Optimization and Model Reduction of Time Dependent PDE-Constrained Optimization Problems

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Outline

Outline

The Problem

- We consider optimal control problems governed by advection diffusion equations

$$\frac{\partial}{\partial t} y(x,t) - \nabla(k(x)\nabla y(x,t)) + V(x) \cdot \nabla y(x,t)) = f(x,t)$$

in $\Omega \times (0,T)$. The optimization variables are related to the right hand side f or to boundary data.

- After (finite element) discretization in space the optimal control problems are of the form

$$\min J(\mathbf{u}) \equiv \frac{1}{2}\int_0^T \|\mathbf{C}\mathbf{y}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t)\|^2 dt,$$

where $\mathbf{y}(t) = \mathbf{y}(\mathbf{u};t)$ is the solution of

$$\begin{aligned} \mathbf{M}\mathbf{y}'(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{u}(t), \qquad t \in (0,T), \\ \mathbf{y}(0) &= \mathbf{y}_0. \end{aligned}$$

Here $\mathbf{y}(t) \in \mathbb{R}^N$, $\mathbf{M}, \mathbf{A} \in \mathbb{R}^{N\times N}$, $\mathbf{B} \in \mathbb{R}^{N\times m}$, with N large.

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The Reduced Order Problem

- Projection matrices $\mathbf{W}, \mathbf{V} \in \mathbb{R}^{N \times n}$ with $n \ll N$ small.
- Replace states $\mathbf{y}(t)$ by $\mathbf{V}\widehat{\mathbf{y}}(t)$ and project state equation by $\mathbf{W}$. This gives reduced order state equation

$$\underbrace{\mathbf{W}^T\mathbf{M}\mathbf{V}}_{=\widehat{\mathbf{M}}}\widehat{\mathbf{y}}'(t) = \underbrace{\mathbf{W}^T\mathbf{A}\mathbf{V}}_{=\widehat{\mathbf{A}}}\widehat{\mathbf{y}}(t) + \underbrace{\mathbf{W}^T\mathbf{B}}_{=\widehat{\mathbf{B}}}\mathbf{u}(t)$$

and reduced order objective function

$$\int_0^T \| \underbrace{\mathbf{C}\mathbf{V}}_{=\widehat{\mathbf{C}}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t)\|^2 dt.$$

- The reduced optimal control problem is

$$\min \widehat{J}(\mathbf{u}) \equiv \frac{1}{2}\int_0^T \|\widehat{\mathbf{C}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t)\|^2 dt$$

where $\widehat{\mathbf{y}}(t) = \widehat{\mathbf{y}}(\mathbf{u}; t)$ solves

$$\begin{aligned} \widehat{\mathbf{M}}\widehat{\mathbf{y}}'(t) &= \widehat{\mathbf{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t), \qquad t \in (0, T), \\ \widehat{\mathbf{y}}(0) &= \widehat{\mathbf{y}}_0. \end{aligned}$$

Here $\widehat{\mathbf{y}}(t) \in \mathbb{R}^n$, $\widehat{\mathbf{M}}, \widehat{\mathbf{A}} \in \mathbb{R}^{n \times n}$, $\widehat{\mathbf{B}} \in \mathbb{R}^{n \times m}$, with $n \ll N$ small.

Error Analysis (Standard)

- $\mathbf{U}$ Hilbert space.
- Let $\mathbf{u}_* = \text{argmin}_{\mathbf{u}\in\mathbf{U}} J(\mathbf{u})$ be the minimizer of the original problem and let $\widehat{\mathbf{u}}_* = \text{argmin}_{\mathbf{u}\in\mathbf{U}} \widehat{J}(\mathbf{u})$ a minimizer of the reduced problem.
- Assume that J is a strictly convex quadratic function, i.e., that there exists $\kappa > 0$ such that

$$\langle \mathbf{u}-\mathbf{w}, \nabla J(\mathbf{u}) - \nabla J(\mathbf{w})\rangle_{\mathbf{U}} \geq \kappa \|\mathbf{u}-\mathbf{w}\|_{\mathbf{U}}^2 \text{ for all } \mathbf{u},\mathbf{w}\in\mathbf{U}.$$

- Set $\mathbf{u} = \mathbf{u}_*$ and $\mathbf{w} = \widehat{\mathbf{u}}_*$ and use

$$\nabla J(\mathbf{u}_*) = \nabla \widehat{J}(\widehat{\mathbf{u}}_*) = 0$$

  to get

$$\begin{aligned} &\|\mathbf{u}_* - \widehat{\mathbf{u}}_*\|_{\mathbf{U}} \|\nabla \widehat{J}(\widehat{\mathbf{u}}_*) - \nabla J(\widehat{\mathbf{u}}_*)\|_{\mathbf{U}} \\ &= \|\mathbf{u}_* - \widehat{\mathbf{u}}_*\|_{\mathbf{U}} \|\nabla J(\mathbf{u}_*) - \nabla J(\widehat{\mathbf{u}}_*)\|_{\mathbf{U}} \\ &\geq \langle \mathbf{u}_* - \widehat{\mathbf{u}}_*, \nabla J(\mathbf{u}_*) - \nabla J(\widehat{\mathbf{u}}_*)\rangle_{\mathbf{U}} \geq \kappa \|\mathbf{u}_* - \widehat{\mathbf{u}}_*\|_{\mathbf{U}}^2. \end{aligned}$$

- Hence

$$\|\mathbf{u}_* - \widehat{\mathbf{u}}_*\|_{\mathbf{U}} \leq \kappa^{-1} \|\nabla \widehat{J}(\widehat{\mathbf{u}}_*) - \nabla J(\widehat{\mathbf{u}}_*)\|_{\mathbf{U}}.$$

- Need to estimate error in the gradients to get estimate for error in the solution.

Gradient Computation

- For the original problem

$$\begin{aligned} \mathbf{M}\mathbf{y}'(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{u}(t), && t \in (0,T), \quad \mathbf{y}(0) = \mathbf{y}_0, \\ \mathbf{z}(t) &= \mathbf{C}\mathbf{y}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t), && t \in (0,T) \\ -\mathbf{M}^T\boldsymbol{\lambda}'(t) &= \mathbf{A}^T\boldsymbol{\lambda}(t) + \mathbf{C}^T\mathbf{z}(t), && t \in (0,T), \quad \boldsymbol{\lambda}(T) = 0, \\ \nabla J(\mathbf{u}) = \mathbf{q}(t) &= \mathbf{B}^T\boldsymbol{\lambda}(t) + \mathbf{D}^T\mathbf{z}(t), && t \in (0,T) \end{aligned}$$

- For the reduced problem

$$\begin{aligned} \widehat{\mathbf{M}}\widehat{\mathbf{y}}'(t) &= \widehat{\mathbf{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t), && t \in (0,T) \quad \widehat{\mathbf{y}}(0) = \widehat{\mathbf{y}}_0, \\ \widehat{\mathbf{z}}(t) &= \widehat{\mathbf{C}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t), && t \in (0,T) \\ -\widehat{\mathbf{M}}^T\widehat{\boldsymbol{\lambda}}'(t) &= \widehat{\mathbf{A}}^T\widehat{\boldsymbol{\lambda}}(t) + \widehat{\mathbf{C}}^T\widehat{\mathbf{z}}(t), && t \in (0,T) \quad \widehat{\boldsymbol{\lambda}}(T) = 0, \\ \nabla \widehat{J}(\mathbf{u}) = \widehat{\mathbf{q}}(t) &= \widehat{\mathbf{B}}^T\widehat{\boldsymbol{\lambda}}(t) + \mathbf{D}^T\widehat{\mathbf{z}}(t), && t \in (0,T) \end{aligned}$$

Requirement on Reduced Order Model

- Need to approximte state system

$$\begin{aligned} \mathbf{M}\mathbf{y}'(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{u}(t), \quad t \in (0,T) \\ \mathbf{z}(t) &= \mathbf{C}\mathbf{y}(t) + \mathbf{D}\mathbf{u}(t), \quad t \in (0,T) \end{aligned}$$

  and corresponding adjoint system

$$\begin{aligned} -\mathbf{M}\boldsymbol{\lambda}'(t) &= \mathbf{A}^T\boldsymbol{\lambda}(t) + \mathbf{C}\mathbf{w}(t), \quad t \in (0,T) \\ \mathbf{q}(t) &= \mathbf{B}^T\boldsymbol{\lambda}(t) + \mathbf{D}^T\mathbf{w}(t), \quad t \in (0,T) \end{aligned}$$

- Need to approximate input-to-output maps

$$\mathbf{u} \mapsto \mathbf{z} \quad \text{and} \quad \mathbf{w} \mapsto \mathbf{q}.$$

- We assume $\mathbf{y}_0 = \mathbf{0}$ to simplify presentation. Inhomogeneous initial data can be handled with modification (Heinkenschloss, Reis, Antoulas 2011).

