Modeling, Simulation and Optimization of Surface Acoustic Wave Driven Microfluidic Biochips

Ronald H.W. Hoppe[1,2]

[1] Department of Mathematics, University of Houston
[2] Institute of Mathematics, University of Augsburg

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Department of Mathematics, University of Houston
Institut für Mathematik, Universität Augsburg

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A. Gantner, D. Köster, C. Linsenmann (Inst. of Math., Augsburg)

S. Braunmüller, T. Franke, A. Wixforth (Inst. of Phys.)

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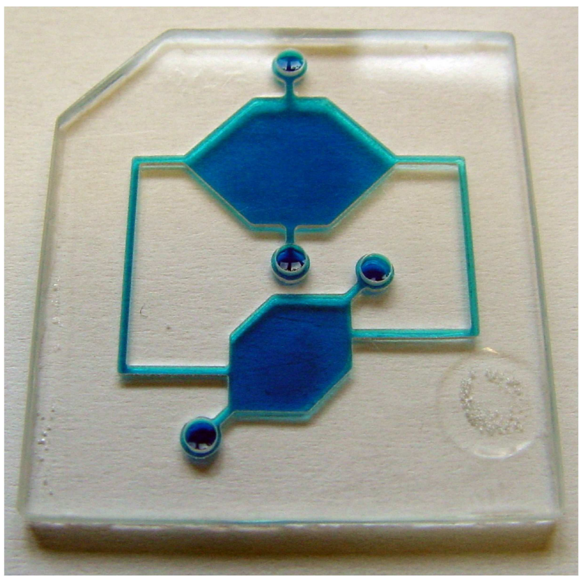
Modeling and Simulation of SAW Driven Microfluidic Biochips

- Multiphysics: Coupling of piezoelectrics and compressible Navier-Stokes
- Multiscale: Homogenization of the Navier-Stokes equations
- Multilevel: Simulation by multilevel finite element discretizations

Optimization of SAW Driven Microfluidic Biochips

- Projection Based Model Reduction
- Domain Decomposition & Balanced Truncation
- Optimal Design of Capillary Barriers

Applications of Active Microfluidic Biochips

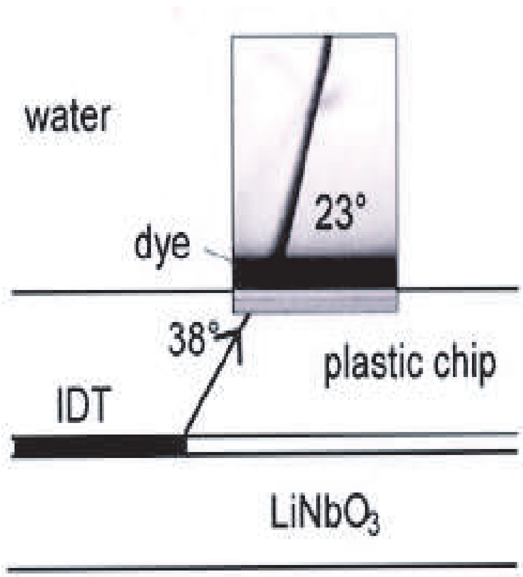


Biomedical Analysis

Biochips of the microarray type are controllable biochemical labs (lab-on-a-chip) that are used for combinatorial chemical and biological analysis in pharmocology, molecular biology, and cli--nical diagnostics.

The current trend is to design active biochips based on nanopumps featuring piezoelectrically actuated SAWs (Surface Acoustic Waves) propagating on the surface of the chip like a miniaturized earthquake. The elastic waves interact with the fluid and produce a streaming pattern.

Application of Active Microfluidic Biochips



Acoustic streaming induced by surface acoustic waves

The surface acoustic waves are excited by interdigital transducers and are diffracted into the device where they propagate through the base and enter the fluid filled microchannel creating a sharp jet on a time-scale of nanoseconds.
The acoustic waves undergo a significant damping along the microchannel resulting in an acoustic streaming on a time-scale of milliseconds.
The induced fluid flow transports the probes to reservoirs within the network where a chemical analysis is performed.

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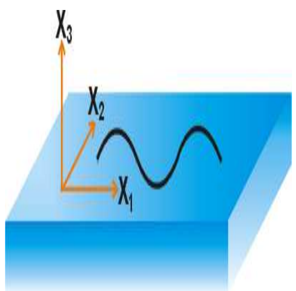
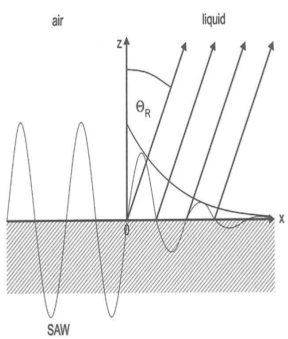
Coupling Surface Acoustic Waves and Fluid Flow





Piezoelectric Equations

$$\rho_1 \frac{\partial^2 u_i}{\partial t^2} - c_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} - e_{kij} \frac{\partial^2 \Phi}{\partial x_j \partial x_k} = 0 ,$$

$$e_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} - \epsilon_{ij} \frac{\partial^2 \Phi}{\partial x_i \partial x_j} = 0 .$$

Compressible Navier-Stokes Equations

$$\rho_2 \left(\frac{\partial v}{\partial t} + (v \cdot \nabla) v\right) = - \nabla p + \eta \, \Delta v + (\xi + \frac{\eta}{3}) \nabla (\nabla \cdot v) ,$$

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 v) = 0 ,$$

$$v(x + u(x,t), t) = \frac{\partial u}{\partial t}(x,t) \quad \text{on the boundary} .$$

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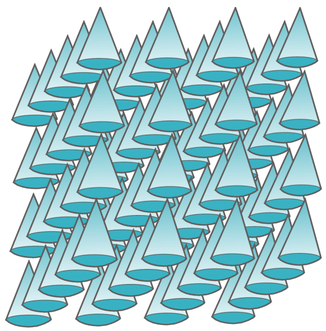
Piezoelectrically Actuated Surface Acoustic Waves

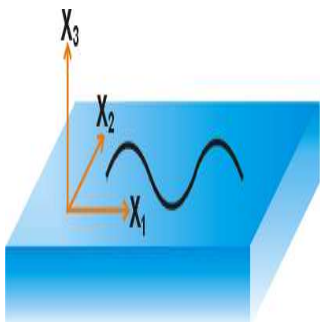


Piezoelectric effect in materials with a polar axis:
Outer electric field $\mathbf{E}$ causes mechanical displacement

$$\rho_1 \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, \mathbf{E}) = 0 \quad \text{in } Q := \Omega \times (0, T) ,$$
$$\nabla \cdot \mathbf{D}(\mathbf{u}, \mathbf{E}) = 0 \quad \text{in } Q := \Omega \times (0, T) .$$

The stress tensor $\boldsymbol{\sigma}(\mathbf{u}, \mathbf{E})$ is related to the linearized strain tensor $\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ by the generalized Hooke's law

$$\sigma_{ij}(\mathbf{u}, \mathbf{E}) = c_{ijkl}\, \varepsilon_{kl}(\mathbf{u}) + e_{kij}\, E_k .$$



The displacement field satisfies the constitutive equation

$$D_i(\mathbf{u}, \mathbf{E}) = \epsilon_{ij}\, E_j + P_i$$

with the polarization $P_i = e_{ikl}\varepsilon_{kl}(\mathbf{u})$.

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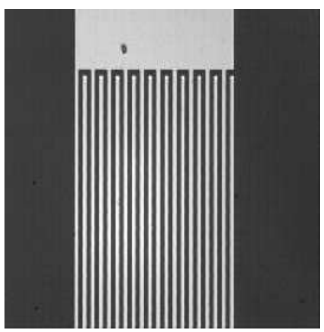
Surface Acoustic Waves: Time-Harmonic Approach

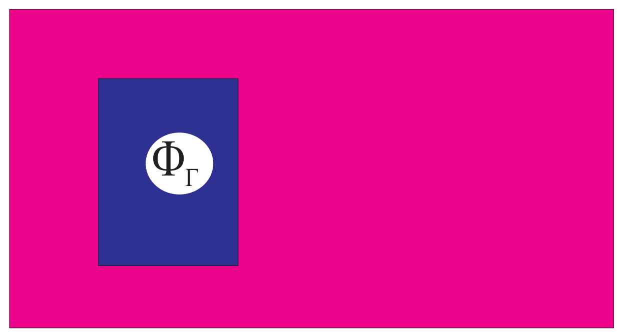
SAWs are usually excited by interdigital transducers located at Γ_Φ operating at a frequency $f \approx 100$ MHz with wavelength $\lambda = 40\ \mu$m. The time-harmonic ansatz leads to the saddle point problem

$$\int_\Omega c_{ijkl}\ \varepsilon_{kl}(u)\ \varepsilon_{ij}(\bar{v})\ dx\ -\ \omega^2 \int_\Omega u_i\ \bar{v}_i\ dx\ +\ \int_\Omega e_{kij}\ \frac{\partial \Phi}{\partial x_k}\ \varepsilon_{ij}(\bar{v})\ dx\ =\ <\boldsymbol{\sigma}_n, v>\ ,\ \ v \in V\ ,$$

$$\int_\Omega e_{ijk}\ \varepsilon_{ij}(u)\ \frac{\partial \bar{\Psi}}{\partial x_k}\ dx\ -\ \int_\Omega \epsilon_{ij}\ \frac{\partial \Phi}{\partial x_i}\ \frac{\partial \bar{\Psi}}{\partial x_j}\ dx\ =\ <D_n, \Psi>\ ,\ \ \Psi \in W\ .$$



Interdigital transducer



Position of IDT on PE substrate

Time-Harmonic Approach: Fredholm Alternative

The saddle point problem can be written in operator form as follows

$$(A - \omega^2 I)u \ + \ B\Phi \ = \ f \ ,$$
$$B^* u \ - \ C\Phi \ = \ g \ .$$

Here, $A : V \subset H^1(\Omega)^d \to V^*$, $B : H^1(\Omega) \to V^*$ and $C : W \subset H^1(\Omega) \to W^*$ are bounded linear operators. Moreover, A is symmetric, V-elliptic, and C is symmetric and W-elliptic. Elimination of Φ results in the Schur complement system

$$(*) \qquad S_\omega u \ := \ (S - \omega^2 I)u \ = \ f \ + \ BC^{-1}g \quad , \quad S \ := \ A \ + \ BC^{-1}B* \ .$$

Theorem. The Schur complement S has at most countably many real eigenvalues $\omega_1^2 > 0, i \in \mathbb{N}$. If ω^2 is not an eigenvalue of S, then $(*)$ has a unique solution $u \in V$. Otherwise, $(*)$ is solvable, if $f + BC^{-1}g \in \mathrm{Ker}\ S_\omega^o$. In either case

$$(**) \qquad \inf_{v \neq 0} \ \sup_{w \neq 0} \ \frac{|< S_\omega v, w >|}{\|v\|_{1,\Omega} \|w\|_{1,\Omega}} \ \geq \ \beta \ > \ 0 \ .$$

Finite Element Discretization of the Time-Harmonic Problem

Discretization in space by P1 conforming FE elements w.r.t. an adaptively generated hierarchy of triangulations leads to the discrete saddle point problem resp. to the discrete Schur complement system

$$\begin{aligned} (A_h - \omega^2 I_h) u_h \; + \; B_h \, \Phi_h &= f_h \\ B_h^* u_h \; - \; C_h \Phi_h &= g_h \end{aligned} \quad , \quad S_{h,\omega} u_h \; := \; (S_h - \omega^2 I_h) u_h \; = \; f_h \; + \; B_h C_h^{-1} g_h \; ,$$

where $S_h := A_h + B_h C_h^{-1} B_h^*$.

