Here, g_{ref} = hard wall solution

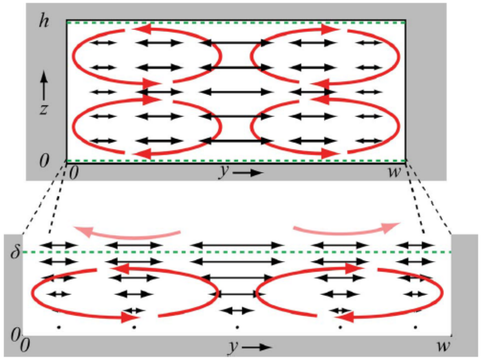


Acoustic fields



$$\mathbf{n}\cdot\nabla p_1 = i\frac{\omega\rho_0}{\rho_m c_m}p_1$$

Bulk Acoustic Wave (BAW) Device



P. Augustsson *et al*, Lab Chip, 2011, 11, 4152–4164.

$$\delta = \sqrt{\frac{2\nu}{\omega}}$$

Particle tracking

Radiation Force

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

M. Settnes and H. Bruus, Phys Rev E, vol. 85, p. 016327, 2012.

$$f_1 = 1 - \frac{\kappa_p}{\kappa_0} \quad \text{and} \quad f_2 = \frac{2(1-\gamma)(\rho_p - \rho_0)}{2\rho_p + \rho_0(1-3\gamma)}$$

$$\gamma = -\tfrac{3}{2}[1 + \imath(1+\tilde{\delta})]\tilde{\delta}, \quad \tilde{\delta} = \frac{\delta}{a}, \quad \delta = \sqrt{\frac{\mu}{\pi f \rho_0}}$$

Hydrodynamic Drag Force

$$\mathbf{F}^{\mathrm{drag}} = 6\pi\mu a\big(\langle \mathbf{v}_2 \rangle - \mathbf{v}^{\mathrm{bead}}\big)$$