- Want reduced order state and adjoint systems

$$\widehat{\mathbf{M}}\widehat{\mathbf{y}}'(t) = \widehat{\mathbf{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t), \quad t \in (0,T)$$
$$\widehat{\mathbf{z}}(t) = \widehat{\mathbf{C}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t), \quad t \in (0,T),$$
$$\widehat{\mathbf{M}}^T\widehat{\boldsymbol{\lambda}}'(t) = \widehat{\mathbf{A}}^T\widehat{\boldsymbol{\lambda}}(t) + \widehat{\mathbf{C}}^T\mathbf{w}(t), \quad t \in (0,T)$$
$$\widehat{\mathbf{q}}(t) = \widehat{\mathbf{B}}^T\widehat{\boldsymbol{\lambda}}(t) + \mathbf{D}^T\mathbf{w}(t), \quad t \in (0,T)$$

  with $\widehat{\mathbf{M}} = \mathbf{W}^T\mathbf{M}\mathbf{V}$, $\widehat{\mathbf{A}} = \mathbf{W}^T\mathbf{A}\mathbf{V}$, $\widehat{\mathbf{B}} = \mathbf{W}^T\mathbf{B}$, and $\widehat{\mathbf{C}} = \mathbf{C}\mathbf{V}$,
- such that we have error bounds

$$\|\mathbf{z} - \widehat{\mathbf{z}}\|_{L^2} \leq \text{ tol } \|\mathbf{u}\|_{L^2} \quad \text{and} \quad \|\mathbf{q} - \widehat{\mathbf{q}}\|_{L^2} \leq \text{ tol } \|\mathbf{w}\|_{L^2}. \qquad (*)$$

  for any given inputs $\mathbf{u}$ and $\mathbf{w}$, where tol is a user specified tolerance.

- Want reduced order state and adjoint systems

$$\widehat{\mathbf{M}}\widehat{\mathbf{y}}'(t) = \widehat{\mathbf{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t), \quad t \in (0,T)$$
$$\widehat{\mathbf{z}}(t) = \widehat{\mathbf{C}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t), \quad t \in (0,T),$$
$$\widehat{\mathbf{M}}^T\widehat{\boldsymbol{\lambda}}'(t) = \widehat{\mathbf{A}}^T\widehat{\boldsymbol{\lambda}}(t) + \widehat{\mathbf{C}}^T\mathbf{w}(t), \quad t \in (0,T)$$
$$\widehat{\mathbf{q}}(t) = \widehat{\mathbf{B}}^T\widehat{\boldsymbol{\lambda}}(t) + \mathbf{D}^T\mathbf{w}(t), \quad t \in (0,T)$$

  with $\widehat{\mathbf{M}} = \mathbf{W}^T\mathbf{M}\mathbf{V}$, $\widehat{\mathbf{A}} = \mathbf{W}^T\mathbf{A}\mathbf{V}$, $\widehat{\mathbf{B}} = \mathbf{W}^T\mathbf{B}$, and $\widehat{\mathbf{C}} = \mathbf{C}\mathbf{V}$,
- such that we have error bounds

$$\|\mathbf{z} - \widehat{\mathbf{z}}\|_{L^2} \leq \text{ tol } \|\mathbf{u}\|_{L^2} \quad \text{and} \quad \|\mathbf{q} - \widehat{\mathbf{q}}\|_{L^2} \leq \text{ tol } \|\mathbf{w}\|_{L^2}. \qquad (*)$$

  for any given inputs $\mathbf{u}$ and $\mathbf{w}$, where tol is a user specified tolerance.
- If the system is stable ($\text{Re}(\lambda(\mathcal{A})) < 0$), controllable and observable, we can use Balanced Truncation Model Reduction (BTMR).
  BTMR error bound: For any given inputs $\mathbf{u}$ and $\mathbf{w}$

$$\|\mathbf{z} - \widehat{\mathbf{z}}\|_{L^2} \leq 2(\sigma_{n+1} + \ldots + \sigma_N)\ \|\mathbf{u}\|_{L^2},$$
$$\|\mathbf{q} - \widehat{\mathbf{q}}\|_{L^2} \leq 2(\sigma_{n+1} + \ldots + \sigma_N)\ \|\mathbf{w}\|_{L^2},$$

  where $\sigma_1 \geq \ldots \geq \sigma_n \geq \sigma_{n+1} \geq \ldots \sigma_N \geq 0$ are the Hankel singular values.

- Want reduced order state and adjoint systems

$$\begin{aligned} \widehat{\mathbf{M}}\widehat{\mathbf{y}}'(t) &= \widehat{\mathbf{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t), \quad t \in (0,T) \\ \widehat{\mathbf{z}}(t) &= \widehat{\mathbf{C}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t), \quad t \in (0,T), \\ \widehat{\mathbf{M}}^T\widehat{\boldsymbol{\lambda}}'(t) &= \widehat{\mathbf{A}}^T\widehat{\boldsymbol{\lambda}}(t) + \widehat{\mathbf{C}}^T\mathbf{w}(t), \quad t \in (0,T) \\ \widehat{\mathbf{q}}(t) &= \widehat{\mathbf{B}}^T\widehat{\boldsymbol{\lambda}}(t) + \mathbf{D}^T\mathbf{w}(t), \quad t \in (0,T) \end{aligned}$$

  with $\widehat{\mathbf{M}} = \mathbf{W}^T\mathbf{M}\mathbf{V}$, $\widehat{\mathbf{A}} = \mathbf{W}^T\mathbf{A}\mathbf{V}$, $\widehat{\mathbf{B}} = \mathbf{W}^T\mathbf{B}$, and $\widehat{\mathbf{C}} = \mathbf{C}\mathbf{V}$,
- such that we have error bounds

$$\|\mathbf{z} - \widehat{\mathbf{z}}\|_{L^2} \leq \text{ tol } \|\mathbf{u}\|_{L^2} \quad \text{and} \quad \|\mathbf{q} - \widehat{\mathbf{q}}\|_{L^2} \leq \text{ tol } \|\mathbf{w}\|_{L^2}. \qquad (*)$$

  for any given inputs $\mathbf{u}$ and $\mathbf{w}$, where tol is a user specified tolerance.
- If the system is stable (Re$(\lambda(\mathcal{A})) < 0$), controllable and observable, we can use Balanced Truncation Model Reduction (BTMR).
  BTMR error bound: For any given inputs $\mathbf{u}$ and $\mathbf{w}$

$$\begin{aligned} \|\mathbf{z} - \widehat{\mathbf{z}}\|_{L^2} &\leq 2(\sigma_{n+1} + \ldots + \sigma_N)\ \|\mathbf{u}\|_{L^2}, \\ \|\mathbf{q} - \widehat{\mathbf{q}}\|_{L^2} &\leq 2(\sigma_{n+1} + \ldots + \sigma_N)\ \|\mathbf{w}\|_{L^2}, \end{aligned}$$

  where $\sigma_1 \geq \ldots \geq \sigma_n \geq \sigma_{n+1} \geq \ldots \sigma_N \geq 0$ are the Hankel singular values.
- We use BTMR in our numerics, but theoretical results only rely on error bound (*). Other model reduction approaches that have an error bound (*) can be used as well. We state results with tol $= 2(\sigma_{n+1} + \ldots + \sigma_N)$.

Back to Gradient Error Estimates

- For the original problem

$$
\begin{aligned}
\mathbf{M}\mathbf{y}'(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{u}(t), && t \in (0,T), \quad \mathbf{y}(0) = \mathbf{y}_0,\\
\mathbf{z}(t) &= \mathbf{C}\mathbf{y}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t), && t \in (0,T)\\
-\mathbf{M}\boldsymbol{\lambda}'(t) &= \mathbf{A}^T\boldsymbol{\lambda}(t) + \mathbf{C}^T\mathbf{z}(t), && t \in (0,T), \quad \boldsymbol{\lambda}(T) = 0,\\
\nabla J(\mathbf{u}) = \mathbf{q}(t) &= \mathbf{B}^T\boldsymbol{\lambda}(t) + \mathbf{D}^T\mathbf{z}(t), && t \in (0,T)
\end{aligned}
$$

- For the reduced problem

$$
\begin{aligned}
\widehat{\mathbf{y}}'(t) &= \widehat{\mathbf{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}}\mathbf{u}(t), && t \in (0,T) \quad \widehat{\mathbf{y}}(0) = \widehat{\mathbf{y}}_0,\\
\widehat{\mathbf{z}}(t) &= \widehat{\mathbf{C}}\widehat{\mathbf{y}}(t) + \mathbf{D}\mathbf{u}(t) - \mathbf{d}(t), && t \in (0,T)\\
-\widehat{\boldsymbol{\lambda}}'(t) &= \widehat{\mathbf{A}}^T\widehat{\boldsymbol{\lambda}}(t) + \widehat{\mathbf{C}}^T\widehat{\mathbf{z}}(t), && t \in (0,T) \quad \widehat{\boldsymbol{\lambda}}(T) = 0,\\
\nabla \widehat{J}(\mathbf{u}) = \widehat{\mathbf{q}}(t) &= \widehat{\mathbf{B}}^T\widehat{\boldsymbol{\lambda}}(t) + \mathbf{D}^T\widehat{\mathbf{z}}(t), && t \in (0,T)
\end{aligned}
$$

- We can *almost* apply BTMR error bounds, but need same inputs $\mathbf{w}$ in full and reduced order adjoint system.
- Easy to fix: Introduce auxiliary adjoint $\widetilde{\boldsymbol{\lambda}}$ as solution of the original adjoint, but with input $\widehat{\mathbf{z}}$ instead of $\mathbf{z}$.

