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

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Motivation

- Use domain decomposition to explore problem structure in shape optimization.

Nonlinearity due to shape variation is localized in small subdomain $\Omega_2(\alpha)$.

- Use Model Reduction to reduce the linear subproblem corresponding to subdomain Ω₁.
- Need to optimize potentially much smaller system that approximates the original, large system.
- Can handle other localized nonlinearities in the PDE in a similar manner.







Outline

Model Reduction

Model Reduction and Optimal Control of the Advection Diffusion Equation

Model Reduction and Shape Optimization of the Advection Diffusion Equation

Model Reduction and Shape Optimization of the Stokes Equation

Uncertainty

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Reduced-Order Dynamical Systems

$$\begin{split} \dot{\mathbf{y}}(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{z}(t) &= \mathbf{C}\mathbf{y}(t) \end{split}$$

 $\dot{\mathbf{y}}(t) = f(\mathbf{y}(t), \mathbf{u}(t), t)$ $\mathbf{z}(t) = g(\mathbf{y}(t), t)$

Replace $\mathbf{y}(t) \in \mathbb{R}^N$ by $\mathcal{V}\widehat{\mathbf{y}}(t) = \sum_{i=1}^n \mathbf{v}_i \widehat{y}_i(t)$, $\widehat{\mathbf{y}} \in \mathbb{R}^n$ where $n \ll N$ and multiply the state equation by \mathcal{W}^T .

$$\begin{split} \dot{\widehat{\mathbf{y}}} &= \mathcal{W}^T \mathbf{A} \mathcal{V} \widehat{\mathbf{y}} + \mathcal{W}^T \mathbf{B} \mathbf{u} \\ \widehat{\mathbf{z}} &= \mathbf{C} \mathcal{V} \widehat{\mathbf{y}} \end{split}$$

Two main questions:

- Accuracy of the reduced order model? Approximation of the input-to-output map u → z.
- Efficiency of the reduced order model?

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Projection Based Model Reduction Approaches

- Proper Orthogonal Decomposition (POD) or Karhunen Loeve (KL) expansion
 - Very often used, especially for nonlinear problems.
 - Data driven.
 - Quality of reduced order model limited by sampling of snapshots.
- Balanced Truncation Model Reduction.
 - Theory and efficient algorithms for linear time invariant (LTI) problems.
 - Extensions to nonlinear problems proposed, but depend on sampling and are missing theory at level available for LTI problems.
- Optimization Based Approach
 - In theory applicable to large class of problems.
 - Can be tailored to different measures of approximation.
 - Ideal formulation is computationally intractable, approximate variants exist.

Review of Balanced Truncation Model Reduction

Consider

$$\begin{aligned} \frac{d}{dt}\mathbf{y}(t) &= \mathcal{A}\mathbf{y}(t) + \mathcal{B}\mathbf{u}(t), \quad t \in (0,T) \\ \mathbf{z}(t) &= \mathcal{C}\mathbf{y}(t) + \mathcal{D}\mathbf{u}(t), \quad t \in (0,T) \\ \mathbf{y}(0) &= 0. \end{aligned}$$

- ▶ Projection methods for model reduction produce n × k matrices V, W with n ≪ N and with W^TV = I_n.
- \blacktriangleright One obtains a reduced form by setting $\mathbf{y}=\mathcal{V}\widehat{\mathbf{y}}$ and projecting so that

$$\mathcal{W}^{T}[\mathcal{V}\frac{d}{dt}\widehat{\mathbf{y}}(t) - \mathcal{A}\mathcal{V}\widehat{\mathbf{y}}(t) - \mathcal{B}\mathbf{u}(t)] = 0, \quad t \in (0,T).$$

 \blacktriangleright This leads to a reduced order system of order n given by

$$\begin{aligned} \frac{d}{dt}\widehat{\mathbf{y}}(t) &= \widehat{\mathcal{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathcal{B}}\mathbf{u}(t), \quad t \in (0,T) \\ \widehat{\mathbf{z}}(t) &= \widehat{\mathcal{C}}\widehat{\mathbf{y}}(t) + \mathcal{D}\mathbf{u}(t), \quad t \in (0,T) \\ \widehat{\mathbf{y}}(0) &= 0. \end{aligned}$$

with $\widehat{\mathcal{A}} = \mathcal{W}^T \mathcal{A} \mathcal{V}$, $\widehat{\mathcal{B}} = \mathcal{W}^T \mathcal{B}$, and $\widehat{\mathcal{C}} = \mathcal{C} \mathcal{V}$.

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Controllability and Observability Gramians

Recall

$$\mathbf{y}'(t) = \mathcal{A}\mathbf{y}(t) + \mathcal{B}\mathbf{u}(t), \quad t \in (0,T)$$
$$\mathbf{z}(t) = \mathcal{C}\mathbf{y}(t) + \mathcal{D}\mathbf{u}(t), \quad t \in (0,T).$$

Assume the system is stable ($\text{Re}(\lambda(A)) < 0$), controllable and observable.