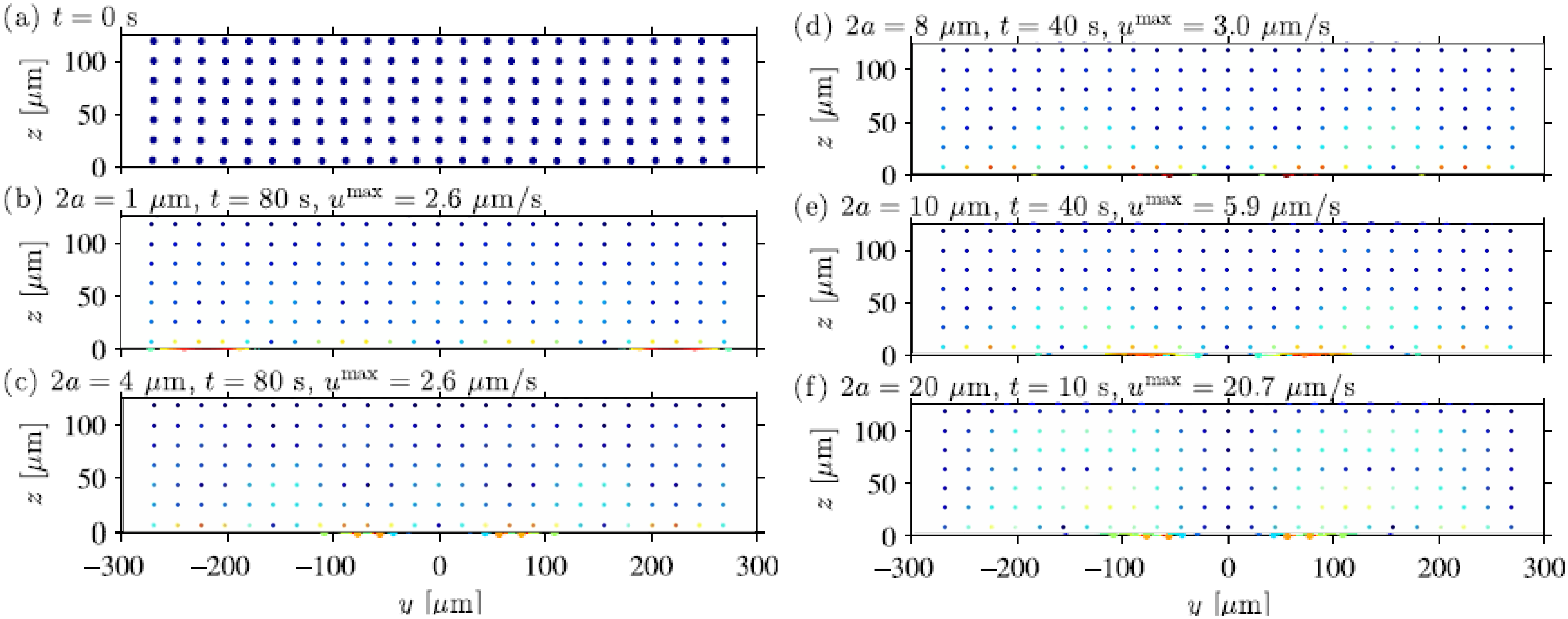
Newton's Second Law

$$m_{\mathrm{p}}\mathbf{a}_{\mathrm{p}} = \mathbf{F}^{\mathrm{rad}} + \mathbf{F}^{\mathrm{drag}}$$

Particle Velocity

$$\mathbf{v}^{\mathrm{bead}} = \langle \mathbf{v}_2 \rangle + \frac{\mathbf{F}^{\mathrm{rad}}}{6\pi\mu a}$$

Particle tracking



(a) $t = 0$ s

(b) $2a = 1\ \mu m$, $t = 80$ s, $u^{max} = 2.6\ \mu m/s$

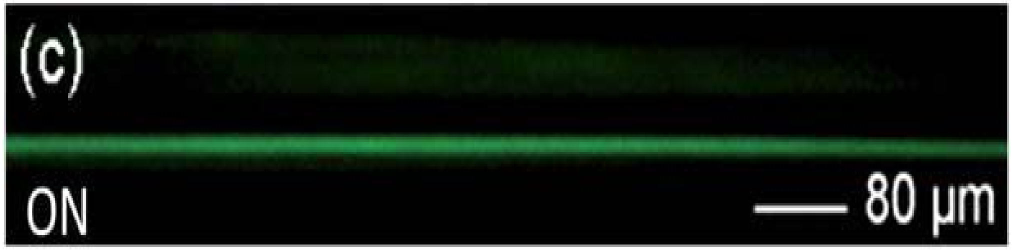
(c) $2a = 4\ \mu m$, $t = 80$ s, $u^{max} = 2.6\ \mu m/s$