Error Estimate

- Assume that there exists $\alpha > 0$ such that

$$\mathbf{v}^T \mathbf{A} \mathbf{v} \leq -\alpha \mathbf{v}^T \mathbf{M} \mathbf{v}, \qquad \forall \mathbf{v} \in \mathbb{R}^N.$$

  For any $\mathbf{u} \in L^2$ let $\widehat{\mathbf{y}}(\mathbf{u})$ be the corresponding reduced state and $\widehat{\mathbf{z}}(\mathbf{u}) = \widehat{\mathbf{C}}\widehat{\mathbf{y}}(\mathbf{u}) + \mathbf{D}\mathbf{u} - \mathbf{d}$.

- There exists $c > 0$ such that the error in the gradients obeys

$$\|\nabla J(\mathbf{u}) - \nabla \widehat{J}(\mathbf{u})\|_{L^2} \leq 2 \left(c\|\mathbf{u}\|_{L^2} + \|\widehat{\mathbf{z}}(\mathbf{u})\|_{L^2} \right) (\sigma_{n+1} + \ldots + \sigma_N)$$

  for all $\mathbf{u} \in L^2$!

- Consequently, the error between the solutions satisfies

$$\|\mathbf{u}_* - \widehat{\mathbf{u}}_*\|_{L^2} \leq \frac{2}{\kappa} \left(c\|\widehat{\mathbf{u}}_*\|_{L^2} + \|\widehat{\mathbf{z}}_*\|_{L^2} \right) (\sigma_{n+1} + \ldots + \sigma_N).$$

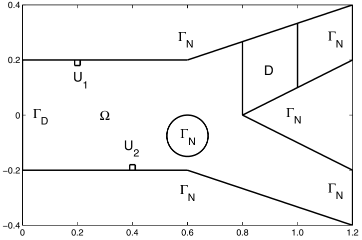
Example Problem (modeled after Dede/Quarteroni 2005)

$$\text{Minimize } \frac{1}{2}\int_0^T \int_D (y(x,t) - d(x,t))^2 dx\, dt + \frac{10^{-4}}{2}\int_0^T \int_{U_1 \cup U_2} u^2(x,t) dx\, dt,$$

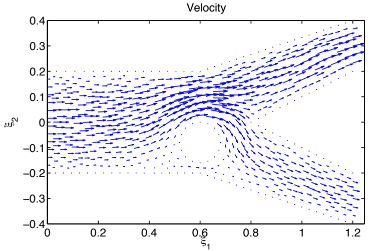
subject to

$$\frac{\partial}{\partial t} y(x,t) - \nabla(k \nabla y(x,t)) + \mathbf{V}(x) \cdot \nabla y(x,t)$$
$$= u(x,t)\chi_{U_1}(x) + u(x,t)\chi_{U_2}(x) \qquad \text{in } \Omega \times (0,4),$$

with boundary conditions $y(x,t) = 0$ on $\Gamma_D \times (0,4)$, $\frac{\partial}{\partial n} y(x,t) = 0$ on $\Gamma_N \times (0,4)$ and initial conditions $y(x,0) = 0$ in Ω.



Ω with boundary conditions for the advection diffusion equation



the velocity field $\mathbf{v}$

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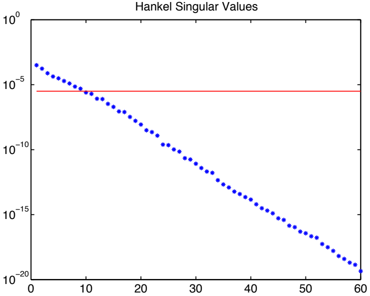
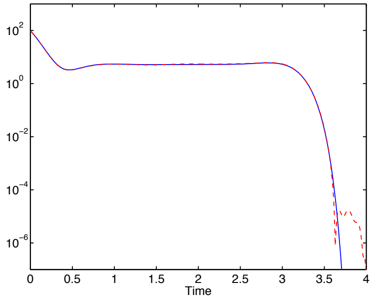
grid	m	k	N	n
1	168	9	1545	9
2	283	16	2673	9
3	618	29	6036	9

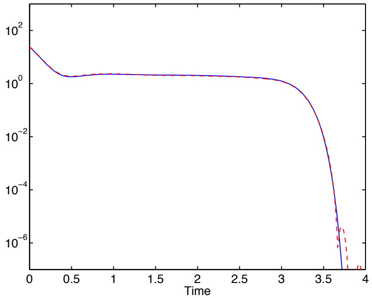
The number m of observations, the number k of controls, the size N of the full order system, and the size n of the reduced order system for three discretizations.



The largest Hankel singular values and the threshold $10^{-4}\sigma_1$ (fine grid)

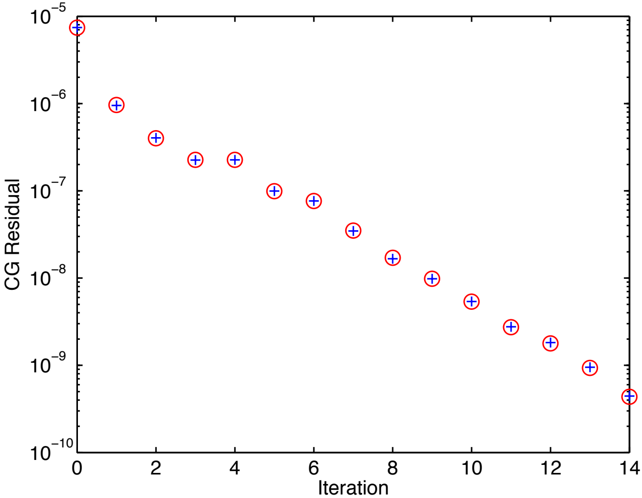


Integrals $\int_{U_1} u_*^2(x,t)dx$ (solid blue line) and $\int_{U_1} \widehat{u}_*^2(x,t)dx$ (dashed red line) of the optimal controls computed using the full and and the reduced order model.



Integrals $\int_{U_2} u_*^2(x,t)dx$ (solid blue line) and $\int_{U_2} \widehat{u}_*^2(x,t)dx$ (dashed red line) of the optimal controls computed using the full and and the reduced order model.

The full and reduced order model solutions are in excellent agreement: $\|u_* - \widehat{u}_*\|_{L^2}^2 = 6.2 \cdot 10^{-3}$.



The convergence histories of the Conjugate Gradient algorithm applied to the full ($+$) and the reduced (o) order optimal control problems.

Recall error bound for the gradients:

$$\|\nabla J(\mathbf{u}) - \nabla \widehat{J}(\mathbf{u})\|_{L^2} \leq 2\left(c\|\mathbf{u}\|_{L^2} + \|\widehat{\mathbf{z}}(\mathbf{u})\|_{L^2}\right)(\sigma_{n+1} + \ldots + \sigma_N)$$

for all $\mathbf{u} \in L^2$!

Outline

Shape Optimization Problem

- Consider the minimization problem

$$\min_{\theta \in \Theta_{ad}} J(\theta) := \int_0^T \int_{\Omega(\theta)} \ell(y(x,t;\theta),t,\theta)dx\ dt$$

where $y(x,t;\theta)$ solves

$$\begin{aligned}
\frac{\partial}{\partial t} y(x,t) - \nabla(k(x)\nabla y(x,t)) & \\
+V(x)\cdot\nabla y(x,t)) &= f(x,t) \qquad (x,t) \in \Omega(\theta)\times(0,T),\\
k(x)\nabla y(x,t)\cdot n &= g(x,t) \qquad (x,t)\in \Gamma_N(\theta)\times(0,T),\\
y(x,t) &= u(x,t) \qquad (x,t)\in\Gamma_D(\theta)\times(0,T),\\
y(x,0) &= y_0(x) \qquad x\in\Omega_D(\theta)
\end{aligned}$$

- Semidiscretization in space leads to

$$\min_{\theta \in \Theta_{ad}} J(\theta) := \int_0^T \ell(\mathbf{y}(t;\theta),t,\theta)\ dt$$

where $\mathbf{y}(t;\theta)$ solves

$$\begin{aligned}
\mathbf{M}(\theta)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\theta)\mathbf{y}(t) &= \mathbf{B}(\theta)\mathbf{u}(t), \quad t\in[0,T],\\
\mathbf{M}(\theta)\mathbf{y}(0) &= \mathbf{M}(\theta)\mathbf{y}_0.
\end{aligned}$$

- We would like to replace the large scale problem

$$\min_{\theta \in \Theta_{ad}} J(\theta) := \int_0^T \ell(\mathbf{y}(t;\theta), t, \theta)\ dt$$

where $\mathbf{y}(t;\theta)$ solves

$$\begin{aligned} \mathbf{M}(\theta)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\theta)\mathbf{y}(t) &= \mathbf{B}(\theta)\mathbf{u}(t), \quad t \in [0,T], \\ \mathbf{M}(\theta)\mathbf{y}(0) &= \mathbf{M}(\theta)\mathbf{y}_0 \end{aligned}$$

- by a reduced order problem

$$\min_{\theta \in \Theta_{ad}} \widehat{J}(\theta) := \int_0^T \ell(\widehat{\mathbf{y}}(t;\theta), t, \theta)\ dt$$

where $\widehat{\mathbf{y}}(t;\theta)$ solves

$$\begin{aligned} \widehat{\mathbf{M}(\theta)}\frac{d}{dt}\widehat{\mathbf{y}}(t) + \widehat{\mathbf{A}(\theta)}\mathbf{y}(t) &= \widehat{\mathbf{B}(\theta)}\mathbf{u}(t), \quad t \in [0,T], \\ \widehat{\mathbf{M}(\theta)}\widehat{\mathbf{y}}(0) &= \widehat{\mathbf{M}(\theta)}\widehat{\mathbf{y}}_0. \end{aligned}$$

- Problem is that we need a reduced order model that approximates the full order model for all $\theta \in \Theta_{ad}$!