Controllability Gramian.

$$\blacktriangleright \mathcal{P} = \int_0^\infty e^{\mathcal{A}t} \mathcal{B} \mathcal{B}^T e^{\mathcal{A}^T t} dt.$$

- Eigenspaces corresponding to large eigenvalues are 'easy' to control (control has smaller energy).
- Controllability Gramian solves the Lyapunov equation

$$\mathcal{AP} + \mathcal{PA}^T + \mathcal{BB}^T = 0.$$

Observability Gramian.

$$\blacktriangleright \mathcal{Q} = \int_0^\infty e^{\mathcal{A}^T t} \mathcal{C}^T \mathcal{C} e^{\mathcal{A} t} dt.$$

- Eigenspaces corresponding to large eigenvalues are 'easy' to observe.
- Observability Gramian solves the Lyapunov equation

$$\mathcal{A}^T \mathcal{Q} + \mathcal{Q} \mathcal{A} + \mathcal{C}^T \mathcal{C} = 0.$$

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• Compute controllability and observability gramians $\mathcal{P}, \mathcal{Q} \mathcal{P} = \mathbf{U}\mathbf{U}^T$ and $\mathcal{Q} = \mathbf{L}\mathbf{L}^T$ in factored form, i.e., solve

$$\mathcal{AP} + \mathcal{PA}^{T} + \mathcal{BB}^{T} = 0,$$

$$\mathcal{A}^{T}\mathcal{Q} + \mathcal{QA} + \mathcal{C}^{T}\mathcal{C} = 0.$$

- Compute the SVD $\mathbf{U}^T \mathbf{L} = \mathbf{Z} \mathbf{S} \mathbf{Y}^T$, where $\mathbf{S}_n = diag(\sigma_1, \sigma_2, \dots, \sigma_n)$ with $\mathbf{S} = \mathbf{S}_N$, and $\sigma_1 \ge \sigma_2 \ge \dots$.
- Set V = UZ_nS_n^{-1/2}, W = LY_nS_n^{-1/2}, where n is selected to be the smallest positive integer such that σ_{n+1} < τσ₁. Here τ > 0 is a prespecified constant. The matrices Z_n, Y_n consist of the corresponding leading n columns of Z, Y.
- It is easily verified that $\mathcal{PW} = \mathcal{VS}_n$ and that $\mathcal{QV} = \mathcal{WS}_n$.
- Hence

$$0 = \mathcal{W}^{T}(\mathcal{AP} + \mathcal{PA}^{T} + \mathcal{BB}^{T})\mathcal{W} = \widehat{\mathcal{A}}\mathbf{S}_{n} + \mathbf{S}_{n}\widehat{\mathcal{A}}^{T} + \widehat{\mathcal{B}}\widehat{\mathcal{B}}^{T},$$

$$0 = \mathcal{V}^{T}(\mathcal{A}^{T}\mathcal{Q} + \mathcal{QA} + \mathcal{C}^{T}\mathcal{C})\mathcal{V} = \widehat{\mathcal{A}}^{T}\mathbf{S}_{n} + \mathbf{S}_{n}\widehat{\mathcal{A}} + \widehat{\mathcal{C}}^{T}\widehat{\mathcal{C}}.$$

Two important properties of balanced trunction model reduction:

- $\widehat{\mathcal{A}}$ is stable
- \blacktriangleright For any given input ${\bf u}$ we have

$$\|\mathbf{z} - \widehat{\mathbf{z}}\|_{\mathcal{L}_2} \le 2\|\mathbf{u}\|_{\mathcal{L}_2}(\sigma_{n+1} + \ldots + \sigma_N)$$

where $\widehat{\mathbf{z}}$ is the output (response) of the reduced model (Glover 1984).

Consider state system

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

and corresponding adjoint system

$$\boldsymbol{\lambda}'(t) = \mathcal{A}^T \boldsymbol{\lambda}(t) + \mathcal{C} \mathbf{w}(t), \quad t \in (0, T)$$
$$\mathbf{q}(t) = \mathcal{B}^T \boldsymbol{\lambda}(t) + \mathcal{D}_a \mathbf{w}(t), \quad t \in (0, T)$$

▶ Apply BTMR to compute $\mathcal{V}, \mathcal{W} \in \mathbb{R}^{n \times k}$, the reduced state system

$$\frac{d}{dt}\widehat{\mathbf{y}}(t) = \widehat{\mathcal{A}}\widehat{\mathbf{y}}(t) + \widehat{\mathcal{B}}\mathbf{u}(t), \quad t \in (0,T)$$
$$\widehat{\mathbf{z}}(t) = \widehat{\mathcal{C}}\widehat{\mathbf{y}}(t) + \mathcal{D}_s\mathbf{u}(t), \quad t \in (0,T)$$

and the reduced adjoint system

$$\frac{d}{dt}\widehat{\boldsymbol{\lambda}}(t) = \widehat{\boldsymbol{\mathcal{A}}}^T\widehat{\boldsymbol{\lambda}}(t) + \widehat{\boldsymbol{\mathcal{C}}}^T\mathbf{w}(t), \quad t \in (0,T)$$
$$\widehat{\mathbf{q}}(t) = \widehat{\boldsymbol{\mathcal{B}}}^T\widehat{\boldsymbol{\lambda}}(t) + \mathcal{D}_a\mathbf{w}(t), \quad t \in (0,T)$$

with $\widehat{\mathcal{A}} = \mathcal{W}^T \mathcal{A} \mathcal{V}$, $\widehat{\mathcal{B}} = \mathcal{W}^T \mathcal{B}$, and $\widehat{\mathcal{C}} = \mathcal{C} \mathcal{V}$.