Theorem. Assume that the continuous operator S_ω fulfills the inf-sup condition $(**)$. Then, there exist $h_{min} > 0$ and $\beta_{min} > 0$ such that for all $h \leq h_{min}$ its discrete counterpart $S_{h,\omega}$ satisfies

$$\inf_{v_h \neq 0} \; \sup_{w_h \neq 0} \; \frac{| < S_{h,\omega} v_h, w_h > |}{\|v_h\|_{1,\Omega} \|w_h\|_{1,\Omega}} \; \geq \; \beta_h \; \geq \; \beta_{min} \; .$$

Construction of Multilevel Preconditioners

Assume that $\omega \in \mathbb{R}$ has been chosen such that

$$\inf_{\mathbf{U} \neq 0} \sup_{\mathbf{V} \neq 0} \frac{|\mathbf{V}^T \mathcal{A}_\omega \mathbf{U}|}{\|\mathbf{U}\| \|\mathbf{V}\|} \geq \gamma_{\mathcal{A}} > 0 \quad \text{where} \quad \mathcal{A}_\omega \mathbf{U} = \begin{pmatrix} \mathbf{A}_\omega & \mathbf{B} \\ \mathbf{B}^T & -\mathbf{C} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \Phi \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} .$$

Choose $\mathcal{P}^{-1}$ as the block diagonal preconditioner

$$\mathcal{P}^{-1} = \begin{pmatrix} \tilde{\mathbf{A}} & 0 \\ 0 & \tilde{\mathbf{C}} \end{pmatrix} \quad \text{s.th.} \quad \Gamma_{\mathcal{P}}^{-1} \, \mathbf{z}^T \mathbf{z} \leq \mathbf{z}^T \mathcal{P}^{-1} \mathbf{z} \leq \gamma_{\mathcal{P}}^{-1} \mathbf{z}^T \mathbf{z} .$$

Theorem. Under the previous assumptions there holds

$$\gamma_{\mathcal{P}} \, \gamma_{\mathcal{A}} \mathbf{V}^T \mathbf{V} \leq \mathbf{V}^T \mathcal{P}^{1/2} \mathcal{A}_\omega \mathcal{P}^{1/2} \mathbf{V} \leq \Gamma_{\mathcal{P}} \, \|\mathcal{A}_\omega\| \, \mathbf{V}^T \mathbf{V} .$$

Corollary. Let $\gamma_{\mathrm{A}}, \gamma_{\tilde{\mathrm{A}}}, \gamma_{\mathrm{C}}$ be lower bounds for the spectrum of $\mathbf{A}, \tilde{\mathbf{A}}, \mathbf{C}$. Then

$$\|\tilde{\mathbf{A}}\|^{-1} \left(\gamma_{\mathrm{A}} + \|\mathbf{C}\|^{-1} \beta_{\min}^2\right) \mathbf{v}^T \mathbf{v} \leq \mathbf{v}^T \tilde{\mathbf{A}}^{-1/2} \mathbf{S} \tilde{\mathbf{A}}^{-1/2} \mathbf{v} \leq \gamma_{\tilde{\mathrm{A}}}^{-1} \left(\|\mathbf{A}\| + \gamma_{\mathrm{C}}^{-1} \|\mathbf{B}\|^2\right) \mathbf{v}^T \mathbf{v} .$$

Multilevel Preconditioned Iterative Solution

Realization of $\tilde{A}$ and $\tilde{C}$ by multilevel preconditioners of BPX-type and

- solution of the preconditioned Schur complement system by CG,
- solution of the preconditioned saddle point problem by BICGSTAB , GMRES.

Level	SC-CG		BICGST		GMRES		Level	SC-PCG		PBICGST		PGMRES	
	time	iter	time	iter	time	iter		time	iter	time	iter	time	iter
3	0.15	74	0.10	65	0.14	17	5	2.5	48	1.1	33	1.2	6
4	1.4	148	0.75	137	1.7	56	6	12	52	5.2	39	5.9	7
5	29	311	7.6	324	32	206	7	70	55	23	41	25	7
6	440	872	75	678	530	758	8	290	57	92	44	100	8

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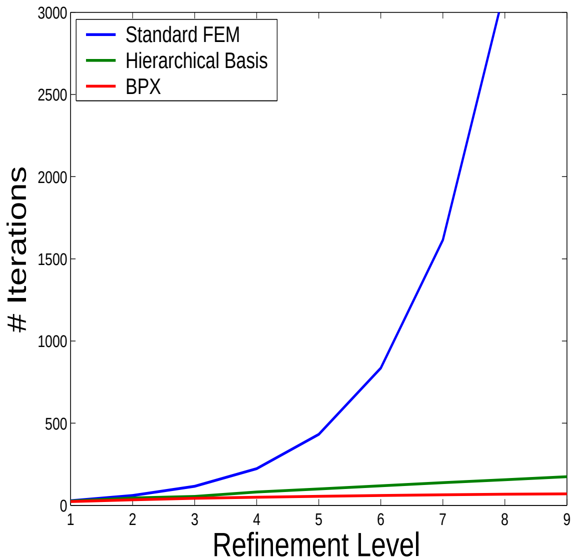
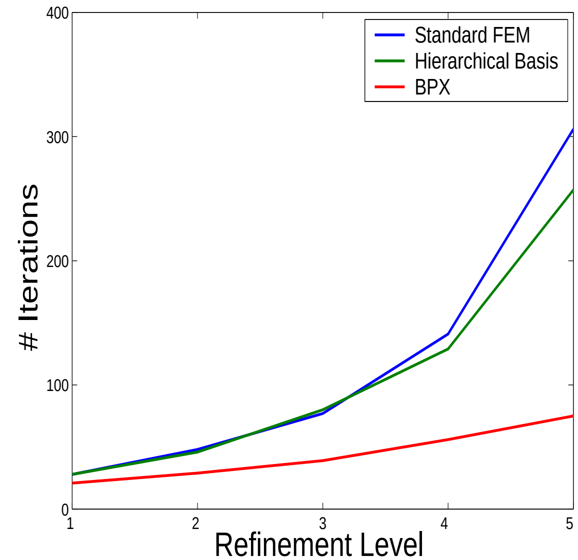
Performance of the Multilevel Preconditioned Iterative Solver



2D Simulation



3D Simulation

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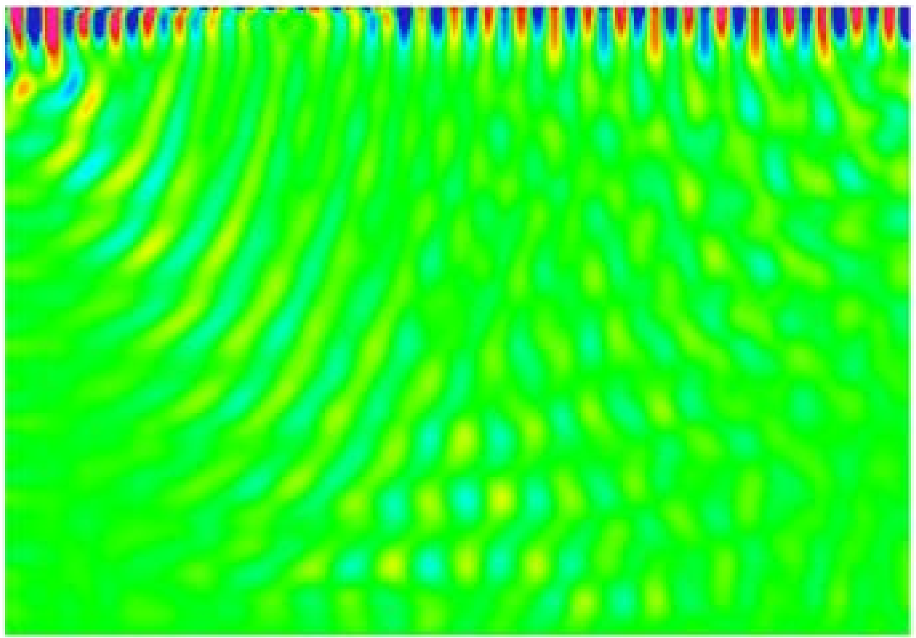
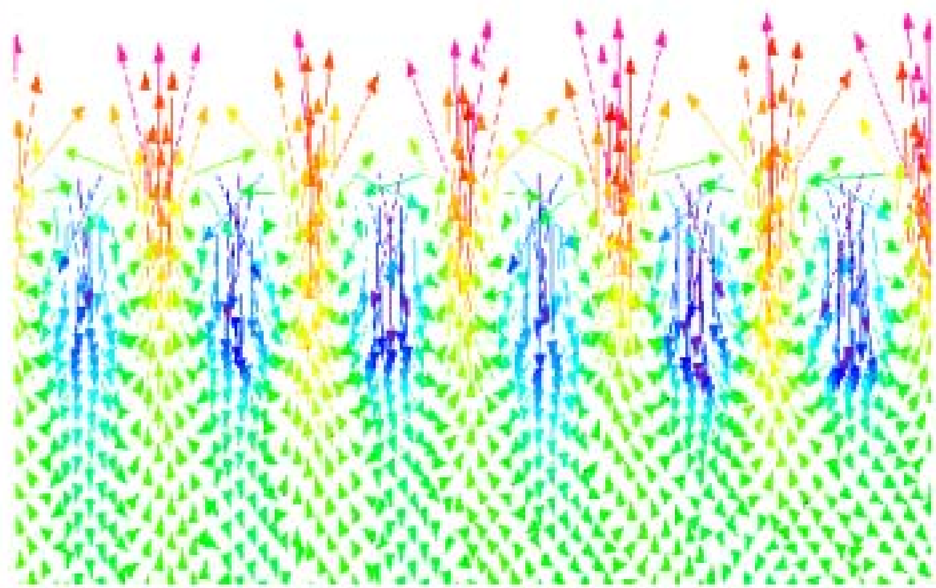
Numerical Simulation: Surface Acoustic Waves



Electric Potential Wave (100 MHz)



Displacement Vectors

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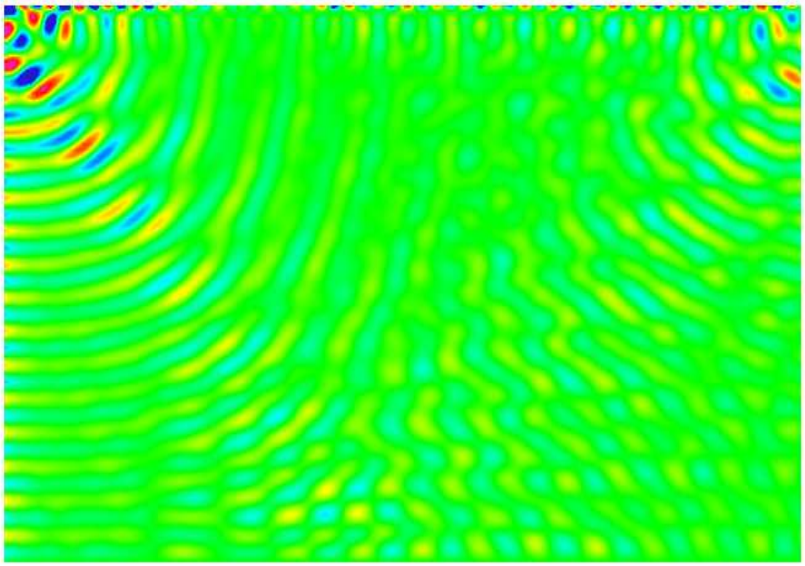
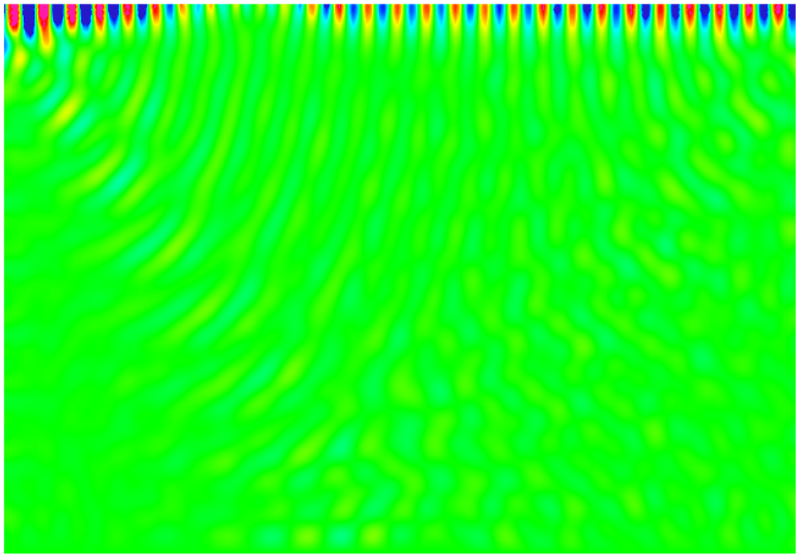
Numerical Simulation: Surface Acoustic Waves