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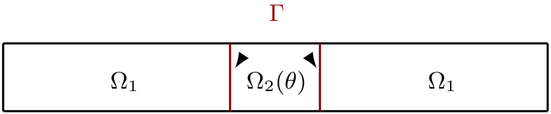
Consider Problems with Local Nonlinearity

- Consider classes of problems where the shape parameter θ only influences a (small) subdomain:

$$\bar{\Omega}(\theta) := \bar{\Omega}_1 \cup \bar{\Omega}_2(\theta), \quad \Omega_1 \cap \Omega_2(\theta) = \emptyset, \quad \Gamma = \bar{\Omega}_1 \cap \bar{\Omega}_2(\theta).$$



- The FE stiffness matrix times vector can be decomposed into

$$\mathbf{A}\mathbf{y} = \begin{pmatrix} \mathbf{A}_1^{II} & \mathbf{A}_1^{I\Gamma} & 0 \\ \mathbf{A}_1^{\Gamma I} & \mathbf{A}^{\Gamma\Gamma}(\theta) & \mathbf{A}_2^{\Gamma I}(\theta) \\ 0 & \mathbf{A}_2^{I\Gamma}(\theta) & \mathbf{A}_2^{II}(\theta) \end{pmatrix} \begin{pmatrix} \mathbf{y}_1^I \\ \mathbf{y}^\Gamma \\ \mathbf{y}_2^I \end{pmatrix}$$

  where $\mathbf{A}^{\Gamma\Gamma}(\theta) = \mathbf{A}_1^{\Gamma\Gamma} + \mathbf{A}_2^{\Gamma\Gamma}(\theta)$.
  The matrices $\mathbf{M}$, $\mathbf{B}$ admit similar representations.
- Consider objective functions of the type

$$\int_0^T \ell(\mathbf{y}(t), t, \theta)dt = \frac{1}{2}\int_0^T \|\mathbf{C}_1^I \mathbf{y}_1^I - \mathbf{d}_1^I(t)\|_2^2 + \widetilde{\ell}(\mathbf{y}^\Gamma(t), \mathbf{y}_2^I(t), t, \theta)dt.$$

Our Optimization problem

$$\min_{\theta\in\Theta_{ad}} J(\theta) := \int_0^T \ell(\mathbf{y}(t;\theta), t, \theta)\ dt$$

where $\mathbf{y}(t;\theta)$ solves

$$\begin{aligned}\mathbf{M}(\theta)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\theta)\mathbf{y}(t) &= \mathbf{B}(\theta)\mathbf{u}(t), \quad t\in[0,T],\\ \mathbf{M}(\theta)\mathbf{y}(0) &= \mathbf{M}(\theta)\mathbf{y}_0\end{aligned}$$

can now be written as

$$\min_{\theta\in\Theta_{ad}} J(\theta) := \frac{1}{2}\int_0^T \|\mathbf{C}_1^I\mathbf{y}_1^I - \mathbf{d}_1^I(t)\|_2^2 + \widetilde{\ell}(\mathbf{y}^\Gamma(t), \mathbf{y}_2^I(t), t, \theta) dt.$$

where $\mathbf{y}(t;\theta)$ solves

$$\begin{aligned}\mathbf{M}_1^{II}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_1^{II}\mathbf{y}_1^I(t) + \mathbf{A}_1^{I\Gamma}\mathbf{y}^\Gamma(t) &= \mathbf{B}_1^I\mathbf{u}_1^I(t)\\ \mathbf{M}_2^{II}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) + \mathbf{M}_2^{I\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{II}(\theta)\mathbf{y}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\theta)\mathbf{y}^\Gamma(t) &= \mathbf{B}_2^I(\theta)\mathbf{u}_2^I(t)\\ \mathbf{M}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{M}_2^{\Gamma I}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) &\\ +\mathbf{A}_1^{\Gamma I}\mathbf{y}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\theta)\mathbf{y}_2^I(t) &= \mathbf{B}^\Gamma(\theta)\mathbf{u}^\Gamma(t)\end{aligned}$$

Dependence on $\theta\in\Theta_{ad}$ is now localized. The fixed subsystem 1 is large. The variable subsystem 2 is small. Idea: Reduce subsystem 1 only.

First Order Optimality Conditions

- The first order necessary optimality conditions are

$$
\begin{aligned}
\mathbf{M}(\theta)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\theta)\mathbf{y}(t) &= \mathbf{B}(\theta)\mathbf{u}(t) \quad t \in [0,T], \\
\mathbf{M}(\theta)\mathbf{y}(0) &= \mathbf{y}_0, \\
-\mathbf{M}(\theta)\frac{d}{dt}\boldsymbol{\lambda}(t) + \mathbf{A}^T(\theta)\boldsymbol{\lambda}(t) &= -\nabla_{\mathbf{y}}\ell(\mathbf{y},t,\theta) \quad t \in [0,T], \\
\mathbf{M}(\theta)\boldsymbol{\lambda}(T) &= 0. \\
\nabla_\theta L(\mathbf{y}(t),\boldsymbol{\lambda}(t),\theta)(\widetilde{\theta} - \theta) \geq 0, &\quad \widetilde{\theta} \in \Theta_{ad}
\end{aligned}
$$

- Gradient of J is given by $\nabla J(\theta) = \nabla_\theta \ell(\mathbf{y}(t),\boldsymbol{\lambda}(t),\theta)$.

Using the DD structure, the state and adjoint equations can be written as

$$
\begin{aligned}
\mathbf{M}_1^{II}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_1^{II}\mathbf{y}_1^I(t) + \mathbf{A}_1^{I\Gamma}\mathbf{y}^\Gamma(t) &= \mathbf{B}_1^I\mathbf{u}_1^I(t)\\
\mathbf{M}_2^{II}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) + \mathbf{M}_2^{I\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{II}(\theta)\mathbf{y}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\theta)\mathbf{y}^\Gamma(t) &= \mathbf{B}_2^I(\theta)\mathbf{u}_2^I(t)\\
\mathbf{M}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{M}_2^{\Gamma I}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t)&\\
+\mathbf{A}_1^{\Gamma I}\mathbf{y}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\theta)\mathbf{y}_2^I(t) &= \mathbf{B}^\Gamma(\theta)\mathbf{u}^\Gamma(t),
\end{aligned}
$$

Using the DD structure, the state and adjoint equations can be written as

$$\begin{aligned}
\mathbf{M}_1^{II}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_1^{II}\mathbf{y}_1^I(t) + \mathbf{A}_1^{I\Gamma}\mathbf{y}^\Gamma(t) &= \mathbf{B}_1^I\mathbf{u}_1^I(t)\\
\mathbf{M}_2^{II}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) + \mathbf{M}_2^{I\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{II}(\theta)\mathbf{y}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\theta)\mathbf{y}^\Gamma(t) &= \mathbf{B}_2^I(\theta)\mathbf{u}_2^I(t)\\
\mathbf{M}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{M}_2^{\Gamma I}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) &\\
+\mathbf{A}_1^{\Gamma I}\mathbf{y}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\theta)\mathbf{y}_2^I(t) &= \mathbf{B}^\Gamma(\theta)\mathbf{u}^\Gamma(t),
\end{aligned}$$

$$\begin{aligned}
-\mathbf{M}_1^{II}\frac{d}{dt}\boldsymbol{\lambda}_1^I(t) - \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\boldsymbol{\lambda}^\Gamma(t) + \mathbf{A}_1^{II}\boldsymbol{\lambda}_1^I(t) + \mathbf{A}_1^{I\Gamma}\boldsymbol{\lambda}^\Gamma(t) &= -(\mathbf{C}_1^I)^T(\mathbf{C}_1^I\mathbf{y}_1^I(t) - \mathbf{d}_1^I)\\
-\mathbf{M}_2^{II}(\theta)\frac{d}{dt}\boldsymbol{\lambda}_2^I(t) - \mathbf{M}_2^{I\Gamma}(\theta)\frac{d}{dt}\boldsymbol{\lambda}^\Gamma(t) + \mathbf{A}_2^{II}(\theta)\boldsymbol{\lambda}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\theta)\boldsymbol{\lambda}^\Gamma(t) &= -\nabla_{\mathbf{y}_2^I}\widetilde{\ell}(.)\\
-\mathbf{M}_1^{\Gamma I}\frac{d}{dt}\boldsymbol{\lambda}_1^I(t) - \mathbf{M}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\boldsymbol{\lambda}^\Gamma(t) - \mathbf{M}_2^{\Gamma I}(\theta)\frac{d}{dt}\boldsymbol{\lambda}_2^I(t) &\\
+\mathbf{A}_1^{\Gamma I}\boldsymbol{\lambda}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\boldsymbol{\lambda}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\theta)\boldsymbol{\lambda}_2^I(t) &= -\nabla_{\mathbf{y}^\Gamma}\widetilde{\ell}(.),
\end{aligned}$$

To apply model reduction to the system corresponding to fixed subdomain Ω_1, we have to identify how $\mathbf{y}_1^I$ and $\boldsymbol{\lambda}_1^I$ interact with other components.