 \blacktriangleright Error bounds: For any given inputs ${\bf u}$ and ${\bf w}$ we have

$$\|\mathbf{z} - \widehat{\mathbf{z}}\|_{\mathcal{L}_{2}} \leq 2\|\mathbf{u}\|_{\mathcal{L}_{2}}(\sigma_{n+1} + \ldots + \sigma_{N}),$$

$$\|\mathbf{q} - \widehat{\mathbf{q}}\|_{\mathcal{L}_{2}} \leq 2\|\mathbf{w}\|_{\mathcal{L}_{2}}(\sigma_{n+1} + \ldots + \sigma_{N}).$$

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Error bound holds if the system

$$\frac{d}{dt}\mathbf{y}(t) = \mathcal{A}\mathbf{y}(t) + \mathcal{B}\mathbf{u}(t), \quad t \in (0,T)$$
$$\mathbf{z}(t) = \mathcal{C}\mathbf{y}(t) + \mathcal{D}\mathbf{u}(t), \quad t \in (0,T)$$
$$\mathbf{y}(0) = 0$$

has a homogeneous initial condition. For problems with inhomogeneous initial conditions, balanced truncation can be modified and a similar error bound can be proven (Antoulas/H./Reis 2009).

To keep the presentation simple, I assume homogeneous initial conditions.

Descriptor systems

$$\mathcal{E}\frac{d}{dt}\mathbf{y}(t) = \mathcal{A}\mathbf{y}(t) + \mathcal{B}\mathbf{u}(t), \quad t \in (0,T)$$
$$\mathbf{z}(t) = \mathcal{C}\mathbf{y}(t) + \mathcal{D}\mathbf{u}(t), \quad t \in (0,T)$$
$$\mathbf{y}(0) = 0$$

with symmetric positive definite \mathcal{E} can be handled easily. Transform the system $\mathbf{y} \to \mathcal{E}^{1/2}\mathbf{y}$, $\mathcal{A} \to \mathcal{E}^{-1/2}\mathcal{A}\mathcal{E}^{-1/2}$, ...

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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

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

Optimality Conditions

The necessary and sufficient optimality conditions are given by

$$\begin{split} \mathbf{My}'(t) &= \mathbf{Ay}(t) + \mathbf{Bu}(t), & t \in (0,T), \quad \mathbf{y}(0) = \mathbf{y}_0, \\ \mathbf{z}(t) &= \mathbf{Cy}(t) + \mathbf{Du}(t) - \mathbf{d}(t), & t \in (0,T) \\ -\mathbf{M\lambda}'(t) &= \mathbf{A}^T \mathbf{\lambda}(t) + \mathbf{C}^T \mathbf{z}(t), & t \in (0,T), \quad \mathbf{\lambda}(T) = 0, \\ \mathbf{q}(t) &= \mathbf{B}^T \mathbf{\lambda}(t) + \mathbf{D}^T \mathbf{z}(t), & t \in (0,T) \\ \mathbf{q}(t) &= \mathbf{0}, & t \in (0,T). \end{split}$$

This is exactly of the form to which BTMR can be applied!

 \blacktriangleright We use BTMR to compute \mathcal{W}, \mathcal{V} and the reduced optimality system

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

with $\widehat{\mathbf{A}} = \mathcal{W}^T \mathbf{A} \mathcal{V}$, $\widehat{\mathbf{B}} = \mathcal{W}^T \mathbf{B}$, $\widehat{\mathbf{C}} = \mathbf{C} \mathcal{V}$, and $\widehat{\mathbf{y}}_0 = \mathcal{W}^T \mathbf{M} \mathbf{y}_0$. We assume that $\mathbf{y}_0 = \mathbf{0}$.

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Reduced Problem

The reduced optimality system

$$\begin{split} \widehat{\mathbf{y}}'(t) &= \widehat{\mathbf{A}} \widehat{\mathbf{y}}(t) + \widehat{\mathbf{B}} \mathbf{u}(t), & t \in (0, T) & \widehat{\mathbf{y}}(0) = \widehat{\mathbf{y}}_{0}, \\ \widehat{\mathbf{z}}(t) &= \widehat{\mathbf{C}} \widehat{\mathbf{y}}(t) + \mathbf{D} \mathbf{u}(t) - \mathbf{d}(t), & t \in (0, T) \\ -\widehat{\mathbf{\lambda}}'(t) &= \widehat{\mathbf{A}}^{T} \widehat{\mathbf{\lambda}}(t) + \widehat{\mathbf{C}}^{T} \widehat{\mathbf{z}}(t), & t \in (0, T) & \widehat{\mathbf{\lambda}}(T) = 0, \\ \widehat{\mathbf{q}}(t) &= \widehat{\mathbf{B}}^{T} \widehat{\mathbf{\lambda}}(t) + \mathbf{D}^{T} \widehat{\mathbf{z}}(t), & t \in (0, T) \\ \widehat{\mathbf{q}}(t) &= \mathbf{0}, & t \in (0, T), \end{split}$$

is the optimality system for the reduced optimal control problem

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

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

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

Easy to see in this case (but not for other problems). Important to note, since we do reduction on the optimality system, but numerically want to solve an optimization problem!

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Error Analysis (Standard)

- ▶ Let u_{*} be a minimizer of the original objective J and let û_{*} be a minimizer of the reduced objective Ĵ.
- Assume that J is a strictly convex quadratic function, i.e., that there existents κ > 0 such that

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

 \blacktriangleright 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

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

Hence

$$\|\mathbf{u}_* - \widehat{\mathbf{u}}_*\|_{L^2} \le \kappa^{-1} \|\nabla \widehat{J}(\widehat{\mathbf{u}}_*) - \nabla J(\widehat{\mathbf{u}}_*)\|_{L^2}.$$

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

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Gradient Computation

► For the original problem

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

► For the reduced problem

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

Gradient Computation

For the original problem

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

For the original problem

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

- We can *almost* apply BTMR error bounds, but need same inputs w in full and reduced order adjoint system.
- Easy to fix: Introduce auxiliary adjoint λ as solution of the original adjoint, but with input 2 instead of z.