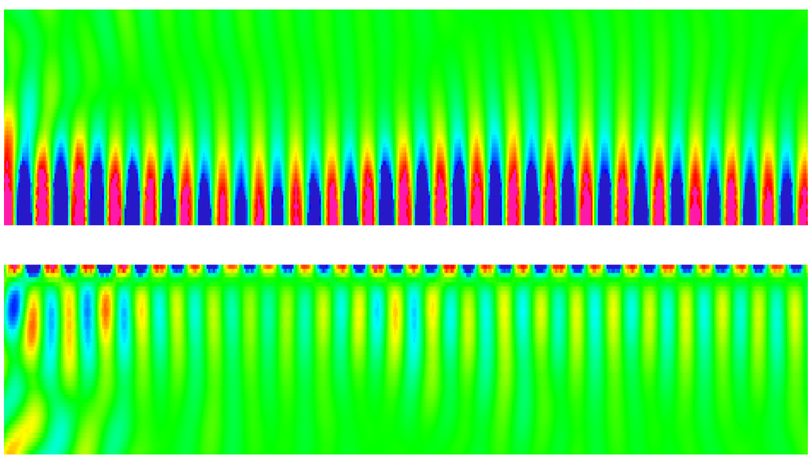


Displacement Wave Amplitude in x_1-direction

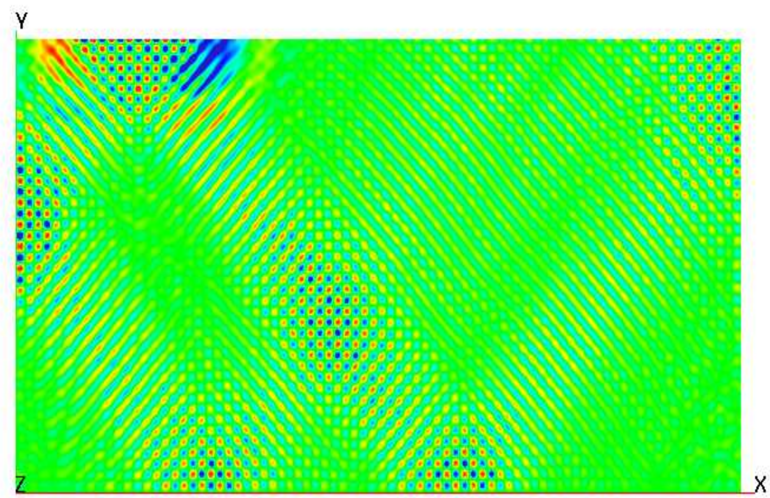


Displacement Wave Amplitude in x_2-direction

Numerical Simulation: Surface Acoustic Waves



Phaseshift of x_1- and x_2-displacements



Bulkwave excitation (200 MHz)

Homogenization of the Compressible Navier-Stokes Equations

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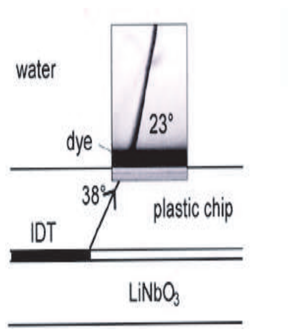
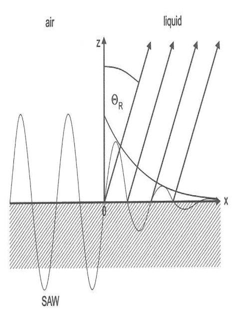
Acoustic Streaming: Compressible Navier-Stokes Equations





The piezoelectrically actuated SAWs penetrate into the microchannel and generate a two-scale fluid flow.

$$\rho_2 \left(\frac{\partial v}{\partial t} + (v\cdot\nabla)v\right) = -\nabla p + \eta\, \Delta v + \left(\xi + \frac{\eta}{3}\right) \nabla(\nabla\cdot v) \ ,$$

$$\frac{\partial \rho_2}{\partial t} + \nabla\cdot(\rho_2\, v) = 0 \quad \text{in } Q_2 := \Omega_2 \times (0, T_2) \ .$$

with boundary conditions

$$v(x + u(x,t), t) = \frac{\partial u}{\partial t}(x,t) \quad \text{on } \Gamma_{2,D} \ .$$

Two time-scales:

- Penetration of SAWs into channel (nanoseconds)
- Induced acoustic streaming (milliseconds)

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Separation of Time-Scales by Homogenization

Consider the expansion of v, p, and ρ in the scale parameter $\varepsilon > 0$ (max. displacement of the walls):

$$\begin{aligned} \mathrm{p} &= \mathrm{p}_0 + \varepsilon\, \mathrm{p}' + \varepsilon^2\, \mathrm{p}'' + O(\varepsilon^3)\ , \\ \rho &= \rho_0 + \varepsilon\, \rho' + \varepsilon^2\, \rho'' + O(\varepsilon^3)\ , \\ \mathrm{v} &= \mathrm{v}_0 + \varepsilon\, \mathrm{v}' + \varepsilon^2\, \mathrm{v}'' + O(\varepsilon^3)\ . \end{aligned}$$

Collecting all terms of order $O(\varepsilon)$ results in the linear system

$$\rho_0 \frac{\partial \mathrm{v}_1}{\partial t} - \eta\, \Delta \mathrm{v}_1 - \left(\xi + \frac{\eta}{3}\right) \nabla(\nabla \cdot \mathrm{v}_1) + \nabla \mathrm{p}_1 = 0 \qquad \text{in } Q_2\ ,$$

$$\frac{\partial \rho_1}{\partial t} + \rho_0\, \nabla \cdot \mathrm{v}_1 = 0 \qquad \text{in } Q_2\ ,$$

$$\mathrm{p}_1 = c_0^2\, \rho_1 \quad \text{in } Q_2 \quad , \quad \mathrm{v}_1 = \frac{\partial \mathrm{u}}{\partial t} \qquad \text{on } \Gamma_{2,D}\ ,$$

where $\mathrm{v}_1 = \varepsilon \mathrm{v}', \mathrm{v}^2 := \varepsilon^2 \mathrm{v}''$ etc. and $c_0^2 := a \gamma \rho_0^{\gamma - 1}$ (small signal sound speed).
The linear system describes the propagation of damped acoustic waves.

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Acoustic Streaming by Time-Averaging

Collecting all terms of order $O(\varepsilon^2)$ and performing the time-averaging

$$\langle w \rangle := \frac{1}{T} \int_{t_0}^{t_0+T} w\, dt \ ,$$

where $T := 2\pi/\omega$, we arrive at the Stokes system:

$$- \eta\ \Delta v_2 \ - \ \left(\xi + \frac{\eta}{3}\right)\ \nabla(\nabla \cdot v_2) \ + \ \nabla p_2 \ = \ \langle -\ \rho_1\ \frac{\partial v_1}{\partial t} \ - \ \rho_0[\nabla v_1]v_1 \rangle \quad \text{in } \Omega_2 \ ,$$

$$\rho_0\ \nabla \cdot v_2 \ = \ \langle -\nabla \cdot (\rho_1 v_1) \rangle \quad \text{in } \Omega_2 \ ,$$

$$v_2 \ = \ - \ \langle [\nabla v_1] u \rangle \quad \text{on } \Gamma_{2,D} \ .$$

The Stokes system describes the stationary flow pattern caused by the high frequency surface acoustic waves (acoustic streaming).

Periodic Solutions and Oscillating Equilibrium States

Theorem (Existence and uniqueness of periodic solutions)

Assume that the forcing term is a periodic function of period T. Then, the compressible Navier-Stokes equations have a unique weak periodic solution

$$(v_{per}, p_{per}) \in H^1((0,T); H^{-1}(\Omega) \times L^2_0(\Omega)) \ .$$

Theorem (Convergence to an oscillating equilibrium state)

Let $(\tilde{v}, \tilde{p})$ resp. $(\tilde{v}_{per}, \tilde{p}_{per})$ be extensions of the solution resp. the periodic solution of the Navier-Stokes equation with periodic forcing term to arbitrary large $\tau > 0$ and assume $(\tilde{v}'', \tilde{p}'')$, $(\tilde{v}''_{per}, \tilde{p}''_{per}) \in L^2((0,\tau); H)$, where $H := L^2(\Omega) \times L^2_0(\Omega)$. Then, there holds

$$\|(\tilde{v}(t), \tilde{p}(t)) - (\tilde{v}_{per}(t), \tilde{p}_{per}(t))\|_H \ \le \ C \ t^{-1/2} \ .$$

Numerical Simulation Tools for the Homogenized Navier-Stokes Equations

- First Order System (Periodic Navier-Stokes Equations)
  - Discretization in time by the Θ-scheme until a specific condition for periodicity is reached.
  - Discretization in space by Taylor-Hood elements w.r.t. adaptive generated hierarchies of simplicial triangulations.
- Second Order Equations (Time-Averaged Stokes System)
  - Same techniques as for the time-harmonic acoustic problem.

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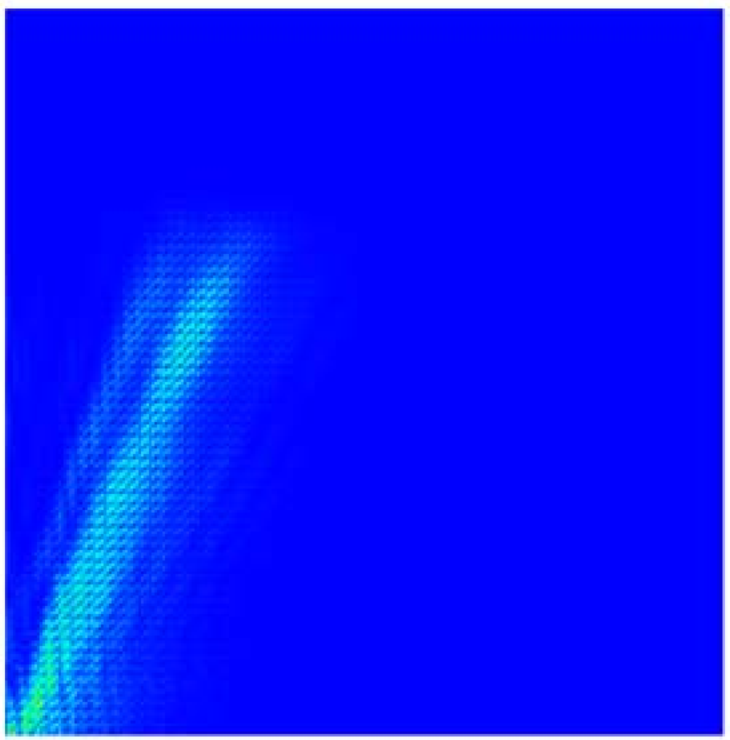
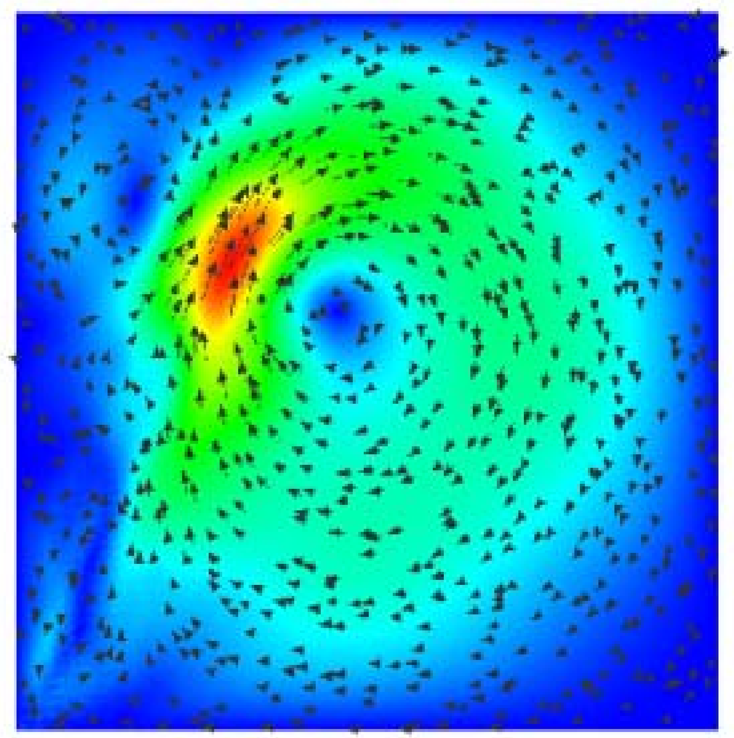
Numerical Simulation: Acoustic Streaming