Model Reduction of Fixed Subdomain Problem

We need to reduce

$$
\begin{aligned}
\mathbf{M}_1^{II}\frac{d}{dt}\mathbf{y}_1^I(t) &= -\mathbf{A}_1^{II}\mathbf{y}_1^I(t) - \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{B}_1^I\mathbf{u}_1^I(t) - \mathbf{A}_1^{I\Gamma}\mathbf{y}^\Gamma(t)\\
\mathbf{z}_1^I &= \mathbf{C}_1^I\mathbf{y}_1^I(t) - \mathbf{d}_1^I\\
\mathbf{z}_1^\Gamma &= -\mathbf{M}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I - \mathbf{A}_1^{\Gamma I}\mathbf{y}_1^I,\\
-\mathbf{M}_1^{II}\frac{d}{dt}\boldsymbol{\lambda}_1^I(t) &= -\mathbf{A}_1^{II}\boldsymbol{\lambda}_1^I(t) + \mathbf{M}_1^{I\Gamma}\frac{d}{dt}\boldsymbol{\lambda}^\Gamma(t) - (\mathbf{C}_1^I)^T\mathbf{z}_1^I - \mathbf{A}_1^{I\Gamma}\boldsymbol{\lambda}^\Gamma(t)\\
\mathbf{q}_1^I &= (\mathbf{B}_1^I)^T\boldsymbol{\lambda}_1^I\\
\mathbf{q}_1^\Gamma &= \mathbf{M}_1^{\Gamma I}\frac{d}{dt}\boldsymbol{\lambda}_1^I - \mathbf{A}_1^{\Gamma I}\boldsymbol{\lambda}_1^I
\end{aligned}
$$

For simplicity we assume that

$$\mathbf{M}_1^{I\Gamma} = 0 \quad \mathbf{M}_1^{\Gamma I} = 0,$$

We get

$$
\begin{aligned}
\mathbf{M}_1^{II}\frac{d}{dt}\mathbf{y}_1^I(t) &= -\mathbf{A}_1^{II}\mathbf{y}_1^I(t) + (\mathbf{B}_1^I \mid -\mathbf{A}_1^{I\Gamma})\begin{pmatrix} \mathbf{u}_1^I \\ \mathbf{y}^\Gamma \end{pmatrix}, \\
\begin{pmatrix} \mathbf{z}_1^I \\ \mathbf{z}_1^\Gamma \end{pmatrix} &= \begin{pmatrix} -\mathbf{C}_1^I \\ -\mathbf{A}_1^{\Gamma I} \end{pmatrix}\mathbf{y}_1^I + \begin{pmatrix} \mathbf{I} \\ 0 \end{pmatrix}\mathbf{d}_1^I, \\
-\mathbf{M}_1^{II}\frac{d}{dt}\boldsymbol{\lambda}_1^I(t) &= -\mathbf{A}_1^{II}\boldsymbol{\lambda}_1^I(t) + (-(\mathbf{C}_1^I)^T \mid -\mathbf{A}_1^{I\Gamma})\begin{pmatrix} \mathbf{z}_1^I \\ \boldsymbol{\lambda}^\Gamma \end{pmatrix}, \\
\begin{pmatrix} \mathbf{q}_1^I \\ \mathbf{q}_1^\Gamma \end{pmatrix} &= \begin{pmatrix} (\mathbf{B}_1^I)^T \\ -\mathbf{A}_1^{\Gamma I} \end{pmatrix}\boldsymbol{\lambda}_1^I.
\end{aligned}
$$

This system is exactly of the form needed for balanced truncation model reduction.

Reduced Optimization Problem

- We apply BTMR to the fixed subdomain problem with inputs and output determined by the original inputs to subdomain 1 as well as the interface conditions.
- In the optimality conditions replace the fixed subdomain problem by its reduced order model.
- We can interpret the resulting reduced optimality system as the optimality system of the following reduced optimization problem

$$\min \int_0^T \frac{1}{2}\|\widehat{\mathbf{C}}_1^I \widehat{\mathbf{y}}_1^I - \mathbf{d}_1^I(t)\|_2^2 + \widetilde{\ell}(\mathbf{y}^\Gamma(t), \mathbf{y}_2^I(t), t, \theta)dt$$

subject to

$$\begin{aligned}
\widehat{\mathbf{M}}_1^{II}\frac{d}{dt}\widehat{\mathbf{y}}_1^I(t) + \widehat{\mathbf{M}}_1^{I\Gamma}\frac{d}{dt}\mathbf{y}^\Gamma(t) + \widehat{\mathbf{A}}_1^{II}\widehat{\mathbf{y}}_1^I(t) + \widehat{\mathbf{A}}_1^{I\Gamma}\mathbf{y}^\Gamma(t) &= \widehat{\mathbf{B}}_1^I\mathbf{u}_1^I(t) \\
\mathbf{M}_2^{II}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) + \mathbf{M}_2^{I\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{II}(\theta)\mathbf{y}_2^I(t) + \mathbf{A}_2^{I\Gamma}(\theta)\mathbf{y}^\Gamma(t) &= \mathbf{B}_2^I(\theta)\mathbf{u}_2^I(t) \\
\widehat{\mathbf{M}}_1^{\Gamma I}\frac{d}{dt}\mathbf{y}_1^I(t) + \mathbf{M}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{M}_2^{\Gamma I}(\theta)\frac{d}{dt}\mathbf{y}_2^I(t) & \\
+\widehat{\mathbf{A}}_1^{\Gamma I}\mathbf{y}_1^I(t) + \mathbf{A}^{\Gamma\Gamma}(\theta)\frac{d}{dt}\mathbf{y}^\Gamma(t) + \mathbf{A}_2^{\Gamma I}(\theta)\mathbf{y}_2^I(t) &= \mathbf{B}^\Gamma(\theta)\mathbf{u}^\Gamma(t) \\
\widehat{\mathbf{y}}_1^I(0) = \widehat{\mathbf{y}}_{1,0}^I\ \mathbf{y}_2^I(0) = \mathbf{y}_{2,0}^I,\ \mathbf{y}^\Gamma(0) = \mathbf{y}_0^\Gamma, & \\
\theta \in \Theta_{ad} &
\end{aligned}$$

Error Estimate

If

- there exists $\alpha > 0$ such that
$$\mathbf{v}^T \mathbf{A} \mathbf{v} \leq -\alpha \mathbf{v}^T \mathbf{M} \mathbf{v}, \qquad \forall \mathbf{v} \in \mathbb{R}^N,$$
- the gradients $\nabla_{\mathbf{y}_I^{(2)}} \widetilde{\ell}(\mathbf{y}_I^{(2)}, \mathbf{y}_\Gamma, t, \theta)$, $\nabla_{\mathbf{y}_\Gamma} \widetilde{\ell}(\mathbf{y}_I^{(2)}, \mathbf{y}_\Gamma, t, \theta)$, $\nabla_\theta \widetilde{\ell}(\mathbf{y}_I^{(2)}, \mathbf{y}_\Gamma, t, \theta)$, are Lipschitz continuous in $\mathbf{y}_I^{(2)}, \mathbf{y}_\Gamma$
- for all $\|\widetilde{\theta}\| \leq 1$ and all $\theta \in \Theta$ the following bound holds
$$\max \left\{ \|D_\theta \mathbf{M}^{(2)}(\theta)\widetilde{\theta}\|, \|D_\theta \mathbf{A}^{(2)}(\theta)\widetilde{\theta}\|, \|D_\theta \mathbf{B}^{(2)}(\theta)\widetilde{\theta}\| \right\} \leq \gamma,$$

then there exists $c > 0$ dependent on $\mathbf{u}$, $\widehat{\mathbf{y}}$, and $\widehat{\boldsymbol{\lambda}}$ such that
$$\|\nabla J(\theta) - \nabla \widehat{J}(\theta)\|_{L^2} \leq \frac{c}{\alpha}(\sigma_{n+1} + \ldots + \sigma_N).$$

If we assume the convexity condition
$$(\nabla J(\widehat{\theta}_*) - \nabla J(\theta_*))^T (\widehat{\theta}_* - \theta_*) \geq \kappa \|\widehat{\theta}_* - \theta_*\|^2,$$

then we obtain the error bound
$$\|\theta_* - \widehat{\theta}_*\| \leq \frac{c}{\alpha\kappa}(\sigma_{n+1} + \ldots + \sigma_N).$$

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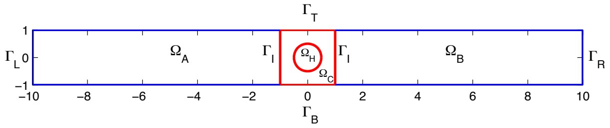
Example 1: Shape Optim. Governed by Parabolic Eqn.