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Error Estimate

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

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

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

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

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

Consequently, the error between the solutions satisfies

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

Example Problem (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

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

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



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)





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



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:

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

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Shape Optimization Problem

Consider the minimization problem

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

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

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

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

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

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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

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

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

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

Problem is that we need a reduced order model that approximates the full order model for all θ ∈ Θ_{ad}! Cannot be done using BTMR. I am not aware of any MR method that can do this with guaranteed error bounds.

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Restrict Problem Class

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

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

$$\Gamma$$

$$\Omega_1 \qquad \Omega_2(\theta) \qquad \Omega_1$$

> 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

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

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Our Optimization problem

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

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

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

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

$$\begin{split} \mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{y}_{1}^{I}(t) + \mathbf{M}_{1}^{I\Gamma} \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{A}_{1}^{II} \mathbf{y}_{1}^{I}(t) + \mathbf{A}_{1}^{I\Gamma} \mathbf{y}^{\Gamma}(t) &= \mathbf{B}_{1}^{I} \mathbf{u}_{1}^{I}(t) \\ \mathbf{M}_{2}^{II}(\theta) \frac{d}{dt} \mathbf{y}_{2}^{I}(t) + \mathbf{M}_{2}^{I\Gamma}(\theta) \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{A}_{2}^{II}(\theta) \mathbf{y}_{2}^{I}(t) + \mathbf{A}_{2}^{I\Gamma}(\theta) \mathbf{y}^{\Gamma}(t) &= \mathbf{B}_{2}^{I}(\theta) \mathbf{u}_{2}^{I}(t) \\ \mathbf{M}_{1}^{\Gamma I} \frac{d}{dt} \mathbf{y}_{1}^{I}(t) + \mathbf{M}^{\Gamma\Gamma}(\theta) \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{M}_{2}^{\Gamma I}(\theta) \frac{d}{dt} \mathbf{y}_{2}^{I}(t) \\ &+ \mathbf{A}_{1}^{\Gamma I} \mathbf{y}_{1}^{I}(t) + \mathbf{A}^{\Gamma\Gamma}(\theta) \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{A}_{2}^{\Gamma I}(\theta) \mathbf{y}_{2}^{I}(t) &= \mathbf{B}^{\Gamma}(\theta) \mathbf{u}^{\Gamma}(t) \end{split}$$

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.

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First Order Optimality Conditions

Lagrangian

$$L(\mathbf{y}, \mathbf{p}, \theta) = J(\theta) + \int_0^T \mathbf{p}(t)^T \left(\mathbf{M}(\theta) \frac{d}{dt} \mathbf{y}(t) + \mathbf{A}(\theta) \mathbf{y}(t) - \mathbf{B}(\theta) \mathbf{u}(t) \right) dt$$

The first order necessary optimality conditions are

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

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

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

$$\begin{split} \mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{y}_{1}^{I}(t) + \mathbf{M}_{1}^{I\Gamma} \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{A}_{1}^{II} \mathbf{y}_{1}^{I}(t) + \mathbf{A}_{1}^{I\Gamma} \mathbf{y}^{\Gamma}(t) &= \mathbf{B}_{1}^{I} \mathbf{u}_{1}^{I}(t) \\ \mathbf{M}_{2}^{II}(\theta) \frac{d}{dt} \mathbf{y}_{2}^{I}(t) + \mathbf{M}_{2}^{I\Gamma}(\theta) \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{A}_{2}^{II}(\theta) \mathbf{y}_{2}^{I}(t) + \mathbf{A}_{2}^{I\Gamma}(\theta) \mathbf{y}^{\Gamma}(t) &= \mathbf{B}_{2}^{I}(\theta) \mathbf{u}_{2}^{I}(t) \\ \mathbf{M}_{1}^{\Gamma I} \frac{d}{dt} \mathbf{y}_{1}^{I}(t) + \mathbf{M}^{\Gamma \Gamma}(\theta) \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{M}_{2}^{\Gamma I}(\theta) \frac{d}{dt} \mathbf{y}_{2}^{I}(t) \\ &+ \mathbf{A}_{1}^{\Gamma I} \mathbf{y}_{1}^{I}(t) + \mathbf{M}^{\Gamma \Gamma}(\theta) \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{A}_{2}^{\Gamma I}(\theta) \mathbf{y}_{2}^{I}(t) &= \mathbf{B}^{\Gamma}(\theta) \mathbf{u}^{\Gamma}(t), \\ -\mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{p}_{1}^{I}(t) - \mathbf{M}_{1}^{I\Gamma} \frac{d}{dt} \mathbf{p}^{\Gamma}(t) + \mathbf{A}_{1}^{I\Gamma} \mathbf{p}_{1}^{I}(t) + \mathbf{A}_{1}^{I\Gamma} \mathbf{p}^{\Gamma}(t) &= -(\mathbf{C}_{1}^{I})^{T} (\mathbf{C}_{1}^{I} \mathbf{y}_{1}^{I}(t) - \mathbf{d}_{1}^{I} \\ -\mathbf{M}_{2}^{II}(\theta) \frac{d}{dt} \mathbf{p}_{2}^{I}(t) - \mathbf{M}_{2}^{I\Gamma}(\theta) \frac{d}{dt} \mathbf{p}^{\Gamma}(t) + \mathbf{A}_{2}^{II}(\theta) \mathbf{p}_{2}^{I}(t) + \mathbf{A}_{2}^{I\Gamma}(\theta) \mathbf{p}^{\Gamma}(t) &= -\nabla_{\mathbf{y}_{2}^{I} \tilde{\ell}(.) \\ \end{split}$$