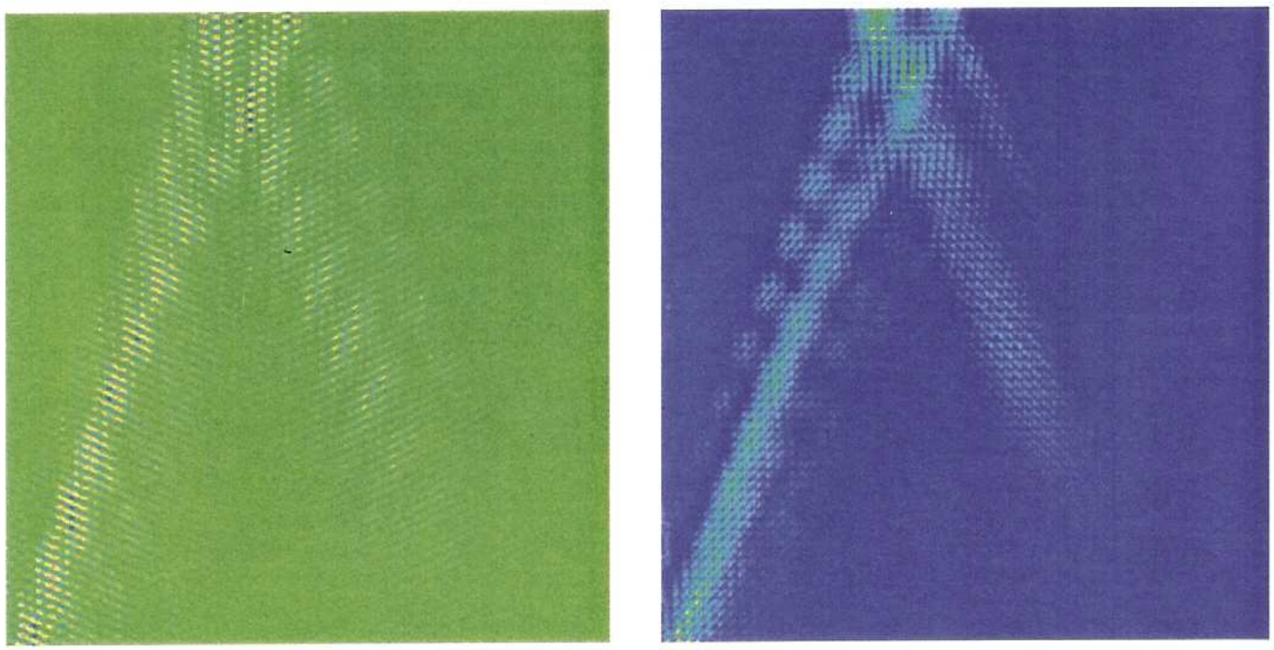


Effective force



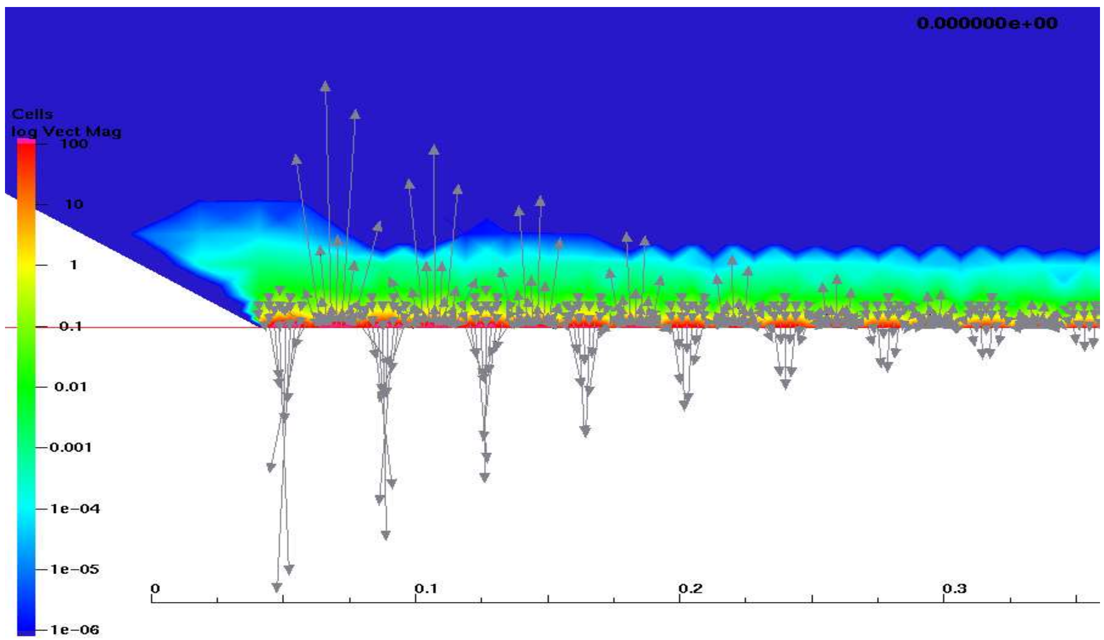
Velocity field

Numerical Results: Pressure Distribution and Effective Force



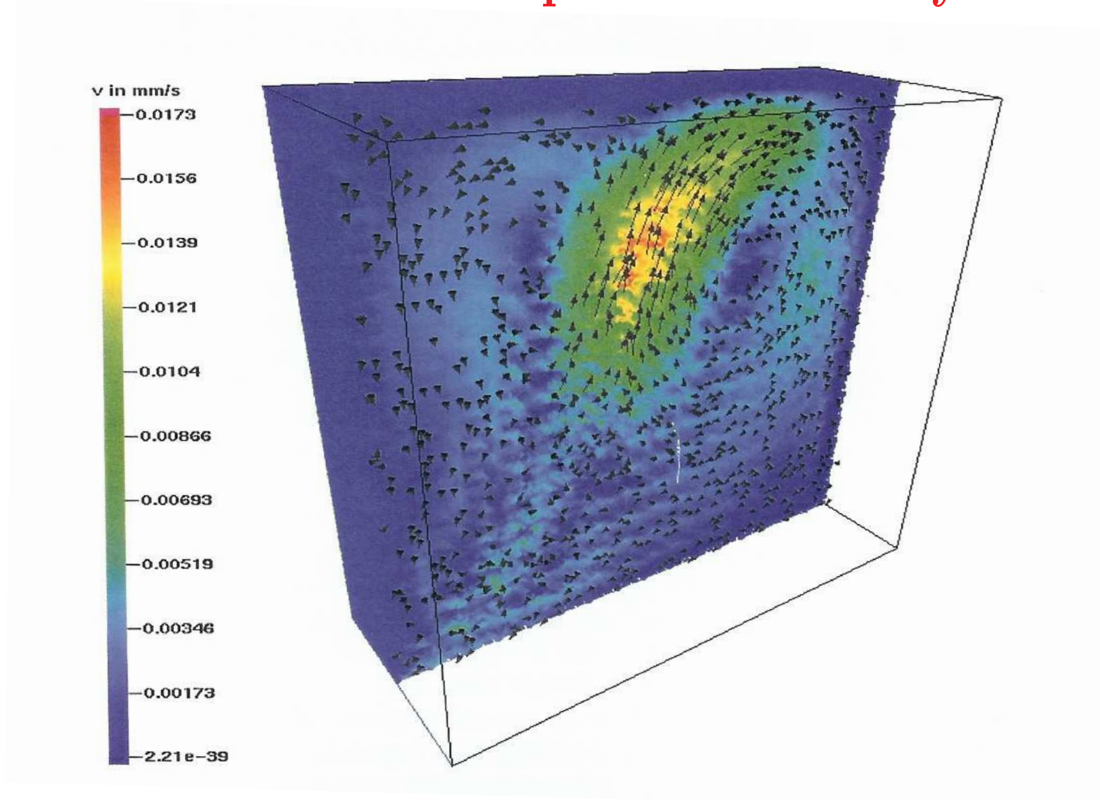
Left: Pressure $p^{(1)}$ at $t = 1.42\ \mu s$, Right: Effective force (with reflection)

Numerical Simulation: Acoustic Streaming



Strong damping of SAWs after penetration into fluid

Numerical Results: Snapshot of Velocity Field



Acoustic streaming: Velocity field $v^{(2)}$ in slab $x_3 \geq 0$

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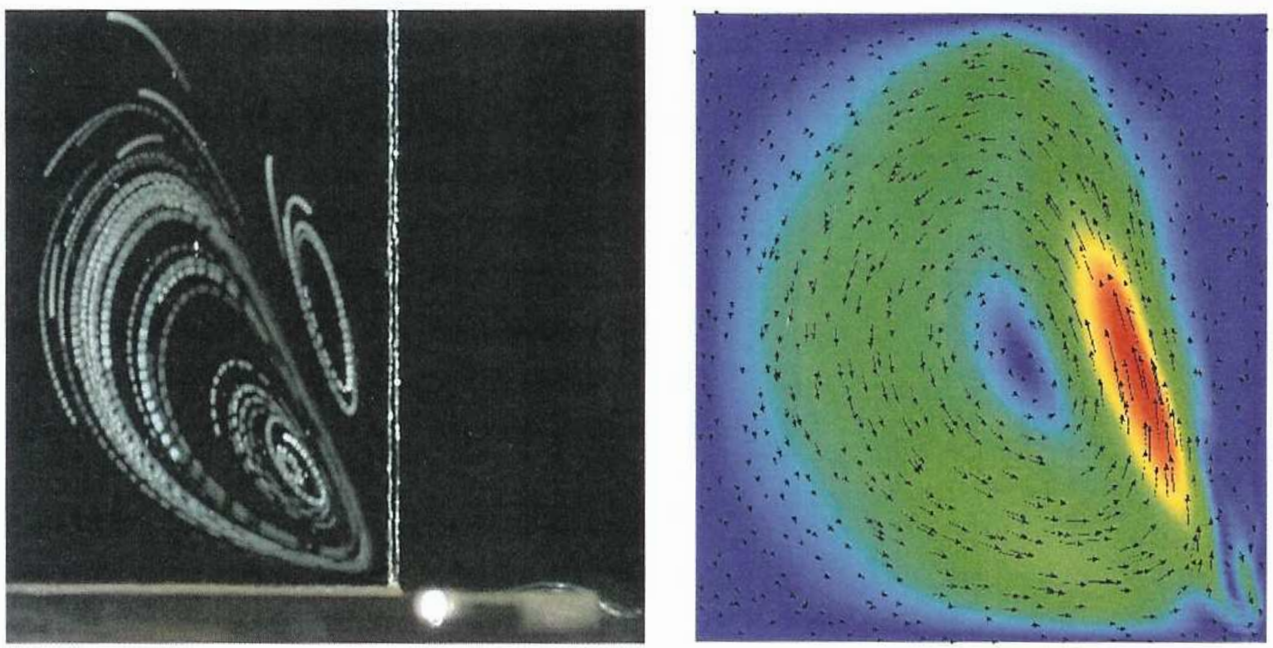
Acoustic Streaming: Model Validation based on Experimental Data



Left: Experimental measurement , Right: Results of numerical simulation

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Optimal Design of Microfluidic Biochips

Projection Based Model Reduction

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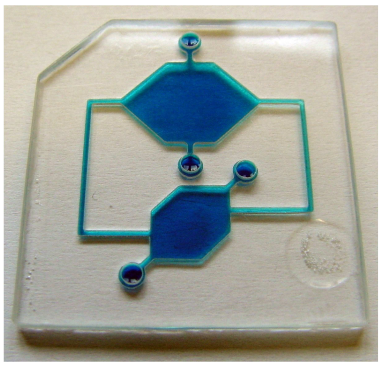
Shape Optimization of the Stokes System



Left: Microfluidic biochip with lithographically produced network of channels and reservoirs.

Given a velocity field $v^d = (v_1^d, v_2^d)^T$ and a pressure distribution p^d, we want to design the microfluidic biochip such that

$$\inf_{v,p,\theta} J(v,p,\theta) := \frac{1}{2} \int_0^T \int_{\Omega(\theta)} \left(|v - v^d|^2 + |p - p^d|^2 + \alpha \, |u|^2 \right) dx \, dt$$

subject to the PDE constraints (Stokes flow) on the state (v, p)

$$\frac{\partial v}{\partial t} - \nu \Delta v + \nabla p = u \quad \text{in } \Omega(\theta) ,$$

$$\nabla \cdot v = 0 \quad \text{in } \Omega(\theta) ,$$

and subject to bilateral constraints on the design variable θ.

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Institut für Mathematik, Universität Augsburg

Semi-Discretized Shape Optimization Problem for the Stokes System

Let $\Theta := \{\boldsymbol{\theta} \in \mathbb{R}^d \mid \theta_i^{(\min)} \le \theta_i \le \theta_i^{(\max)}, 1 \le i \le d\}$, and $A(\boldsymbol{\theta}), M(\boldsymbol{\theta}) \in \mathbb{R}^{n\times n}, B(\boldsymbol{\theta}) \in \mathbb{R}^{m\times n}$, as well as $C(\boldsymbol{\theta}) \in \mathbb{R}^{q\times n}, D(\boldsymbol{\theta}) \in \mathbb{R}^{q\times m}, F(\boldsymbol{\theta}) \in \mathbb{R}^{q\times k}$, and $d(t) \in \mathbb{R}^q$.