- Reference domain Ω_{ref}



- Optimization problem

$$\min \int_0^T \int_{\Gamma_L \cup \Gamma_R} |y - y^d|^2 ds dt + \int_0^T \int_{\Omega_2(\theta)} |y - y^d|^2 dx dt$$

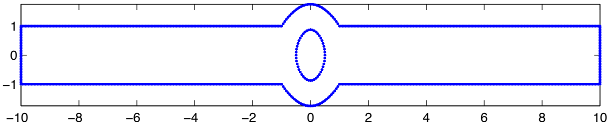
subject to the differential equation

$$\begin{aligned} y_t(x,t) - \Delta y(x,t) + y(x,t) &= 100 && \text{in } \Omega(\theta) \times (0,T), \\ n \cdot \nabla y(x,t) &= 0 && \text{on } \partial\Omega(\theta) \times (0,T), \\ y(x,0) &= 0 && \text{in } \Omega(\theta) \end{aligned}$$

and design parameter constraints $\theta^{min} \leq \theta \leq \theta^{max}$.

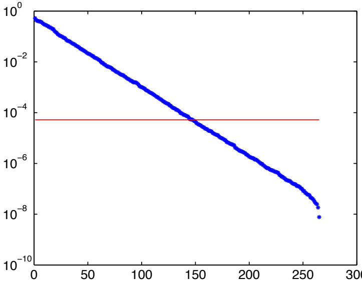
- We use $k_T = 3, k_B = 3$ Bézier control points to specify the top and the bottom boundary of the variable subdomain $\Omega_2(\theta)$.
The desired temperature y^d is computed by specifying the optimal parameter θ_* and solving the state equation on $\Omega(\theta_*)$.

- We use automatic differentiation to compute the derivatives with respect to the design variables θ.
- The semi-discretized optimization problems are solved using a projected BFGS method with Armijo line search. The optimization algorithm is terminated when the norm of projected gradient is less than $\epsilon = 10^{-4}$.
- The optimal domain



	$N_{dof}^{(1)}$	N_{dof}
Reduced	147	581
Full	4280	4714

Sizes of the full and the reduced order problems



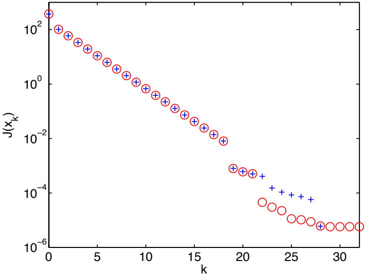
The largest Hankel singular values and the threshold $10^{-4}\sigma_1$

Error in solutions: $\|\theta^* - \widehat{\theta}^*\|_2 = 2.3 \cdot 10^{-4}$

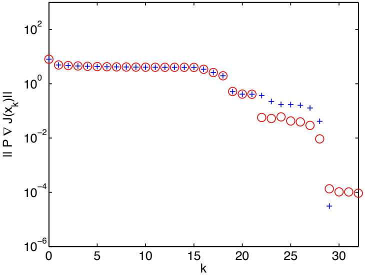
Optimal shape parameters θ_* and $\widehat{\theta}_*$ (rounded to 5 digits) computed by minimizing the full and the reduced order model.

θ_*	(1.00, 2.0000, 2.0000, -2.0000, -2.0000, -1.00)
$\widehat{\theta}_*$	(1.00, 1.9999, 2.0001, -2.0001, -1.9998, -1.00)

The convergence histories of the projected BFGS algorithm applied to the full and the reduced order problems.

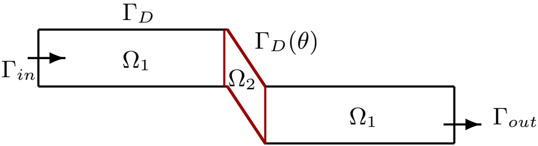


convergence history of the objective functionals for the full (+) and reduced (o) order model.



convergence history of the projected gradients for the full (+) and reduced (o) order model.

Example 2: Shape Optim. Governed by Stokes Eqns.



$$\min_{\theta \in \Theta_{ad}} J(\theta) := \int_0^T \int_{\Omega(\theta)} \ell(\mathbf{v}(\theta), p(\theta), t, \theta) dx\, dt$$

where $\mathbf{v}(\theta), p(\theta)$ solve the Stokes equations

$$\begin{aligned}
\frac{\partial}{\partial t}\mathbf{v}(x,t) - \nu \Delta \mathbf{v}(x,t) + \nabla p(x,t) &= \mathbf{f}(x,t) && \text{in } \Omega(\theta) \times (0,T]\,, \\
\text{div } \mathbf{v}(x,t) &= 0 && \text{in } \Omega(\theta) \times (0,T]\,, \\
(\nu \nabla \mathbf{v}(x,t) + p(x,t)) &= 0 && \text{on } \Gamma_{out}(\theta) \times (0,T]\,, \\
\mathbf{v}(x,t) &= \mathbf{u}(x,t) && \text{on } (\Gamma_D(\theta) \cup \Gamma_{in}) \times (0,T]\,, \\
\mathbf{v}(x,0) &= \mathbf{v}_0(x) && \text{in } \Omega(\theta).
\end{aligned}$$

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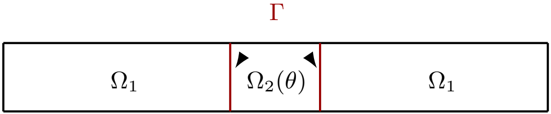
- We apply the same approach
  - Assume that only a small part of the domain depends on the shape parameter θ.
  - Use DD to isolate the quantities that depend on θ.
  - Use BMTR to reduced the subdomain problem that corresponds to the fixed domain.

- We apply the same approach
  - Assume that only a small part of the domain depends on the shape parameter θ.
  - Use DD to isolate the quantities that depend on θ.
  - Use BMTR to reduced the subdomain problem that corresponds to the fixed domain.
- But (discretized) Stokes eqns. lead to a DAE (Hessenberg index 2), which makes approach and analysis more complicated.
  - Standard BTMR cannot be used. Extension for Stokes type systems exist (Stykel 2006, Heinkenschloss/Sorensen/Sun 2008).
  - Spatial domain decomposition for the Stokes system requires care to ensure well-posedness of the coupled problem as well as of the subdomain problems. See, e.g., Toselli/Widlund book for approaches.
  - We use discretization with discontinuous pressures along the subdomain interface. Subdomain pressures are represented as a constant plus a pressure with zero spatial average.
  - Error analysis for the shape optimization exists for the case when the objective function corresponding to the fixed subdomain does not explicitly depend on pressure (A.,Heinkenschloss,Hoppe 2011).

Domain Decomposition: Discontinuous Pressure



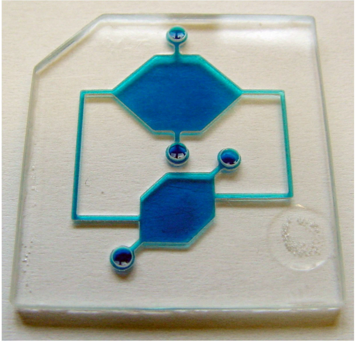
- On each subdomain, the pressure is written as the sum of a constant pressure plus a pressure with zero spatial average. $\mathbf{p}_j^I$ is the pressure in Ω_j with average 0; $\mathbf{p}_0$ the vector constant pressures. There is no pressure associated with the interface.
- The Stokes matrix times vector multiplication can be decomposed into

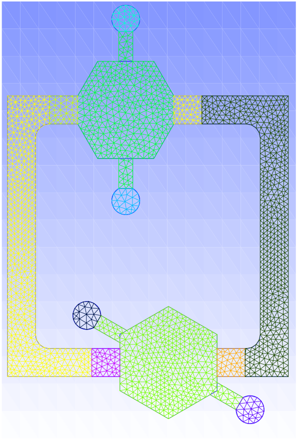
$$\mathbf{S}\mathbf{y} = \left(\begin{array}{cc|cc|cc} \mathbf{A}_1^{II} & (\mathbf{B}_1^{II})^T & 0 & 0 & \mathbf{A}_1^{I\Gamma} & 0 \\ \mathbf{B}_1^{II} & 0 & 0 & 0 & \mathbf{B}_1^{\Gamma I} & 0 \\ \hline 0 & 0 & \mathbf{A}_2^{II} & (\mathbf{B}_2^{II})^T & \mathbf{A}_2^{I\Gamma} & 0 \\ 0 & 0 & \mathbf{B}_2^{II} & 0 & \mathbf{B}_2^{\Gamma I} & 0 \\ \hline \mathbf{A}_1^{\Gamma I} & (\mathbf{B}_1^{\Gamma I})^T & \mathbf{A}_2^{\Gamma I} & (\mathbf{B}_2^{\Gamma I})^T & \mathbf{A}^{\Gamma\Gamma} & (\mathbf{B}_0)^T \\ 0 & 0 & 0 & 0 & \mathbf{B}_0 & 0 \end{array}\right) \left(\begin{array}{c} \mathbf{v}_1^I \\ \mathbf{p}_1^I \\ \hline \mathbf{v}_2^I \\ \mathbf{p}_2^I \\ \hline \mathbf{v}^\Gamma \\ \mathbf{p}_0 \end{array}\right)$$

- Zeros 0 in last row and column block are important to derive error bound for the coupled reduced problem (A.,Heinkenschloss,Hoppe 2011).