$$\begin{split} -\mathbf{M}_{1}^{\Gamma I} \frac{d}{dt} \mathbf{p}_{1}^{I}(t) - \mathbf{M}^{\Gamma\Gamma}(\theta) \frac{d}{dt} \mathbf{p}^{\Gamma}(t) - \mathbf{M}_{2}^{\Gamma I}(\theta) \frac{d}{dt} \mathbf{p}_{2}^{I}(t) \\ +\mathbf{A}_{1}^{\Gamma I} \mathbf{p}_{1}^{I}(t) + \mathbf{A}^{\Gamma\Gamma}(\theta) \frac{d}{dt} \mathbf{p}^{\Gamma}(t) + \mathbf{A}_{2}^{\Gamma I}(\theta) \mathbf{p}_{2}^{I}(t) \ = \ -\nabla_{\mathbf{y}^{\Gamma}} \widetilde{\ell}(.), \end{split}$$

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

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Model Reduction of Fixed Subdomain Problem

We need to reduce

$$\begin{split} \mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{y}_{1}^{I}(t) &= -\mathbf{A}_{1}^{II} \mathbf{y}_{1}^{I}(t) - \mathbf{M}_{1}^{I\Gamma} \frac{d}{dt} \mathbf{y}^{\Gamma}(t) + \mathbf{B}_{1}^{I} \mathbf{u}_{1}^{I}(t) - \mathbf{A}_{1}^{I\Gamma} \mathbf{y}^{\Gamma}(t) \\ \mathbf{z}_{1}^{I} &= \mathbf{C}_{1}^{I} \mathbf{y}_{1}^{I}(t) - \mathbf{d}_{1}^{I} \\ \mathbf{z}_{1}^{\Gamma} &= -\mathbf{M}_{1}^{\Gamma I} \frac{d}{dt} \mathbf{y}_{1}^{I} - \mathbf{A}_{1}^{\Gamma I} \mathbf{y}_{1}^{I}, \\ -\mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{p}_{1}^{I}(t) &= -\mathbf{A}_{1}^{II} \mathbf{p}_{1}^{I}(t) + \mathbf{M}_{1}^{I\Gamma} \frac{d}{dt} \mathbf{p}^{\Gamma}(t) - (\mathbf{C}_{1}^{I})^{T} \mathbf{z}_{1}^{I} - \mathbf{A}_{1}^{I\Gamma} \mathbf{p}^{\Gamma}(t) \\ \mathbf{q}_{1}^{I} &= (\mathbf{B}_{1}^{I})^{T} \mathbf{p}_{1}^{I} \\ \mathbf{q}_{1}^{\Gamma} &= \mathbf{M}_{1}^{\Gamma I} \frac{d}{dt} \mathbf{p}_{1}^{I} - \mathbf{A}_{1}^{\Gamma I} \mathbf{p}_{1}^{I} \end{split}$$

For simplicity we assume that

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

we get

$$\begin{split} \mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{y}_{1}^{I}(t) &= -\mathbf{A}_{1}^{II} \mathbf{y}_{1}^{I}(t) + (\mathbf{B}_{1}^{I} \mid -\mathbf{A}_{1}^{I\Gamma}) \begin{pmatrix} \mathbf{u}_{1}^{I} \\ \mathbf{y}^{\Gamma} \end{pmatrix}, \\ & \begin{pmatrix} \mathbf{z}_{1}^{I} \\ \mathbf{z}_{1}^{\Gamma} \end{pmatrix} = \begin{pmatrix} -\mathbf{C}_{1}^{I} \\ -\mathbf{A}_{1}^{\Gamma I} \end{pmatrix} \mathbf{y}_{1}^{I} + \begin{pmatrix} \mathbf{I} \\ 0 \end{pmatrix} \mathbf{d}_{1}^{I}, \\ -\mathbf{M}_{1}^{II} \frac{d}{dt} \mathbf{p}_{1}^{I}(t) &= -\mathbf{A}_{1}^{II} \mathbf{p}_{1}^{I}(t) + (-(\mathbf{C}_{1}^{I})^{T} \mid -\mathbf{A}_{1}^{I\Gamma}) \begin{pmatrix} \mathbf{z}_{1}^{I} \\ \mathbf{p}^{\Gamma} \end{pmatrix}, \\ & \begin{pmatrix} \mathbf{q}_{1}^{I} \\ \mathbf{q}_{1}^{\Gamma} \end{pmatrix} = \begin{pmatrix} (\mathbf{B}_{1}^{I})^{T} \\ -\mathbf{A}_{1}^{\Gamma I} \end{pmatrix} \mathbf{p}_{1}^{I}. \end{split}$$