Consider the optimization problem

$$\inf_{\boldsymbol{\theta} \in \Theta} J(v,p,\boldsymbol{\theta}) \quad , \quad J(v,p,\boldsymbol{\theta}) := \int_0^T |C(\boldsymbol{\theta})v(t) + D(\boldsymbol{\theta})p(t) + F(\boldsymbol{\theta})u(t) - d(t)|^2 \, dt$$

subject to

$$\begin{pmatrix} M(\boldsymbol{\theta}) & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} v(t) \\ p(t) \end{pmatrix} = - \begin{pmatrix} A(\boldsymbol{\theta}) & B^T(\boldsymbol{\theta}) \\ B(\boldsymbol{\theta}) & 0 \end{pmatrix} \begin{pmatrix} v(t) \\ p(t) \end{pmatrix} + \begin{pmatrix} K(\boldsymbol{\theta}) \\ L(\boldsymbol{\theta}) \end{pmatrix} u(t) \quad , \quad t \in (0,T] \, ,$$

$$Mv(0) = v^0 \, ,$$

where $K(\boldsymbol{\theta}) \in \mathbb{R}^{n\times k}, L(\boldsymbol{\theta}) \in \mathbb{R}^{m\times k}$.

Semi-Discretized Time-Dependent Stokes System

Hessenberg index 2 differential-algebraic system:

$$\begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} v(t) \\ p(t) \end{pmatrix} = - \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} v(t) \\ p(t) \end{pmatrix} + \begin{pmatrix} K \\ L \end{pmatrix} u(t) \quad , \quad t \in (0,T] ,$$
$$Mv(0) = v^0 .$$

Theorem (Continuous Dependence on the Data).
Let $A, M \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{m \times n}, m < n$, and assume

(i) M is symmetric positive definite,

(ii) A is symmetric positive definite on $\mathrm{Ker}\, B$,

(iii) B has full row rank m.

Then there holds

$$\begin{pmatrix} \|v\|_{L^2} \\ \|p\|_{L^2} \end{pmatrix} \le C_1 \, \|v^0\| + C_2 \begin{pmatrix} \|u\|_{L^2} \\ \|u\|_{L^2} + \|\frac{d}{dt} u\|_{L^2} \end{pmatrix} .$$

Proof. We introduce

$$\Pi \ := \ I \ - \ B^T(BM^{-1}B^T)^{-1}BM^{-1}$$

as the projection onto Ker B^T along Im B and split $v(t) = v_H(t) + v_P(t)$, where

$$v_H(t) \in \text{Ker } B \quad \text{and} \quad v_P(t) := M^{-1}B^T(BM^{-1}B^T)^{-1}Lu(t)$$

is a particular solution of the second equation of the Stokes system.
The Stokes system transforms to

$$\underbrace{\Pi M \Pi^T}_{=: \ \bar{M}} \frac{d}{dt} v_H(t) \ = \ - \underbrace{\Pi A \Pi^T}_{=: \bar{A}} v_H(t) \ + \ \Pi \widetilde{K} u(t) \quad , \quad t \in (0,T] \ ,$$

$$\underbrace{\Pi M \Pi^T}_{=: \ \bar{M}} v_H(0) \ = \Pi v^0 \ .$$

The pressure p can be recovered according to

$$p(t) \ = \ (BM^{-1}B^T)^{-1}\Big(BM^{-1}\Big(- Av_H(t) + \widetilde{K}u(t)\Big) \ - \ L\frac{d}{dt}u(t)\Big) \ ,$$

where $\widetilde{K} := K - AM^{-1}B^T(BM^{-1}B^T)^{-1}L$.

Projection Based Model Reduction

Projection Based Model Reduction

$$\frac{d}{dt}y(t) = Ay(t) + Bu(t), \qquad z(t) = Cy(t)$$

$$\frac{d}{dt}y(t) = f(y(t), u(t), t), \qquad z(t) = g(y(t), t)$$

Replace $y(t) \in \mathbb{R}^N$ by $V\hat{y}(t)$, $\hat{y}(t) \in \mathbb{R}^n$, $n \ll N$, where $V \in \mathbb{R}^{N\times n}$ and multiply the state equation by $W^T \in \mathbb{R}^{n\times N}$ $(W^T V = I \in \mathbb{R}^{n\times n})$.

$$\frac{d}{dt}\hat{y}(t) = W^T AV\hat{y}(t) + W^T Bu(t), \qquad \hat{z}(t) = C\hat{y}(t)$$

$$\frac{d}{dt}\hat{y}(t) = W^T f(V\hat{y}(t), u(t), t), \qquad \hat{z}(t) = g(V\hat{y}(t), t)$$

Issues: Construction of the projectors, accuracy of the ROM.

Projection Based Model Reduction

- Proper Orthogonal Decomposition (POD)
  - Wide range of applicability (incl. nonlinear problems),
  - Data driven,
  - Quality of ROM depends on the selection of snapshots.
- Balanced Truncation Model Reduction (BTMR)
  - Theory & Algorithms for linear time-invariant systems,
  - Extension to nonlinear problems in progress (no theory so far).
- Reduced Basis Methods (RBM)
  - In theory applicable to a large problem class,
  - Can be tailored to different measures of approximation,
  - Ideal formulation computationally intractable (approximate variants).

Projection Based Model Reduction

Antoulas [2005] , Bai/DeWilde/Freund [2005]

Benner/Freund/Sorensen/Varga [2006] , Benner/Mehrmann/Sorensen [2005]

Dullerud/Paganini [2000] , Freund [2003]

Grepl/Patera [2005] , Grepl/Maday/Nguyen/Patera [2007]

Volkwein [2008] , Zhou/Doyle/Glover [1996]

Balanced Truncation Model Reduction for the Semi-Discrete Stokes System

BTMR for DAEs including semi-discrete Stokes systems

Antil/Heinkenschloss/H [2009]

Cao/Li/Petzold/Serban [2000]

Mehrmann/Stykel [2005]

Stykel [2006,2008]

Balanced Truncation MR of the Stokes Optimality System

a) State Equations

$$\begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} v(t) \\ p(t) \end{pmatrix} = - \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} v(t) \\ p(t) \end{pmatrix} + \begin{pmatrix} K \\ L \end{pmatrix} u(t) \quad , \quad t \in (0,T] \, ,$$

$$z(t) = Cv(t) + Dp(t) + Fu(t) \quad , \quad t \in (0,T] \, ,$$

$$Mv(0) = v^0 \, .$$

b) Adjoint Equations:

$$- \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \lambda(t) \\ \kappa(t) \end{pmatrix} = - \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \lambda(t) \\ \kappa(t) \end{pmatrix} + \begin{pmatrix} C^T \\ D^T \end{pmatrix} z(t) \quad , \quad t \in (0,T] \, ,$$

$$q(t) = K^T \lambda(t) + L^T \kappa(t) + F^T z(t) \quad , \quad t \in (0,T] \, ,$$

$$M\lambda(T) = \lambda^{(T)} \, .$$

Balanced Truncation MR of the Stokes Optimality System

Projection Method: Choose matrices $\mathbf{V}, \mathbf{W} \in \mathbb{R}^{n \times p}$ such that

$$\mathbf{V} = \Pi^T \mathbf{V} \quad , \quad \mathbf{W} = \Pi^T \mathbf{W} \quad , \quad \mathbf{W}^T \mathbf{M} \mathbf{V} = \mathbf{I} \, .$$

Multiplying the state equations by $\mathbf{W}^T$ and the adjoint equations by $\mathbf{V}^T$ results in:

Reduced Order Optimality System

$$\begin{aligned}
\frac{d}{dt}\widehat{v}_H(t) &= -\widehat{A}\widehat{v}_H(t) + \widehat{K}u(t) \quad , \quad t \in (0,T] \, , \\
\widehat{z}(t) &= \widehat{C}\widehat{v}_H(t) + \widehat{G}u(t) - \widehat{H}\frac{d}{dt}u(t) \quad , \quad t \in (0,T] \, , \\
\widehat{v}_H(0) &= \widehat{v}_H^0 \, ,
\end{aligned}$$

$$\begin{aligned}
-\frac{d}{dt}\widehat{\lambda}_H(t) &= -\widehat{A}^T\widehat{\lambda}_H(t) + \widehat{C}^T\widehat{z}(t) \quad , \quad t \in (0,T] \, , \\
\widehat{q}(t) &= \widehat{K}^T\widehat{\lambda}_H(t) + \widehat{G}^T\widehat{z}(t) - \widehat{H}\frac{d}{dt}\widehat{z}(t) \quad , \quad t \in (0,T] \, , \\
\widehat{\lambda}_H(T) &= \widehat{\lambda}^{(T)} \, .
\end{aligned}$$

Realization of the Balanced Truncation Model Reduction

Compute the controllability and observability Gramians $P, Q \in \mathbb{R}^{n \times n}$ as the solutions of the Lyapunov equations

$$\bar{A}P\bar{M} + \bar{M}P\bar{A} + \bar{K}\bar{K}^T = 0 \quad , \quad \bar{A}Q\bar{M} + \bar{M}Q\bar{A} + \bar{C}^T\bar{C} = 0 \, .$$

Factorize $P = UU^T, Q = EE^T$ and perform the Singular Value Decomposition

$$U^TME = ZS_nY^T \quad , \quad S_n := \mathrm{diag}(\sigma_1, \cdots, \sigma_n) \, , \; \sigma_i > \sigma_{i+1} \, , \; 1 \le i \le n-1 \, .$$

Compute V, W according to

$$V = UZ_pS_p^{-1/2} \quad , \quad W = EY_pS_p^{-1/2} \, .$$

where $1 \le p \le n$ is chosen such that $\sigma_{p+1} < \tau\sigma_1$ for some $\tau > 0$.

Note that $V^TPW = W^TQV = S_p$.

Balanced Truncation Model Reduction of the Optimality System

Theorem (Balanced Truncation Error Bound).
Let $z(t), q(t), t \in [0,T]$, and $\hat{z}(t), \hat{q}(t), t \in [0,T]$, be the observations/outputs of the full order and the reduced order optimality system and let $\sigma_i, 1 \le i \le n$, be the Hankel singular values from the singular value decomposition. Then, there holds

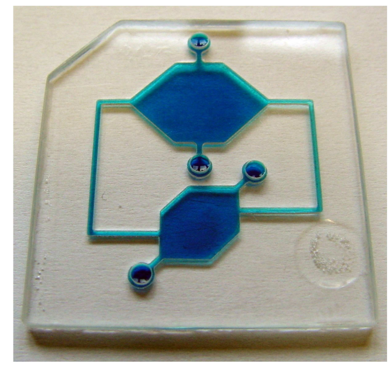
$$\|z - \hat{z}\|_{L^2} \le 2 \; \|u\|_{L^2} \left(\sigma_{p+1} + \cdots + \sigma_n \right) ,$$
$$\|q - \hat{q}\|_{L^2} \le 2 \; \|\hat{z}\|_{L^2} \left(\sigma_{p+1} + \cdots + \sigma_n \right) .$$

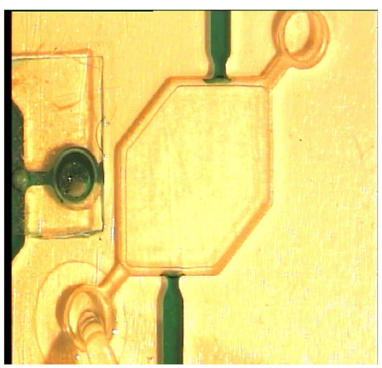
ROM Based Shape Optimization:

Domain Decomposition & Balanced Truncation

Domain Decomposition and Balanced Truncation Model Reduction

For design problems associated with linear state equations, where the design only effects a relatively small part of the computational domain, the nonlinearity is thus restricted to that part and motivates to consider a combination of domain decomposition and BTMR.





Such a design problem is, for instance, the optimal design of capillary barriers in microfluidic biochips between the channels and the reservoirs where the objective is to design the barriers such that a filling of the reservoirs with a precise amount of DNA or proteins is guaranteed.