(d) $2a = 8\ \mu m$, $t = 40$ s, $u^{max} = 3.0\ \mu m/s$

(e) $2a = 10\ \mu m$, $t = 40$ s, $u^{max} = 5.9\ \mu m/s$

(f) $2a = 20\ \mu m$, $t = 10$ s, $u^{max} = 20.7\ \mu m/s$

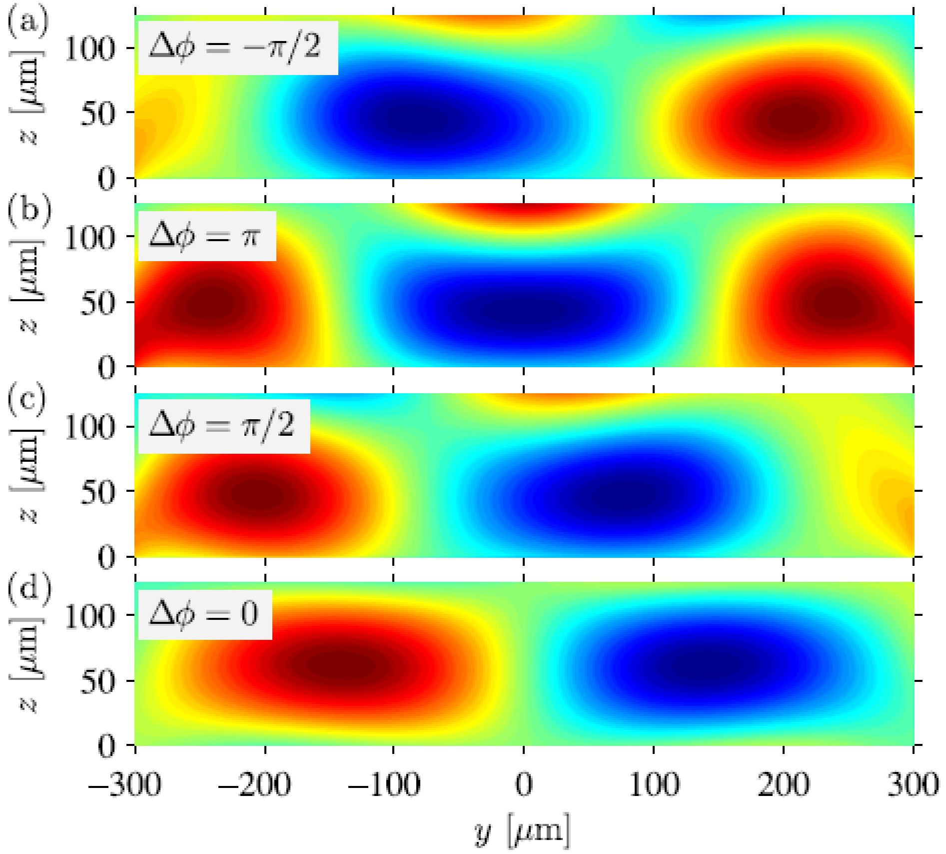
Side View

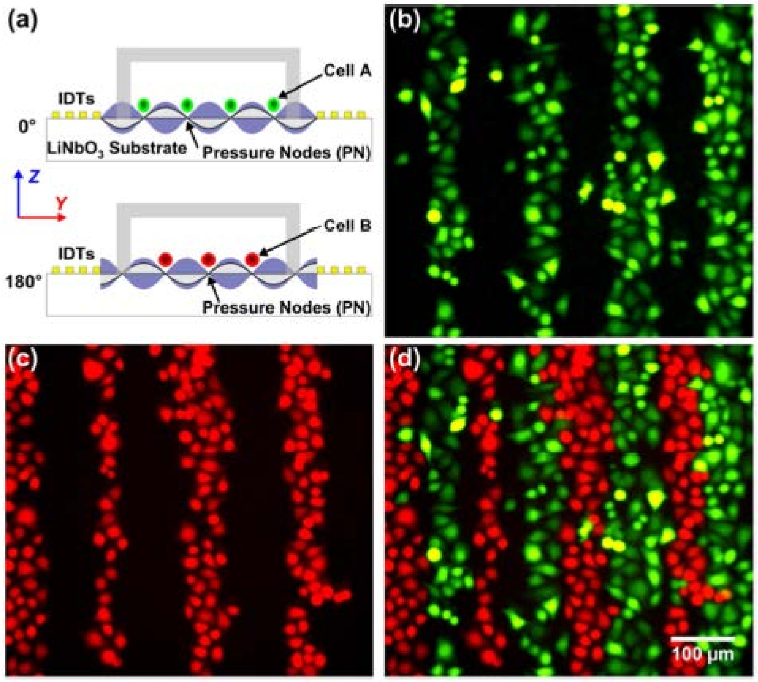


Vertical focusing:
probably due to gravity

Shi *et al,* Lab On a Chip, Vol.11, pp. 2319-2324, 2011.

Application: Phase Sweep





Li *et al*, Lab Chip, Anal. Chem., 86, 9853–9859, 2014.

$$\Delta x = \frac{1}{2k}\varphi = \frac{\lambda}{720^\circ}\varphi \quad \varphi \in [0^\circ, 360^\circ]$$

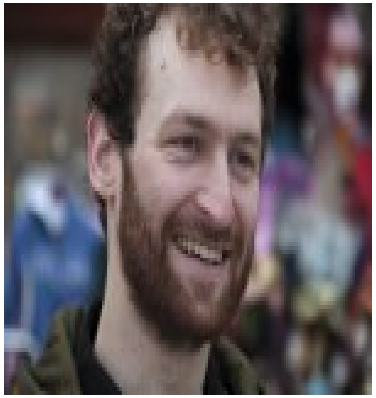
- Displacement of pressure node by changing the phase of one IDT

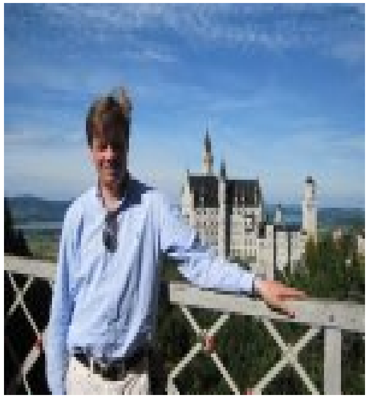
Conclusion and Outlook

- A numerical model for standing SAW based systems is presented.
- The findings are very different from the BAW systems
  - Traveling wave setup in the channel
  - Different boundary layer
  - Leakage of energy to PDMS
- The boundary layer phenomena is yet to be fully understood.
- Quantitative 3D APTV measurements for the experimental verification are in progress.
- More details about the model in the following article:

Nitesh Nama, Rune Barnkob, Zhangming Mao, Christian J. Kähler, Francesco Costanzo, and Tony Jun Huang, **Numerical study of acoustophoretic motion of particles in a PDMS microchannel driven by surface acoustic waves**, *Lab on a Chip*, Vol. 15, pp. 2700-2709, 2015.

Acknowledgments





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