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

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

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Error Estimate

If $\blacktriangleright\,$ there exists $\alpha>0$ such that

$$\begin{split} \mathbf{v}^T \mathbf{A} \mathbf{v} &\leq -\alpha \mathbf{v}^T \mathbf{M} \mathbf{v}, \qquad \forall \mathbf{v} \in \mathbb{R}^N, \\ \blacktriangleright \text{ the gradients } \nabla_{\mathbf{y}_I^{(2)}} \tilde{\ell}(\mathbf{y}_I^{(2)}, \mathbf{y}_{\Gamma}, t, \theta), \ \nabla_{\mathbf{y}_{\Gamma}} \tilde{\ell}(\mathbf{y}_I^{(2)}, \mathbf{y}_{\Gamma}, t, \theta), \\ \nabla_{\theta} \tilde{\ell}(\mathbf{y}_I^{(2)}, \mathbf{y}_{\Gamma}, t, \theta), \text{ are Lipschitz continuous in } \mathbf{y}_I^{(2)}, \mathbf{y}_{\Gamma} \\ \vdash \text{ for all } \|\tilde{\theta}\| \leq 1 \text{ and all } \theta \in \Theta \text{ the following bound holds} \\ \max \left\{ \|D_{\theta} \mathbf{M}^{(2)}(\theta) \tilde{\theta}\|, \|D_{\theta} \mathbf{A}^{(2)}(\theta) \tilde{\theta}\|, \|D_{\theta} \mathbf{B}^{(2)}(\theta) \tilde{\theta}\| \right\} \leq \gamma, \end{split}$$

then there exists c>0 dependent on ${\bf u}$, $\widehat{{\bf y}}$, and $\widehat{{\boldsymbol \lambda}}$ such that

$$\|\nabla J(\theta) - \nabla \widehat{J}(\theta)\|_{L^2} \le \frac{c}{\alpha}(\sigma_{n+1} + \dots + \sigma_N).$$

If we assume the convexity condition

$$(\nabla J(\widehat{\theta}_*) - \nabla J(\theta_*))^T (\widehat{\theta}_* - \theta_*) \ge \kappa \|\widehat{\theta}_* - \theta_*\|^2,$$

then we obtain the error bound

$$\|\theta_* - \widehat{\theta}_*\| \le \frac{c}{\alpha\kappa}(\sigma_{n+1} + \dots + \sigma_N).$$

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Example

• 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

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

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 Ω₂(θ).
 The desired temperature y^d is computed by specifying the optimal parameter θ_{*} and solving the state equation on Ω(θ_{*}).

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- 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



Error in solution between full and reduced order problem: $\|\theta^* - \hat{\theta}^*\|_2 = 2.325 \cdot 10^{-4}$

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

$ heta_*$	(1.00, 2.0000, 2.0000, -2.0000, -2.0000, -1.00)
$\widehat{ heta}_*$	(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.

Outline

Model Reduction

Model Reduction and Optimal Control of the Advection Diffusion Equation

Model Reduction and Shape Optimization of the Advection Diffusion Equation

Model Reduction and Shape Optimization of the Stokes Equation

Uncertainty

Shape Optimization Governed by Stokes System



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

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

- ▶ 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 filed domain.
- But (discretized) Stokes equations leads to a DAE (Hessenberg index 2) and this makes approach and analysis much more complicated.
 - Standard BTMR cannot be used. Extension for Stokes type systems exist (Stykel 2006, H./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., Proceedings of DD Conferences at www.ddm.org or 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 (Antil,H.,Hoppe 2009).

The Semidiscretized Problem

The semi-discretized minimization problem is

$$\min_{\theta \in \Theta_{ad}} J(\theta) := \int_0^T \frac{1}{2} \int_0^T \|\mathbf{C} \mathbf{v}(t,\theta) + \mathbf{F} \mathbf{p}(t,\theta) + \mathbf{D} \mathbf{u}(t) - \mathbf{d}\|^2 dt$$

where $\mathbf{v}(\cdot,\theta)\text{, }p(\cdot,\theta)$ solves the semi-discretized Stokes equations

$$\begin{split} \mathbf{M}(\theta) \frac{d}{dt} \mathbf{v}(t) + \ \mathbf{A}(\theta) \mathbf{v}(t) + \mathbf{B}(\theta) p(t) &= \mathbf{K}(\theta) \mathbf{u}(t) \quad t \in [0, T] ,\\ \mathbf{B}^T(\theta) \mathbf{v}(t) &= \mathbf{L}(\theta) \mathbf{u}(t) \quad t \in [0, T] ,\\ \mathbf{M}(\theta) \mathbf{v}(0) &= \mathbf{M}(\theta) \mathbf{v}_0,\\ \theta &\in \Theta_{ad} \end{split}$$

Optimality Conditions

• The necessary optimality conditions involve the state and the adjoint equations (we omit dependence on θ to simplify notation)

$$\mathbf{M} \frac{d}{dt} \mathbf{v}(t) = \mathbf{A} \mathbf{v}(t) + \mathbf{B}^{T} \mathbf{p}(t) + \mathbf{K} \mathbf{u}(t) ,$$

$$0 = \mathbf{B} \mathbf{v}(t) + \mathbf{L} \mathbf{u}(t) \quad t \in [0, T] ,$$

$$\mathbf{z}(t) = \mathbf{C} \mathbf{v}(t) + \mathbf{F} \mathbf{p}(t) + \mathbf{D} \mathbf{u}(t) - \mathbf{d}(t),$$

$$-\mathbf{M} \frac{d}{dt} \boldsymbol{\lambda}(t) = \mathbf{A} \boldsymbol{\lambda}(t) + \mathbf{B}^{T} \boldsymbol{\pi}(t) + \mathbf{C}^{T} \mathbf{z}(t) ,$$

$$0 = \mathbf{B} \boldsymbol{\lambda}(t) + \mathbf{C}^{T} \mathbf{z}(t) \quad t \in [0, T] ,$$

$$\mathbf{q}(t) = \mathbf{K}^{T} \boldsymbol{\lambda}(t) + \mathbf{L}^{T} \boldsymbol{\pi}(t) + \mathbf{D}^{T} \mathbf{z}(t).$$

We cannot apply balanced truncation model reduction in standard form. Idea: Apply projection to enforce 'incompressibility' constraint and eliminate pressure.