Domain Decomposition & Balanced Truncation

Antil/Heinkenschloss/H [2009]

Antil/Heinkenschloss/H/Sorensen [2009]

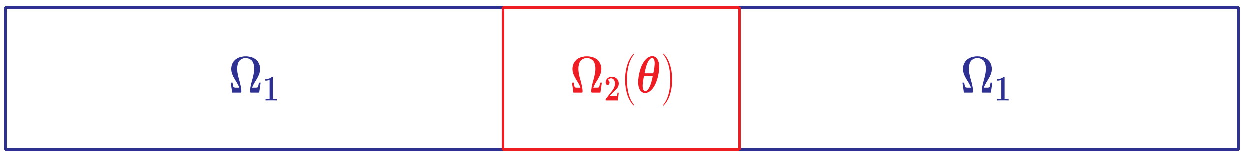
Heinkenschloss/Sorensen/Sun [2008]

Sun/Glowinski/Heinkenschloss/Sorensen [2008]

Domain Decomposition and Balanced Truncation Model Reduction

Consider a decomposition of the spatial domain $\Omega(\theta)$ such that

$$\overline{\Omega(\theta)} \; = \; \overline{\Omega}_1 \cup \overline{\Omega_2(\theta)} \quad , \quad \Omega_1 \cap \Omega_2(\theta) = \emptyset \quad , \quad \Gamma(\theta) := \overline{\Omega}_1 \cap \overline{\Omega_2(\theta)} \; .$$



Domain decomposed shape optimization problem

$$\inf_{\theta \in \Theta} J(v,p,\theta) \quad , \quad J(v,p,\theta) \; = \; J_1(v,p) \; + \; J_2(v,p,\theta) \; ,$$

where

$$J_1(v,p) \; := \; \int_0^T |C_1 v_1(t) + D_1 p_1(t) + F_1 u(t) - d(t)|^2 \; dt \; ,$$

$$J_2(v,p,\theta) \; := \; \int_0^T \ell(v_2(t), p_2(t), v_\Gamma(t), t, \theta) \; dt \; .$$

DDBT Model Reduction: Domain Decomposed State Equation

The domain decomposed semi-discretized state equations are as follows:

$$
\left(\begin{array}{cc|cc|cc}
M_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
- & - & - & - & - & - \\
0 & 0 & M_2(\theta) & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
- & - & - & - & - & - \\
0 & 0 & 0 & 0 & M_\Gamma(\theta) & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{array}\right)
\frac{d}{dt}
\begin{pmatrix} v_1 \\ p_1 \\ - \\ v_2 \\ p_2 \\ - \\ v_\Gamma \\ p_0 \end{pmatrix}
= -
\left(\begin{array}{cc|cc|cc}
A_{11} & B_{11}^T & 0 & 0 & A_{1\Gamma} & 0 \\
B_{11} & 0 & 0 & 0 & B_{1\Gamma} & 0 \\
- & - & - & - & - & - \\
0 & 0 & A_{22}(\theta) & B_{22}^T(\theta) & A_{2\Gamma}(\theta) & 0 \\
0 & 0 & B_{22}(\theta) & 0 & B_{2\Gamma}(\theta) & 0 \\
- & - & - & - & - & - \\
A_{\Gamma 1} & B_{1\Gamma}^T & A_{\Gamma 2}(\theta) & B_{2\Gamma}^T(\theta) & A_{\Gamma\Gamma}(\theta) & B_0^T(\theta) \\
0 & 0 & 0 & 0 & B_0(\theta) & 0
\end{array}\right)
\begin{pmatrix} v_1 \\ p_1 \\ - \\ v_2 \\ p_2 \\ - \\ v_\Gamma \\ p_0 \end{pmatrix}
+
\begin{pmatrix} K_1 \\ L_1 \\ - \\ K_2(\theta) \\ L_2(\theta) \\ - \\ K_\Gamma(\theta) \\ L_0(\theta) \end{pmatrix} u
$$

Balanced truncation model reduction is applied to the subproblem associated with subdomain Ω_1.

DDBT Model Reduction: Optimality System Associated with Ω_1

State equations associated with subdomain Ω_1:

$$\begin{pmatrix} M_1 & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} v_1(t) \\ p_1(t) \end{pmatrix} = - \begin{pmatrix} A_{11} & B_{11}^T \\ B_{11} & 0 \end{pmatrix} \begin{pmatrix} v_1(t) \\ p_1(t) \end{pmatrix} - \begin{pmatrix} A_{1\Gamma} & 0 \\ B_{1\Gamma} & 0 \end{pmatrix} \begin{pmatrix} v_\Gamma(t) \\ p_0(t) \end{pmatrix} + \begin{pmatrix} K_1 \\ L_1 \end{pmatrix} u(t),$$

$$z_1(t) = C_1 v_1(t) + F_1 p_1(t) + F_0 p_0(t) + D_1 u(t) - d(t).$$

Adjoint state equations associated with subdomain Ω_1:

$$- \begin{pmatrix} M_1 & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \lambda_1(t) \\ \kappa_1(t) \end{pmatrix} = - \begin{pmatrix} A_{11} & B_{11}^T \\ B_{11} & 0 \end{pmatrix} \begin{pmatrix} \lambda_1(t) \\ \kappa_1(t) \end{pmatrix} - \begin{pmatrix} A_{1\Gamma} & 0 \\ B_{1\Gamma} & 0 \end{pmatrix} \begin{pmatrix} \lambda_\Gamma(t) \\ \kappa_0(t) \end{pmatrix} - \begin{pmatrix} C_1^T \\ F_1^T \end{pmatrix} z_1(t),$$

$$q_1(t) = K_1^T \lambda_1(t) + L_1^T \kappa_1(t) + D_1^T z_1(t).$$

DDBTMR: Reduced Optimality System Associated with Ω_1

Reduced state equations associated with subdomain Ω_1:

$$\frac{d}{dt}\,\widehat{v}_1(t) = -\ W_1^T A_{11} V_1 \widehat{v}_1(t) - W_1^T \widetilde{B}_1 \begin{pmatrix} \widehat{v}_\Gamma(t) \\ \widehat{p}_0(t) \\ u(t) \end{pmatrix},$$

$$\begin{pmatrix} \widehat{z}_{v,\Gamma}(t) \\ \widehat{z}_{p,\Gamma}(t) \\ \widehat{z}_1(t) \end{pmatrix} = \widetilde{C}_1 V_1 \widehat{v}_1(t) + \widetilde{D}_1 \begin{pmatrix} \widehat{v}_\Gamma(t) \\ \widehat{p}_0(t) \\ u(t) \end{pmatrix} - \widetilde{H}_1 \frac{d}{dt} \begin{pmatrix} \widehat{v}_\Gamma(t) \\ \widehat{p}_0(t) \\ u(t) \end{pmatrix}.$$

Reduced adjoint state equations associated with subdomain Ω_1:

$$-\frac{d}{dt}\,\widehat{\lambda}_1(t) = -\,V_1^T A_{11} W_1 \widehat{\lambda}_1(t) + V_1^T \widetilde{C}_1 \begin{pmatrix} \widehat{\lambda}_1(t) \\ \widehat{\kappa}_0(t) \\ -\widehat{z}_1(t) \end{pmatrix},$$

$$\begin{pmatrix} \widehat{q}_{v,\Gamma}(t) \\ \widehat{q}_{p,\Gamma}(t) \\ \widehat{q}_1(t) \end{pmatrix} = -\,\widetilde{B}_1^T W_1 \widehat{\lambda}_1(t) + \widetilde{D}_1^T \begin{pmatrix} \widehat{\lambda}_1(t) \\ \widehat{\kappa}_0(t) \\ -\widehat{z}_1(t) \end{pmatrix} + \widetilde{H}_1^T \frac{d}{dt} \begin{pmatrix} \widehat{\lambda}_1(t) \\ \widehat{\kappa}_0(t) \\ -\widehat{z}_1(t) \end{pmatrix}.$$

Department of Mathematics, University of Houston
Institut für Mathematik, Universität Augsburg

DDBTMR: Optimality System Associated with $\Omega_2(\theta)$ and $\Gamma(\theta)$

State and adjoint state equations associated with the subdomain $\Omega_2(\theta)$:

$$\begin{pmatrix} M_2(\theta) & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \hat{v}_2(t) \\ \hat{p}_2(t) \end{pmatrix} = - \begin{pmatrix} A_{22}(\theta) & B_{22}^T(\theta) \\ B_{22}(\theta) & 0 \end{pmatrix} \begin{pmatrix} \hat{v}_2(t) \\ \hat{p}_2(t) \end{pmatrix} - \begin{pmatrix} A_{2\Gamma}(\theta) & 0 \\ B_{2\Gamma}(\theta) & 0 \end{pmatrix} \begin{pmatrix} \hat{v}_\Gamma(t) \\ \hat{p}_0(t) \end{pmatrix} + \begin{pmatrix} K_2(\theta) \\ L_2(\theta) \end{pmatrix} u(t),$$

$$-\begin{pmatrix} M_2(\theta) & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \hat{\lambda}_2(t) \\ \hat{\kappa}_2(t) \end{pmatrix} = - \begin{pmatrix} A_{22}(\theta) & B_{22}^T(\theta) \\ B_{22}(\theta) & 0 \end{pmatrix} \begin{pmatrix} \hat{\lambda}_2(t) \\ \hat{\kappa}_2(t) \end{pmatrix} - \begin{pmatrix} A_{2\Gamma}(\theta) & 0 \\ B_{2\Gamma}(\theta) & 0 \end{pmatrix} \begin{pmatrix} \hat{\lambda}_\Gamma(t) \\ \hat{\kappa}_0(t) \end{pmatrix} - \begin{pmatrix} \nabla_{\hat{v}_2} \ell(\hat{v}_2, \hat{p}_2, \hat{v}_\Gamma, \hat{p}_0, t, \theta) \\ \nabla_{\hat{p}_2} \ell(\hat{v}_2, \hat{p}_2, \hat{v}_\Gamma, \hat{p}_0, t, \theta) \end{pmatrix}.$$

State and adjoint state equations associated with the interface $\Gamma(\theta)$:

$$\begin{pmatrix} M_\Gamma(\theta) & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \hat{v}_\Gamma(t) \\ \hat{p}_0(t) \end{pmatrix} = - \begin{pmatrix} A_{\Gamma\Gamma}(\theta) & B_0^T(\theta) \\ B_0(\theta) & 0 \end{pmatrix} \begin{pmatrix} \hat{v}_\Gamma(t) \\ \hat{p}_0(t) \end{pmatrix} + \begin{pmatrix} \hat{z}_{v,\Gamma}(t) \\ \hat{z}_{p,\Gamma}(t) \end{pmatrix} - \begin{pmatrix} A_{2\Gamma}^T(\theta) & B_{2\Gamma}^T(\theta) \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{v}_2(t) \\ \hat{p}_2(t) \end{pmatrix} + \begin{pmatrix} K_\Gamma(\theta) \\ L_0(\theta) \end{pmatrix} u(t),$$

$$-\begin{pmatrix} M_\Gamma(\theta) & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \hat{\lambda}_\Gamma(t) \\ \hat{\kappa}_0(t) \end{pmatrix} = - \begin{pmatrix} A_{\Gamma\Gamma}(\theta) & B_0^T(\theta) \\ B_0(\theta) & 0 \end{pmatrix} \begin{pmatrix} \hat{\lambda}_\Gamma(t) \\ \hat{\kappa}_0(t) \end{pmatrix} + \begin{pmatrix} \hat{q}_{v,\Gamma}(t) \\ \hat{q}_{p,\Gamma}(t) \end{pmatrix} - \begin{pmatrix} A_{2\Gamma}^T(\theta) & B_{2\Gamma}^T(\theta) \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{\lambda}_2(t) \\ \hat{\kappa}_2(t) \end{pmatrix} - \begin{pmatrix} \nabla_{v_\Gamma} \ell(\cdots) \\ \nabla_{p_0} \ell(\cdots) \end{pmatrix}.$$

Theorem [AHH09] (Reduced Order Optimization Problem).
The reduced order optimality system obtained by Domain Decomposition and Balanced Truncation Model Reduction represents the first order necessary optimality conditions for the reduced order optimization problem

$$\inf_{\theta \in \Theta} \widehat{J}(\theta) \quad , \quad \widehat{J}(\theta) := \widehat{J}_1(\widehat{v}_1, \widehat{p}_1, \widehat{v}_\Gamma, \widehat{p}_0) + \widehat{J}_2(\widehat{v}_2, \widehat{p}_2, \widehat{v}_\Gamma, \widehat{p}_0, \theta),$$

where the the reduced order funtionals $\widehat{J}_1$ and $\widehat{J}_2$ are given by

$$\widehat{J}_1(\widehat{v}_1, \widehat{p}_1, \widehat{v}_\Gamma, \widehat{p}_0) := \frac{1}{2} \int_0^T |\widehat{z}_1|^2 dt \quad , \quad \widehat{J}_2(\widehat{v}_2, \widehat{p}_2, \widehat{v}_\Gamma, \widehat{p}_0, \theta) := \int_0^T \ell(\widehat{v}_2, \widehat{p}_2, \widehat{v}_\Gamma, \widehat{p}_0, t, \theta) dt.$$

Analysis of the Modeling Error

Analysis of the Modeling Error

Full Order Model

$$J(\theta^*) = \inf_{\theta \in \Theta} J(\theta)$$

Reduced Order Model

$$\widehat{J}(\widehat{\theta}^*) = \inf_{\theta \in \Theta} \widehat{J}(\theta)$$

Goal: Derive upper bound for the modeling error

$$\|\theta^* - \widehat{\theta}^*\| \le C \left(\sigma_{p+1} + \cdots + \sigma_n \right)$$

in terms of the Hankel singular values in the BTMR of the optimality system for the fixed subdomain Ω_1.