Example

Geometry motivated by biochip





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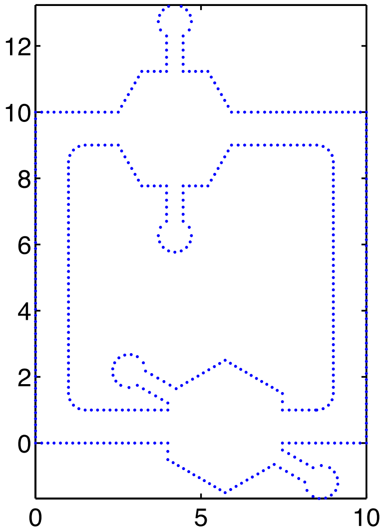
$$\min_{\theta^{min} \le \theta \le \theta^{max}} J(\theta) = \int_0^T \int_{\Omega_{\text{obs}}} \tfrac{1}{2} |\nabla \times \mathbf{v}(x,t;\theta)|^2 dx + \int_{\Omega_2(\theta)} \tfrac{1}{2} |\mathbf{v}(x,t;\theta) - \mathbf{v}^d(x,t)|^2 dx dt$$

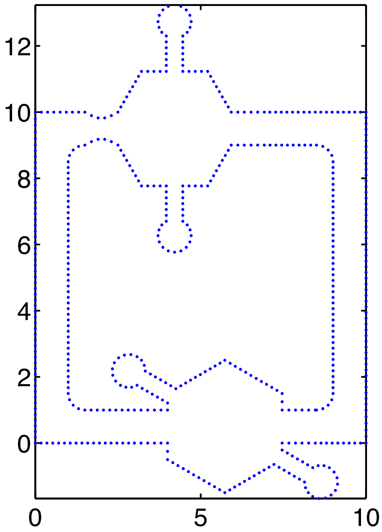
where $\mathbf{v}(\theta)$ and $p(\theta)$ solve the Stokes equations

$$\begin{aligned}
\mathbf{v}_t(x,t) - \mu \Delta \mathbf{v}(x,t) + \nabla p(x,t) &= \mathbf{f}(x,t), && \text{in } \Omega(\theta) \times (0,T),\\
\nabla \cdot \mathbf{v}(x,t) &= 0, && \text{in } \Omega(\theta) \times (0,T),\\
\mathbf{v}(x,t) &= \mathbf{v}_{\text{in}}(x,t) && \text{on } \Gamma_{\text{in}} \times (0,T),\\
\mathbf{v}(x,t) &= \mathbf{0} && \text{on } \Gamma_{\text{lat}} \times (0,T),\\
-(\mu \nabla \mathbf{v}(x,t) - p(x,t) I)\mathbf{n} &= 0 && \text{on } \Gamma_{\text{out}} \times (0,T),\\
\mathbf{v}(x,0) &= \mathbf{0} && \text{in } \Omega(\theta).
\end{aligned}$$

Here $\overline{\Omega(\theta)} = \overline{\Omega_1} \cup \overline{\Omega_2(\theta)}$ and $\overline{\Omega_2(\theta)}$ is the top left yellow, square domain. The observation region Ω_{obs} is part of the two reservoirs.
We have 12 shape parameters, $\theta \in \mathbb{R}^{12}$.



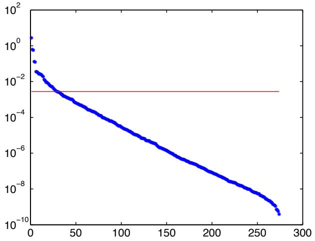
Reference domain Ω_{ref}



Optimal domain

grid	m	$N^{(1)}_{\mathbf{v},dof}$	$N^{(1)}_{\widehat{\mathbf{v}},dof}$	$N_{\mathbf{v},dof}$	$N_{\widehat{\mathbf{v}},dof}$
1	149	4752	23	4862	133
2	313	7410	25	7568	183
3	361	11474	26	11700	252
4	537	16472	29	16806	363

The number m of observations in Ω_{obs}, the number of velocities $N^{(1)}_{\mathbf{v},dof}, N^{(1)}_{\widehat{\mathbf{v}},dof}$ in the fixed subdomain Ω_1 for the full and reduced order model, the number of velocities $N_{\mathbf{v},dof}, N_{\widehat{\mathbf{v}},dof}$ in the entire domain Ω for the full and reduced order model for five discretizations.

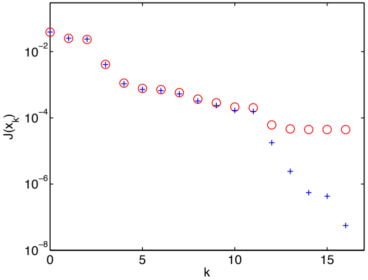


The largest Hankel singular values and the threshold $10^{-3}\sigma_1$

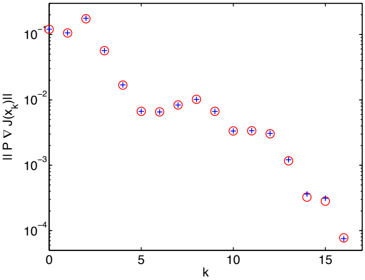
- Error in optimal parameter computed sing the full and the reduced order model (rounded to 5 digits)

θ^*	(9.8987, 9.7510, 9.7496, 9.8994, 9.0991, 9.2499, 9.2504, 9.0989)
$\widehat{\theta}^*$	(9.9026, 9.7498, 9.7484, 9.9021, 9.0940, 9.2514, 9.2511, 9.0956)

- The convergence histories of the projected BFGS algorithm applied to the full and the reduced order problems.



convergence history of the objective functionals for the full (+) and reduced (o) order model.



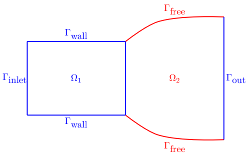
convergence history of the projected gradients for the full (+) and reduced (o) order model.

Outline

Extrude-Swell Problem

(Loading movie ...)

Stokes FBP



$$
\begin{aligned}
-\operatorname{div}(\boldsymbol{\sigma}) = \boldsymbol{f}, \qquad & \operatorname{div}(\boldsymbol{u}) = 0 && \text{in } \Omega \\
\boldsymbol{u} = \boldsymbol{g} & && \text{on } \Gamma_{\text{inlet}} \cup \Gamma_{\text{wall}} \\
\boldsymbol{\sigma}\boldsymbol{\nu} = \boldsymbol{0} & && \text{on } \Gamma_{\text{out}} \\
\boldsymbol{u} \cdot \boldsymbol{\nu} = 0, \qquad & \boldsymbol{\sigma}\boldsymbol{\nu} = \alpha \mathcal{H} \boldsymbol{\nu} && \text{on } \Gamma_{\text{free}},
\end{aligned}
$$

where $\boldsymbol{\sigma} = \eta \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^\top \right) - p\boldsymbol{I}$ is the stress tensor, η is viscosity, α is surface tension.

Formulation challenge

- Try to use the necessary regularity.
- Stokes equations.
  - Oversubscribed boundary conditions.
  - Moving domain.
- The curvature equation.

How to address them?

- Analyze regularity of the free surface.
- Prove well-posedness of the Stokes with mixed B.C.
  - Domain with same regularity of free surface.
- Use non-linear solver techniques.
  - Fixed point, implicit function theorem, etc ...
  - Solve in a reference domain.

Stokes Problem Slip (with friction) Boundary Conditions

- $\Omega \subset \mathbb{R}^n$ is of class $W_s^{2-1/s}$, with $s > n$.
- Start with the Stokes equations

$$-\operatorname{div}\left(\boldsymbol{\sigma}\left(\boldsymbol{u}, p\right)\right) = \boldsymbol{f}, \quad \operatorname{div}\left(\boldsymbol{u}\right) = g \quad \text{in } \Omega,$$

- and add the Navier B.C. i.e. slip with friction

$$\boldsymbol{u} \cdot \boldsymbol{\nu} = \phi, \quad \beta \boldsymbol{T}\boldsymbol{u} + \boldsymbol{T}^\top \boldsymbol{\sigma}\left(\boldsymbol{u}, p\right) \boldsymbol{\nu} = \boldsymbol{\psi} \quad \text{on } \partial\Omega,$$

where $\boldsymbol{T} = \boldsymbol{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$ is the projection operator into the tangent plane of $\partial\Omega$.

$$\boldsymbol{\sigma} = 2\eta\boldsymbol{\varepsilon}(\boldsymbol{u}) - \boldsymbol{I}p, \quad \boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{\nabla u + \nabla u^\top}{2}.$$

Variational Equation (pure slip)

Given $\mathcal{F}$, find $(\boldsymbol{u}, p) \in \mathcal{E}\phi\boldsymbol{\nu} \oplus \mathring{X}_r(\Omega)$ such that

$$\mathcal{S}_\Omega\left(\boldsymbol{u}, p\right)\left(\boldsymbol{v}, q\right) = \mathcal{F}\left(\boldsymbol{v}, q\right) \quad \forall\left(\boldsymbol{v}, q\right) \in \mathring{X}_{r'}(\Omega)$$

and the continuity bounds

$$\left\|(\boldsymbol{u}, p)\right\|_{X_r(\Omega)} \leq C_{\Omega,\eta,n,r}\left(\|\mathcal{F}\|_{X_{r'}(\Omega)} + \|\phi\|_{W_r^{1-1/r}(\partial\Omega)}\right)$$

where the Stokes operator in Ω reads

$$\mathcal{S}_\Omega\left(\boldsymbol{u}, p\right)\left(\boldsymbol{v}, q\right) := \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{u}) : \boldsymbol{\varepsilon}(\boldsymbol{v}) - p\,\mathrm{div}\left(\boldsymbol{v}\right) + q\,\mathrm{div}\left(\boldsymbol{u}\right).$$

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Variational Formulation (Spaces)

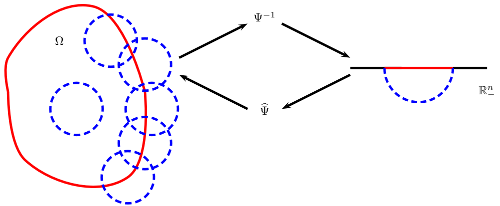
- $\mathring{X}_r := V_r(\Omega) \times L^r_0(\Omega)$, $s' \le r \le s$, $s > n$.
- $V_r(\Omega) := \Big\{ \boldsymbol{v} \in W^1_r(\Omega)/Z(\Omega) : \boldsymbol{v} \cdot \boldsymbol{\nu} = 0 \Big\}$.