- Write $\mathbf{v}(t) = \mathbf{v}_{\mathrm{H}}(t) + \mathbf{v}_{\mathrm{P}}(t)$, where $\mathbf{v}_{\mathrm{P}}(t) = \mathbf{M}^{-1}\mathbf{B}^{T}(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^{T})^{-1}\mathbf{L}\mathbf{u}(t)$ and \mathbf{v}_{H} satisfies $\mathbf{0} = \mathbf{B}\mathbf{v}_{\mathrm{H}}(t)$.
- Define projection $\Pi = \mathbf{I} \mathbf{B}^T (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}$.
- Since $\mathbf{0} = \mathbf{B}\mathbf{v}_{\mathrm{H}}(t)$ we have $\mathbf{\Pi}^T\mathbf{v}_{\mathrm{H}}(t) = \mathbf{v}_{\mathrm{H}}(t)$.
- Insert into Stokes equation and multiply by Π to get

$$\Pi \mathbf{M} \Pi^{T} \frac{d}{dt} \mathbf{v}_{\mathrm{H}}(t) = -\Pi \mathbf{A} \Pi^{T} \mathbf{v}_{\mathrm{H}}(t) + \Pi \widetilde{\mathbf{B}} \mathbf{u}(t),$$
$$\mathbf{z}(t) = \widetilde{\mathbf{C}} \Pi^{T} \mathbf{v}_{\mathrm{H}}(t) + \widetilde{\mathbf{D}} \mathbf{u}(t) - \mathbf{F} (\mathbf{B} \mathbf{M}^{-1} \mathbf{B}^{T})^{-1} \mathbf{L} \frac{d}{dt} \mathbf{u}(t)$$

Similarly for adjoint equations

$$-\mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^{T}\frac{d}{dt}\boldsymbol{\lambda}_{\mathrm{H}}(t) = -\mathbf{\Pi}\mathbf{A}^{T}\mathbf{\Pi}^{T}\boldsymbol{\lambda}_{\mathrm{H}}(t) + \mathbf{\Pi}\widetilde{\mathbf{C}}^{T}\mathbf{z}(t),$$
$$\mathbf{q}(t) = \widetilde{\mathbf{B}}^{T}\mathbf{\Pi}^{T}\boldsymbol{\lambda}_{\mathrm{H}}(t) + \widetilde{\mathbf{D}}^{T}\mathbf{w}(t) + \mathbf{L}^{T}(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^{T})^{-1}\mathbf{F}^{T}\frac{d}{dt}\mathbf{z}(t).$$

 \blacktriangleright We can apply BTMR to these two systems for $v_{\rm H}$ and $\lambda_{\rm H}.$

Note that outputs z, q and pressure

$$\begin{split} \mathbf{p}(t) = & (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1} \Big[-\mathbf{B}\mathbf{M}^{-1}\mathbf{A}\mathbf{v}_{\mathrm{H}}(t) \\ & +\mathbf{B}\mathbf{M}^{-1} \left(\mathbf{K} - \mathbf{A}\mathbf{M}^{-1}\mathbf{B}^T (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L} \right) \mathbf{u}(t) - \mathbf{L}\frac{d}{dt}\mathbf{u}(t) \Big] \\ \text{depend on } \frac{d}{dt}\mathbf{u} \text{ and } \frac{d}{dt}\mathbf{z}. \end{split}$$

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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. p^I_j is the pressure in Ω_j with average 0; p₀ the vector constant pressures. There is no pressure associated with the interface.
- The Stokes matrix times vector multiplication can be decomposed into

$$\mathbf{Sy} = \begin{pmatrix} \mathbf{A}_{1}^{II} & (\mathbf{B}_{1}^{II})^{T} & 0 & 0 & \mathbf{A}_{1}^{I\Gamma} & 0 \\ \mathbf{B}_{1}^{II} & 0 & 0 & \mathbf{B}_{1}^{\Gamma I} & 0 \\ \hline \mathbf{0} & 0 & \mathbf{A}_{2}^{II} & (\mathbf{B}_{2}^{II})^{T} & \mathbf{A}_{2}^{I\Gamma} & 0 \\ \hline \mathbf{0} & 0 & \mathbf{B}_{2}^{II} & \mathbf{0} & \mathbf{B}_{2}^{\Gamma I} & 0 \\ \hline \mathbf{A}_{1}^{\Gamma I} & (\mathbf{B}_{1}^{\Gamma I})^{T} & \mathbf{A}_{2}^{\Gamma I} & (\mathbf{B}_{2}^{\Gamma I})^{T} & \mathbf{A}_{1}^{\Gamma \Gamma} & (\mathbf{B}_{0})^{T} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{B}_{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{v}_{1}^{I} \\ \mathbf{p}_{1}^{I} \\ \mathbf{v}_{2}^{I} \\ \mathbf{p}_{2}^{I} \\ \mathbf{v}_{1}^{\Gamma} \\ \mathbf{p}_{2}^{I} \\ \mathbf{p}_{1}^{I} \end{pmatrix}$$

 Zeros 0 in last row and column block are important to derive error bound for the coupled reduced problem (Antil,H.,Hoppe 2009).