Analysis of the Modeling Error

Lemma [AHH09]. Assume that the objective functional $\mathbf{J}$ is strongly convex

$$(\mathrm{A}_1) \qquad \Big(\nabla \mathbf{J}(\hat{\boldsymbol{\theta}}) - \nabla \mathbf{J}(\boldsymbol{\theta})\Big)^{\mathrm{T}} (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) \;\geq\; \boldsymbol{\kappa}\, \|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2 .$$

Then, if $\boldsymbol{\theta}^* \in \boldsymbol{\Theta}$ and $\hat{\boldsymbol{\theta}}^* \in \boldsymbol{\Theta}$ are the solutions of the full order and the reduced order optimization problem, there holds

$$\|\boldsymbol{\theta}^* - \hat{\boldsymbol{\theta}}^*\| \;\leq\; \boldsymbol{\kappa}^{-1}\, \|\nabla \hat{\mathbf{J}}(\hat{\boldsymbol{\theta}}^*) - \nabla \mathbf{J}(\hat{\boldsymbol{\theta}}^*)\| .$$

Proof. Obviously, we have

$$\left.\begin{array}{rcl} \nabla \mathbf{J}(\boldsymbol{\theta}^*)^{\mathrm{T}}(\boldsymbol{\theta} - \boldsymbol{\theta}^*) & \geq & 0 \\ \nabla \hat{\mathbf{J}}(\hat{\boldsymbol{\theta}}^*)^{\mathrm{T}}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}^*) & \geq & 0 \end{array}\right\} \quad \Longrightarrow \quad \Big(\nabla \mathbf{J}(\boldsymbol{\theta}^*) - \nabla \hat{\mathbf{J}}(\hat{\boldsymbol{\theta}}^*)\Big)^{\mathrm{T}} (\hat{\boldsymbol{\theta}}^* - \boldsymbol{\theta}^*) \;\geq\; 0 .$$

Combining this with the strong convexity of $\mathbf{J}$ allows to conclude.

The estimation of the gradients requires some more assumptions on the objective functionals:

(A_2) The objective functional J_1 does not explicitly depend on the pressure, i.e., it is supposed to be of the form

$$J_1(v_1) = \frac{1}{2} \int_0^T |C_1 v(t) + D_1 u(t) - d(t)|^2 \, dt.$$

(A_3) The integrand ℓ in the objective functional

$$J_2(x_2, x_\Gamma, \theta) = \frac{1}{2} \int_0^T \ell(x_2, x_\Gamma, t, \theta) \, dt,$$

where $x_2 := (v_2, p_2)^T, x_\Gamma := (v_\Gamma, p_0)^T$, satisfies the Lipschitz conditions

$$\|\nabla_w \ell(x_2, x_\Gamma, t, \theta) - \nabla_w \ell(x_2', x_\Gamma', t, \theta)\| \le L_1 \Big(\|x_2 - x_2'\|^2 + \|x_\Gamma - x_\Gamma'\|^2 \Big)^{1/2}$$

uniformly in $\theta \in \Theta$ and $t \in [0, T]$, where $w \in \{v_2, v_\Gamma, p_2, p_0\}$.

Theorem [AHH09] (Estimation of the Gradients of the Objective Functionals).
Assume that $(A_2), (A_3)$ hold true and suppose that the Jacobians of the matrices $M_2(\theta), M_\Gamma(\theta)$ etc. are uniformly bounded in θ.
Then, there exists a constant $C > 0$ such that for $\theta \in \Theta$

$$\|\nabla J(\theta) - \nabla \widehat{J}(\theta)\| \ \leq \ C\left(\left\| \begin{pmatrix} x_2 - \widehat{x}_2 \\ x_\Gamma - \widehat{x}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \mu_2 - \widehat{\mu}_2 \\ \mu_\Gamma - \widehat{\mu}_\Gamma \end{pmatrix} \right\|_{L^2} \right).$$

where $x_2 - \widehat{x}_2$ etc. are given by

$$x_2 - \widehat{x}_2 = \begin{pmatrix} v_2 - \widehat{v}_2 \\ p_2 - \widehat{p}_2 \end{pmatrix} \quad , \quad x_\Gamma - \widehat{x}_\Gamma = \begin{pmatrix} v_\Gamma - \widehat{v}_\Gamma \\ p_0 - \widehat{p}_0 \end{pmatrix},$$

$$\mu_2 - \widehat{\mu}_2 = \begin{pmatrix} \lambda_2 - \widehat{\lambda}_2 \\ \kappa_2 - \widehat{\kappa}_2 \end{pmatrix} \quad , \quad \mu_\Gamma - \widehat{\mu}_\Gamma = \begin{pmatrix} \lambda_\Gamma - \widehat{\lambda}_\Gamma \\ \kappa_0 - \widehat{\kappa}_0 \end{pmatrix}.$$

Proof. For $\tilde{\theta}$ there holds

$$\nabla J(\theta)^T \tilde{\theta} = \int_0^T (\nabla_\theta \ell(x_2, x_\Gamma, t, \theta))^T \tilde{\theta} \, dt \; +$$

$$\int_0^T \begin{pmatrix} \mu_2(t) \\ \lambda_\Gamma(t) \end{pmatrix}^T \begin{pmatrix} (D_\theta P_2(\theta)\tilde{\theta}) x_2(t) - (D_\theta N_2(\theta)\tilde{\theta}) u(t) \\ (D_\theta P_\Gamma(\theta)\tilde{\theta}) x_\Gamma(t) - (D_\theta N_\Gamma(\theta)\tilde{\theta}) u(t) \end{pmatrix} \, dt.$$

Likewise, we have

$$\nabla \widehat{J}(\theta)^T \tilde{\theta} = \int_0^T (\nabla_\theta \ell(\widehat{x}_2, \widehat{x}_\Gamma, t, \theta))^T \tilde{\theta} \, dt \; +$$

$$\int_0^T \begin{pmatrix} \widehat{\mu}_2(t) \\ \widehat{\lambda}_\Gamma(t) \end{pmatrix}^T \begin{pmatrix} (D_\theta P_2(\theta)\tilde{\theta}) \widehat{x}_2(t) - (D_\theta N_2(\theta)\tilde{\theta}) u(t) \\ (D_\theta P_\Gamma(\theta)\tilde{\theta}) \widehat{x}_\Gamma(t) - (D_\theta N_\Gamma(\theta)\tilde{\theta}) u(t) \end{pmatrix} \, dt.$$

Assumptions on the Semi-Discrete Domain Decomposed State Equations

(A_4) The matrix $A(\boldsymbol{\theta}) \in \mathbb{R}^{n \times n}$ is symmetric positive definite and the matrix $B(\boldsymbol{\theta}) \in \mathbb{R}^{m \times n}$ has rank m. The generalized eigenvalues of $(A(\boldsymbol{\theta}), M(\boldsymbol{\theta}))$ have positive real part.

The matrix $A_{11}(\boldsymbol{\theta}) \in \mathbb{R}^{n_1 \times n_1}$ is symmetric positive definite and the matrix $B_{11}(\boldsymbol{\theta}) \in \mathbb{R}^{m_1 \times n_1}$ has rank m_1. The generalized eigenvalues of $(A_{11}(\boldsymbol{\theta}), M_{11}(\boldsymbol{\theta}))$ have positive real part.

Lemma [AHH09] (Estimation of the States and the Observations).

Let $x = (x_1, x_2, x_\Gamma)^T$ with $x_i = (v_i, P_I)^T, 1 \le i \le 2$, $x_\Gamma = (v_\Gamma, p_\Gamma)^T$ and $\hat{x} = (\hat{x}_1, \hat{x}_2, \hat{x}_\Gamma)^T$ with $\hat{x}_1 = \hat{v}_1$, $\hat{x}_2 = (\hat{v}_2, \hat{p}_2)^T$, $\hat{x}_\Gamma = (\hat{v}_\Gamma, \hat{p}_0)^T$, be the states satisfying the optimality systems associated with the full order and the reduced order model.

Then, under assumption (A_4) and for $v_1^{(0)} = 0$ there exists $C > 0$ such that

$$\left\| \begin{pmatrix} v_2 - \hat{v}_2 \\ v_\Gamma - \hat{v}_\Gamma \end{pmatrix} \right\|_{L^2} \le C \left\| \begin{pmatrix} u \\ \hat{x}_\Gamma \end{pmatrix} \right\|_{L^2} \left(\sigma_{p+1} + \cdot + \sigma_n \right),$$

$$\left\| \begin{pmatrix} p_2 - \hat{p}_2 \\ p_0 - \hat{p}_0 \end{pmatrix} \right\|_{L^2} \le C \left\| \begin{pmatrix} u \\ \hat{x}_\Gamma \end{pmatrix} \right\|_{L^2} \left(\sigma_{p+1} + \cdot + \sigma_n \right),$$

$$\left\| \begin{pmatrix} z_1 - \hat{z}_1 \\ z_{v,\Gamma} - \hat{z}_{v,\Gamma} \\ z_{p,\Gamma} - \hat{z}_{p,\Gamma} \end{pmatrix} \right\|_{L^2} \le C \left\| \begin{pmatrix} u \\ \hat{x}_\Gamma \end{pmatrix} \right\|_{L^2} \left(\sigma_{p+1} + \cdot + \sigma_n \right).$$

Proof. We construct an auxiliary system which has the same inputs as the reduced order system:

$$
\begin{aligned}
E_1 \frac{d}{dt} \begin{pmatrix} \tilde{v}_1(t) \\ \tilde{p}_1(t) \end{pmatrix} &= -S_1 \begin{pmatrix} \tilde{v}_1(t) \\ \tilde{p}_1(t) \end{pmatrix} - S_{1,\Gamma} \begin{pmatrix} \widehat{v}_\Gamma(t) \\ \widehat{p}_0(t) \end{pmatrix} + \begin{pmatrix} K_1 \\ L_1 \end{pmatrix} u(t), \\
\tilde{z}_1(t) &= C_1 \tilde{v}_1(t) + F_1 \tilde{p}_1(t) + F_0 \widehat{p}_0(t) + D_1 u(t) - d(t), \\
\begin{pmatrix} \tilde{z}_{v,\Gamma}(t) \\ \tilde{z}_{p,\Gamma}(t) \end{pmatrix} &= -S_{1\Gamma}^T \begin{pmatrix} \tilde{v}_1(t) \\ \tilde{p}_1(t) \end{pmatrix}, \\
M_1 \tilde{v}_1(0) &= v_1^{(0)} \quad , \quad L_1 u(0) = B_{11} M_1^{-1} v_1^{(0)} + B_{1\Gamma} M_\Gamma(\boldsymbol{\theta})^{-1} v_\Gamma^{(0)}(\boldsymbol{\theta}).
\end{aligned}
$$

Hence, the BT error bound gives

$$
\left\| \begin{pmatrix} \tilde{z}_1 - \widehat{z}_1 \\ \tilde{z}_{v,\Gamma} - \widehat{z}_{v,\Gamma} \\ \tilde{z}_{p,\Gamma} - \widehat{z}_{p,\Gamma} \end{pmatrix} \right\|_{L^2} \leq 2 \left(\boldsymbol{\sigma}_{p+1} + \cdots + \boldsymbol{\sigma}_n \right) \left\| \begin{pmatrix} u \\ \widehat{v}_\Gamma \\ \widehat{p}_0 \end{pmatrix} \right\|_{L^2} .
$$

Cont'd proof. Now, we consider the error in the states

$$e_v := (v_1 - \tilde{v}_1, v_2 - \widehat{v}_2, v_\Gamma - \widehat{v}_\Gamma)^T \quad , \quad e_p := (p_1 - \tilde{p}_1, p_2 - \widehat{p}_2, p_0 - \widehat{p}_0)^T,$$

which satisfies the system

$$\begin{aligned} E(\boldsymbol{\theta}) \frac{d}{dt} \begin{pmatrix} e_v(t) \\ e_p(t) \end{pmatrix} &= -S(\boldsymbol{\theta}) \begin{pmatrix} e_v(t) \\ e_p(t) \end{pmatrix} + \begin{pmatrix} g_1(t) \\ 0 \end{pmatrix} \quad , \quad t \in (0,T], \\ M(\boldsymbol{\theta}) &= 0, \end{aligned}$$

where $g_1(t) := (0, 0, \tilde{z}_{v,\Gamma} - \widehat{z}_{v,\Gamma})^T$. Theorem 1 implies

$$\left\| \begin{pmatrix} v_1 - \tilde{v}_1 \\ v_2 - \widehat{v}_2 \\ v_\Gamma - \widehat{v}_\Gamma \end{pmatrix} \right\|_{L^2} \leq C \, \|\tilde{z}_{v,\Gamma} - \widehat{z}_{v,\Gamma}\|_{L^2} \quad , \quad \left\| \begin{pmatrix} p_1 - \tilde{p}_1 \\ p_2 - \widehat{p}_2 \\ p_0 - \widehat{p}_0 \end{pmatrix} \right\|_{L^2} \leq C \, \|\tilde{z}_{v,\Gamma} - \widehat{z}_{v,\Gamma}\|_{L^2}.$$

Department of Mathematics, University of Houston
Institut für Mathematatik, Universität Augsburg

Lemma [AHH09] (Estimation of the Adjoint States).