It is necessary to identify the kernel of $\mathcal{S}_\Omega$

- $L^r_0(\Omega) := L^r(\Omega)/\mathbb{R}$.
- $Z(\Omega) :=$ $\Big\{ \boldsymbol{z}(x) = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b} : \boldsymbol{x} \in \Omega, \boldsymbol{A} = -\boldsymbol{A}^\top \in \mathbb{R}^{n\times n}, \boldsymbol{b} \in \mathbb{R}^n, \boldsymbol{z} \cdot \boldsymbol{\nu}\big|_{\partial\Omega} = 0 \Big\}$.

Earlier result: Amrouche '11 $C^{1,1}$ domain.

Domain Decomposition



- We cover the domain with finite number of balls

$$\overline{\Omega} \subset \cup_{i=1}^{k} B(x_i, \delta_i/2).$$

- Associate to it a smooth partition of unity $\{\varphi_i\}_{i=1}^{k}$.
- And smooth cut-off functions, $\{\varrho_i\}_{i=1}^{k}$, supp $\varrho_i \subset B(x_i, \delta_i)$, $\rho_i = 1$ on $B(x_i, \delta_i/2)$.
- Using Piola transform

$$(\hat{\boldsymbol{v}}, \hat{q}) \mapsto \left(\hat{\boldsymbol{P}}\hat{\boldsymbol{v}}, \hat{q}\right) \circ \Psi^{-1} = (\boldsymbol{v}, q)$$

$$(\boldsymbol{v}, q) \mapsto \left(\boldsymbol{P}^{-1}\boldsymbol{v}, q\right) \circ \hat{\Psi} = (\hat{\boldsymbol{v}}, \hat{q})$$

$$\hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{\nu}} \, \mathrm{d}\hat{s} = \boldsymbol{v} \cdot \boldsymbol{\nu} \, \mathrm{d}s.$$

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Space Decomposition

Restriction map

$$\mathcal{R}_{\varrho_i} : \mathring{X}_r(\Omega) \to \mathring{X}_r(\hat{\Theta}_i)$$

$$(\boldsymbol{u}, p) \mapsto \hat{\mathcal{P}}_i^{-1} (\varrho_i \boldsymbol{u}, \varrho_i p)$$

Projection map

$$\hat{\mathcal{R}}_{\varphi_i} : \mathring{X}_r(\hat{\Theta}_i) \to \mathring{X}_r(\Omega)$$

$$(\hat{\boldsymbol{v}}, \hat{q}) \mapsto \varphi_i \hat{\mathcal{P}}_i (\hat{\boldsymbol{v}}, \hat{q})$$

continuous only when Piola matrix is in $W_s^2(\Omega)$.

- Given $(\boldsymbol{u}, p) \in \mathring{X}_r(\Omega)$, we have

$$(\boldsymbol{u}, p) = \sum_{i=1}^{k} \varphi_i (\boldsymbol{u}, p) = \sum_{i=1}^{k} \varphi_i (\varrho_i \boldsymbol{u}, \varrho_i p) = \sum_{i=1}^{k} \varphi_i \hat{\mathcal{P}}_i \hat{\mathcal{P}}_i^{-1} (\varrho_i \boldsymbol{u}, \varrho_i p)$$

$$= \sum_{i=1}^{k} \hat{\mathcal{R}}_{\varphi_i} \underbrace{\mathcal{R}_{\varrho_i} (\boldsymbol{u}, p)}_{\in \mathring{X}_r(\hat{\Theta}_i)}.$$

  which implies $\mathring{X}_r(\Omega) = \sum_{i=1}^{k} \hat{\mathcal{R}}_{\varphi_i} \mathring{X}_r(\hat{\Theta}_i)$.

- Similarly for the dual space

$$\mathring{X}_r(\Omega)^* = \sum_{i=1}^{k} \hat{\mathcal{R}}_{\varphi_i}^* \mathring{X}_r(\hat{\Theta}_i)^*.$$

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Operator Decomposition

$$
\begin{aligned}
\mathcal{S}_\Omega\left(\boldsymbol{u},p\right)\hat{\mathcal{R}}_{\varphi_i}\left(\hat{\boldsymbol{v}},\hat{q}\right) &= \left(\mathcal{S}_{\Omega_i}\left(\varphi_i\boldsymbol{u},\varphi_i p\right)+\mathcal{K}_i\left(\boldsymbol{u},p\right)\right)\hat{\mathcal{P}}_i\left(\hat{v},\hat{q}\right) \\
&\quad + \left\langle \varepsilon\left(\varphi_i\boldsymbol{u}\right), \varepsilon\left(\hat{\boldsymbol{P}}_i\hat{\boldsymbol{v}}\right)\circ\Psi^{-1}\right\rangle_{\Omega_\lambda} \\
&= \underbrace{\tilde{\mathcal{S}}_i}_{\text{Invertible}}\ \mathcal{R}_{\varphi_i}\left(\boldsymbol{u},p\right)\left(\hat{\boldsymbol{v}},\hat{q}\right) \\
&\quad + \underbrace{\mathcal{C}_{\varphi_i}\mathcal{R}_{\varphi_i}\left(\boldsymbol{u}\right)+\mathcal{K}_i\left(\boldsymbol{u},p\right)\hat{\mathcal{P}}_i\left(\hat{\boldsymbol{v}},\hat{q}\right)}_{\text{Compact}}
\end{aligned}
$$

Pesudo-inverse

Consider the operator

$$\mathcal{S}_\Omega^\dagger := \sum_{i=1}^{k} \hat{\mathcal{R}}_{\varrho_i} \tilde{\mathcal{S}}_i^{-1} \hat{\mathcal{R}}_{\varphi_i}^*.$$

Then

$$\mathcal{S}_\Omega^\dagger \mathcal{S}_\Omega = \mathcal{I}_{X_r(\Omega)} + \sum_{i=1}^{k} \underbrace{\hat{\mathcal{R}}_{\varrho_i} \tilde{\mathcal{S}}_i^{-1} \left(\mathcal{C}_i \mathcal{R}_{\varphi_i} + \hat{\mathcal{P}}_i^* \mathcal{K}_i \right)}_{\text{compact}}.$$

Similarly

$$\mathcal{S}_\Omega \mathcal{S}_\Omega^\dagger = \text{identity} + \text{compact}.$$

Therefore $\mathcal{S}_\Omega$ has a pseudo-inverse, which implies

$$\dim N_{\mathcal{S}_\Omega} < \infty, \quad \operatorname{codim} R_{\mathcal{S}_\Omega} < \infty.$$

$\mathcal{S}_\Omega$ and $\mathcal{S}_\Omega^*$ are Injective

- Problem satisfies the Brezzi's theorem for Hilbert space case. This ensures the uniqueness of solution for

$$2 \leq r \leq s.$$

- Let $r_0 = s' < 2$. Consider the homogeneous problem, we need to show that $(\boldsymbol{u}, p) = 0$.

  Use the method by Galdi-Simader-Sohr '99 to improve the integrability of the function to some $r_k > 2$, to conclude.

Index Theory of Fredholm Operators

Let $\mathcal{A} : X \to Y$ has a pseudo-inverse. $\mathcal{A}$ is bijective if and only if $\mathcal{A}$ and $\mathcal{A}^*$ are injective.

Summary:

- Using index theory we have shown the well-posedness of the Stokes problem with slip boundary condition.
  - under mild domain regularity i.e. $C^{1,\epsilon}$, earlier result Amrouche '11 $C^{1,1}$ domain.
- We have provided a constructive approach based on domain decomposition.
- Extension to slip-with-friction is a direct corollary.

"dimension independent"

Conclusions

- Applied reduced order models in optimization context.
- Important to approximate state and adjoint equations.
- We have integrated domain decomposition and model reduction for systems with small localized nonlinearities. In our case, nonlinearities arise from dependence on shape parameters.
  - We have proven global, a-priori estimates for the error between the solution of the original and the reduced order problem.
  - Error estimates depend on balanced truncation error estimates. (Could use other model reduction techniques).
  - Efficiency of reduced order model depends size of subdomain with nonlinearity, and interface.
- Presented existence theory for Stokes equations with Slip boundary for $C^{1,\epsilon}$ domain, which is much better than earlier known results by Amrouche '11 ($C^{1,1}$) domain.