Example

Geometry motivated by biochip





$$\min_{\theta^{\min} \le \theta \le \theta^{\max}} J(\theta) = \int_{0}^{T} \int_{\Omega_{obs}} \frac{1}{2} |\nabla \times \mathbf{v}(x,t;\theta)|^2 dx + \int_{\Omega_2(\theta)} \frac{1}{2} |\mathbf{v}(x,t;\theta) - \mathbf{v}^d(x,t)|^2 dx dt$$

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

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

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 $\Omega_{\rm obs}$ is part of the two reservoirs. We have 12 shape parameters, $\theta \in \mathbb{R}^{12}$.



grid	m	$N_{\mathbf{v},dof}^{(1)}$	$N_{\widehat{\mathbf{v}},dof}^{(1)}$	$N_{\mathbf{v},dof}$	$N_{\widehat{\mathbf{v}},dof}$
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 $\Omega_{\rm obs}$, the number of velocities $N_{{\bf v},dof}^{(1)},N_{\hat{{\bf v}},dof}^{(1)}$ in the fixed subdomain Ω_1 for the full and reduced order model, the number of velocities $N_{{\bf v},dof},N_{\hat{{\bf v}},dof}$ in the entire domain Ω for the full and reduced order model for five discretizations.



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

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

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

Model Reduction

Model Reduction and Optimal Control of the Advection Diffusion Equation

Model Reduction and Shape Optimization of the Advection Diffusion Equation

Model Reduction and Shape Optimization of the Stokes Equation

Uncertainty

We have considered optimization problems of the form

$$\text{minimize } \int_0^T \ell(\mathbf{y}(t),\mathbf{u}(t),t,\theta) dt,$$

subject to

$$\mathbf{M}(\theta)\frac{d}{dt}\mathbf{y}(t) + \mathbf{A}(\theta)\mathbf{y}(t) = \mathbf{B}(\theta)\mathbf{u}(t), \qquad t \in (0,T),$$
$$\mathbf{M}(\theta)\mathbf{y}(0) = \mathbf{y}_0,$$

where the optimization variables are either \mathbf{u} or θ and where the other quantity (θ or \mathbf{u}) was considered fixed.

We have constructed reduced order optimization problems

minimize
$$\int_0^T \ell(\widehat{\mathbf{y}}(t), \mathbf{u}(t), t, \theta) dt$$
,

subject to

$$\widehat{\mathbf{M}}(\theta) \frac{d}{dt} \widehat{\mathbf{y}}(t) + \widehat{\mathbf{A}}(\theta) \widehat{\mathbf{y}}(t) = \widehat{\mathbf{B}}(\theta) \mathbf{u}(t), \qquad t \in (0, T),$$
$$\widehat{\mathbf{M}}(\theta) \mathbf{y}(0) = \widehat{\mathbf{y}}_0.$$

We have proven error bounds for the gradients of the full and for the reduced problem of the form

$$\|\nabla J - \nabla \widehat{J}\| \le c \|\mathbf{u}\|_{L^2}(\sigma_{n+1} + \ldots + \sigma_N)$$
 for all $\mathbf{u} \in L^2$ and for all $\theta \in \Theta_{ad}$!

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- Since the bound holds for all $\mathbf{u} \in L^2$ and for all $\theta \in \Theta_{ad}$ this is much stronger that what we needed in our context, but can be extremely useful when the other parameter is allowed to vary randomly.
- ► We can replace

minimize
$$\int_0^T \ell(\mathbf{y}(t), \mathbf{u}(t), t, \theta) dt$$
,

subject to

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

by the smaller and computationally much less expensive problem

$$\text{minimize } \int_0^T \ell(\widehat{\mathbf{y}}(t),\mathbf{u}(t),t,\theta) dt, \\$$

subject to

$$\widehat{\mathbf{M}}(\theta) \frac{d}{dt} \widehat{\mathbf{y}}(t) + \widehat{\mathbf{A}}(\theta) \widehat{\mathbf{y}}(t) = \widehat{\mathbf{B}}(\theta) \mathbf{u}(t), \qquad t \in (0, T),$$
$$\widehat{\mathbf{M}}(\theta) \mathbf{y}(0) = \widehat{\mathbf{y}}_{0}.$$

- We are working on the theory.
- Some indication that model reduction can be very useful was given by K. Willcox et.al.

Probabilistic Analysis of Blade Geometry Variation (Courtesy of K. Willcox)

- Two-dimensional model problem governed by the (linearized) Euler equations.
- Our CFD model uses a discontinuous Galerkin formulation, and has 51,504 states per blade passage.
- Reduced order model is generated by an optimization approach (not BTMR, no error bounds available).
- Linearized CFD model and reduced-order model Monte Carlo simulations results. Work per cycle is predicted for blade plunging motion at an interblade phase angle of 180° for 10,000 randomly selected blade geometries.



Comparison of linearized CFD and reduced-order model predictions of WPC for Blade 1. Monte Carlo simulations results are shown for 10,000 blade geometries. The same geometries were analyzed in each case.

	CFD	Reduced
Model size	103,008	201
Offline cost	_	2.8 hours
Online	501.1 hours	0.21 hours
Blade 1 mean	-1.8572	-1.8573
Blade 1 variance	2.687e-4	2.682e-4
Blade 2 mean	-1.8581	-1.8580
Blade 2 variance	2.797e-4	2.799e-4





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Conclusions

- There are many PDE systems with complicated physics, but with few inputs and few outputs.
- How can we extract in a systematic matter the relevant dynamics to get an inexpensive model of the input-output map with a guaranteed error bound?
- 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 estimates for the error between the solution of the original and the reduced order problem.
- Error estimates depend on balanced truncation error estimates.
- Availability of reduced order model techniques for nonlinear or parametrically varying systems with guaranteed error bounds is the bottleneck.
- Our error estimates hold for all parameters and hence make our reduced order models interesting for probabilistic analysis/optimization under uncertainty.