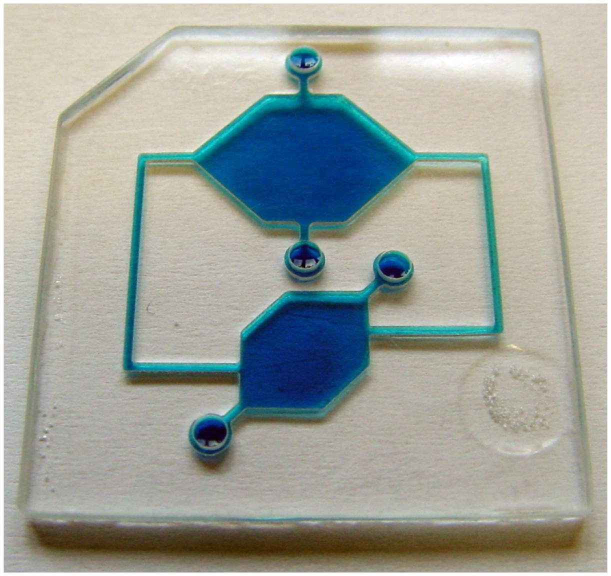
Let x, x_Γ as in Lemma 1 and assume that $\mu := (\mu_1, \mu_2, \mu_\Gamma)^T$ with $\mu_i := (\lambda_i, \kappa_i)^T$, $1 \le i \le 2$, $\mu_\Gamma := (\lambda_\Gamma, \kappa_0)^T$ and $\hat{\mu} := (\hat{\mu}_1, \hat{\mu}_2, \hat{\mu}_\Gamma)^T$ with $\hat{\mu}_1 := \hat{\lambda}_1, \hat{\mu}_2 := (\hat{\lambda}_2, \hat{\kappa}_2)^T$, $\hat{\mu}_\Gamma := (\hat{\lambda}_\Gamma, \hat{\kappa}_0)^T$ satisfy the optimality systems associated with the full order and the reduced order model. Then, under assumptions $(A_2), (A_3)$ and for $\lambda_1^{(T)} = 0$ there exists $C > 0$ such that

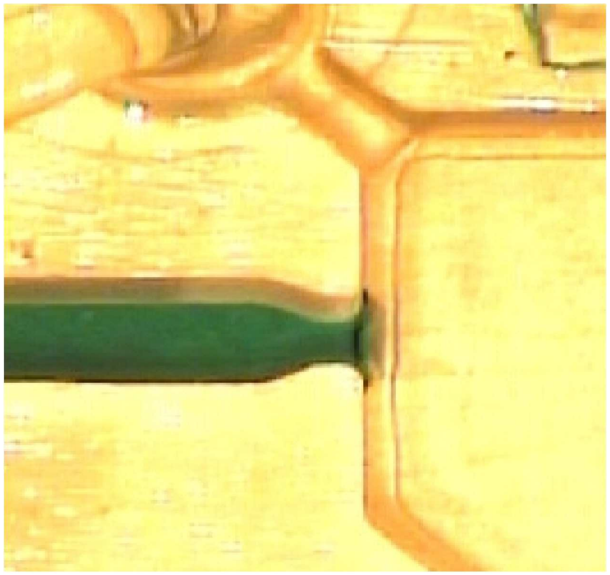
$$\left\| \begin{pmatrix} \lambda_2 - \hat{\lambda}_2 \\ \lambda_\Gamma - \hat{\lambda}_\Gamma \end{pmatrix} \right\|_{L^2} \le C \left(\left\| \begin{pmatrix} u \\ \hat{x}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \hat{z}_1 \\ \hat{\mu}_\Gamma \end{pmatrix} \right\|_{L^2} \right) \left(\sigma_{p+1} + \cdot + \sigma_n \right),$$

$$\left\| \begin{pmatrix} \kappa_2 - \hat{\kappa}_2 \\ \kappa_0 - \hat{\kappa}_0 \end{pmatrix} \right\|_{L^2} \le C \left(\left\| \begin{pmatrix} u \\ \hat{x}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \hat{z}_1 \\ \hat{\mu}_\Gamma \end{pmatrix} \right\|_{L^2} \right) \left(\sigma_{p+1} + \cdot + \sigma_n \right).$$

Optimal Design of Microfluidic Biochips

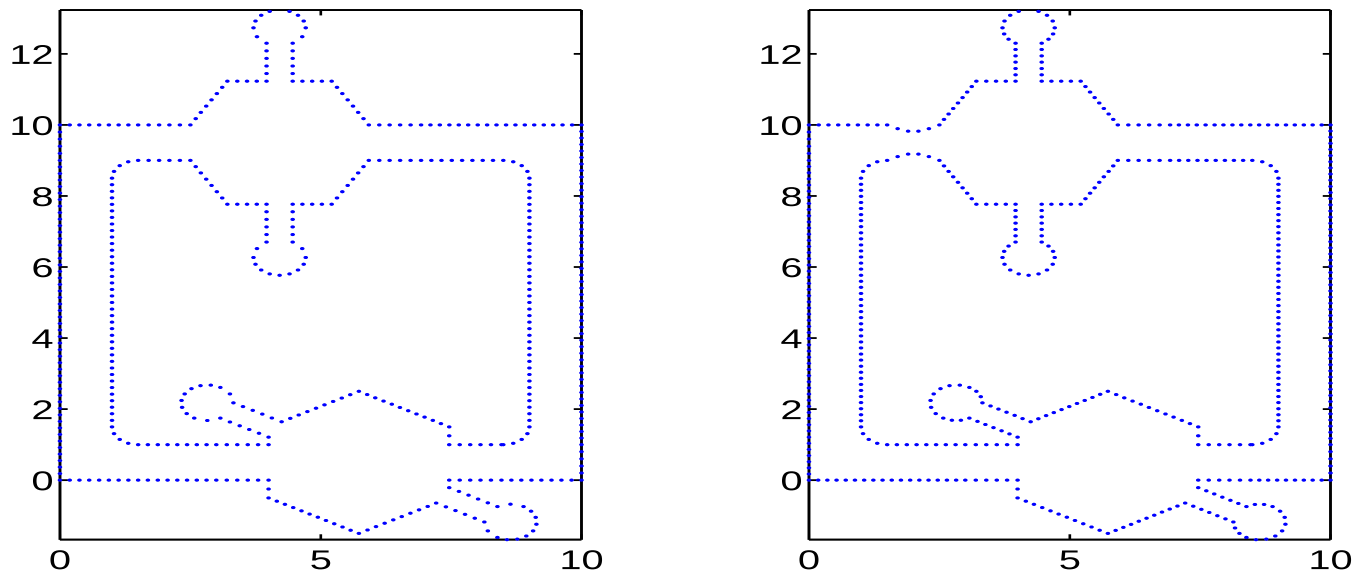
DDBT Model Reduction: Shape Optimization of Microfluidic Biochips





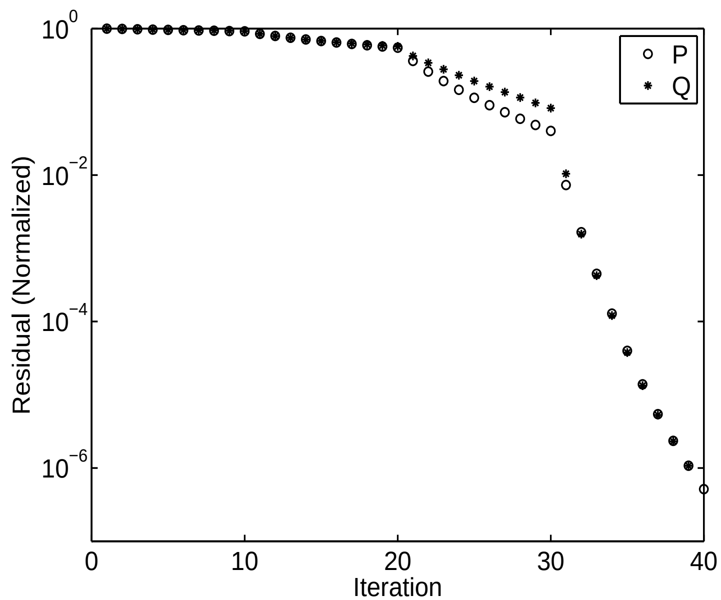
Microfluidic biochip (left) and capillary barrier (right)

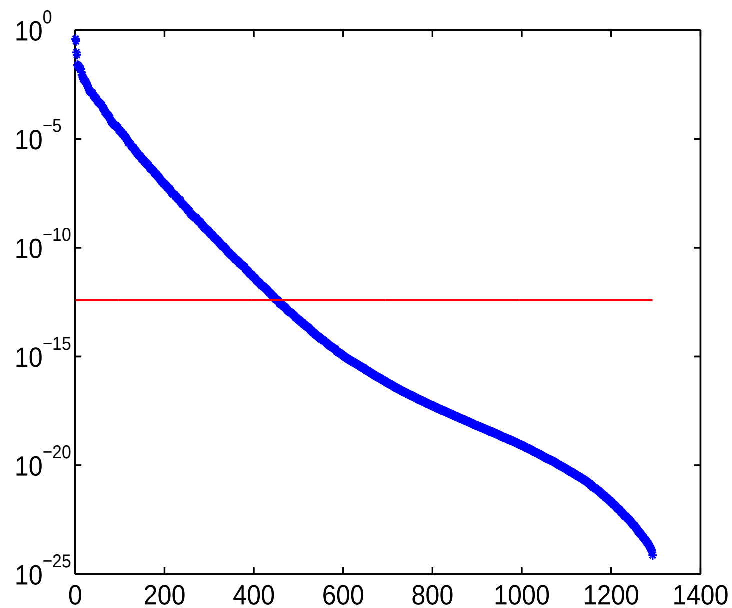
DDBT Model Reduction: Shape Optimization of Microfluidic Biochips



Shape optimization of a capillary barrier:
Initial Configuration (left), optimal design (right)

DDBT Model Reduction: Shape Optimization of Microfluidic Biochips





Convergence of the multishift ADI (left) and Hankel singular values (right)

DDBT Model Reduction: Shape Optimization of Microfluidic Biochips

ℓ	m	$N_{DoF}^{FOM}(\Omega)$	$N_{DoF}^{ROM}(\Omega)$	$N_{DoF}^{FOM}(\Omega_1)$	$N_{DoF}^{ROM}(\Omega_1)$
1	167	7640	509	7482	351
2	195	11668	596	11442	370
3	291	16830	777	16504	451
4	802	49238	1680	48324	766

Grid number ℓ, number of observations m, and Degrees of freedom (DoF) for the FOM and ROM in Ω and Ω_1

DDBT Model Reduction: Shape Optimization of Microfluidic Biochips

θ^*	9.8997	9.7502	9.7498	9.8997	9.1000	9.2497	9.2504	9.0998
$\widehat{\theta}^*$	9.9016	9.7506	9.7498	9.9013	9.0980	9.2489	9.2500	9.0979

Optimal design parameters for the FOM (θ^*) and the ROM ($\widehat{\theta}^*$)