PDE-Constrained Optimization Using Hyper-Reduced Models

Matthew J. Zahr and Charbel Farhat

Institute for Computational and Mathematical Engineering
Farhat Research Group
Stanford University

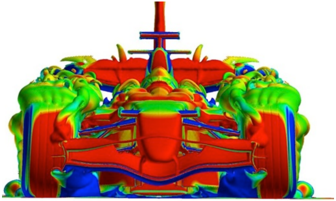
SIAM Conference on Optimization (CP13)
May 19 - 22, 2014
San Diego, CA

Problem Formulation

Goal: Rapidly solve PDE-constrained optimization problems of the form

$$\begin{aligned} \underset{\mathbf{w}\in\mathbb{R}^N,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & f(\mathbf{w}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{R}(\mathbf{w}, \boldsymbol{\mu}) = 0 \end{aligned} \tag{1}$$

where $\mathbf{R} : \mathbb{R}^N \times \mathbb{R}^p \to \mathbb{R}^N$ is the discretized (nonlinear) PDE, $\mathbf{w}$ is the PDE state vector, $\boldsymbol{\mu}$ is the vector of parameters, and N is assumed to be very large.



Reduced-Order Model

- Model Order Reduction (MOR) assumption: *state vector lies in low-dimensional affine subspace*

$$\mathbf{w} = \bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}$$

where $\mathbf{y} \in \mathbb{R}^n$ are the reduced coordinates of $\mathbf{w}$ in the basis $\mathbf{\Phi} \in \mathbb{R}^{N \times n}$ and $n \ll N$

- Substitute assumption into High-Dimensional Model (HDM), $\mathbf{R}(\mathbf{w}, \boldsymbol{\mu}) = 0$

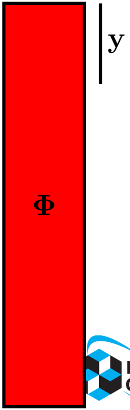
$$\mathbf{R}(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) \approx 0$$

- Require projection of residual in low-dimensional *left subspace*, with basis $\mathbf{\Psi} \in \mathbb{R}^{N \times n}$ to be zero

$$\boxed{\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \mathbf{\Psi}^T \mathbf{R}(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0}$$

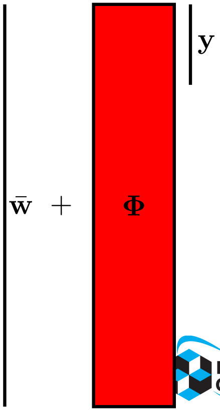
Bottleneck

$$\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0$$



Bottleneck

$$\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0$$



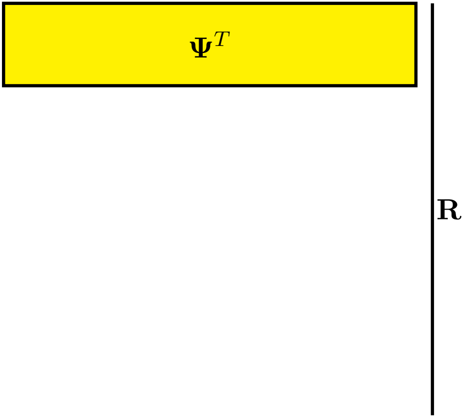
Bottleneck

$$\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0$$

$$\mathbf{R}\left(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}\right)$$

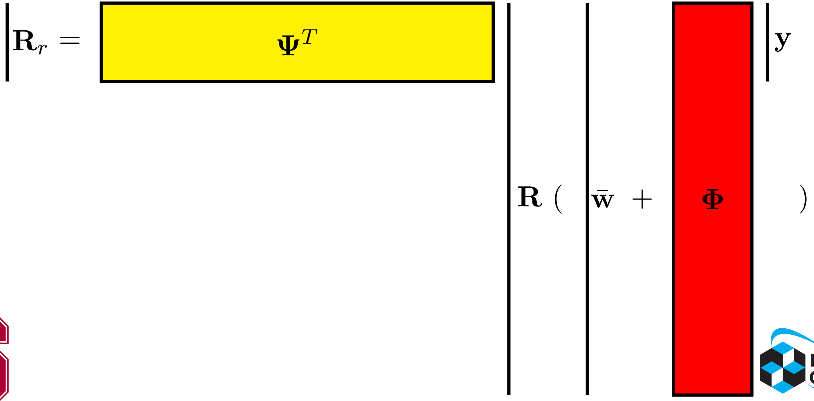
Bottleneck

$$\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0$$



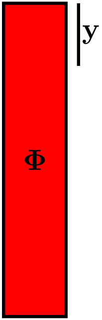
Bottleneck

$$\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0$$



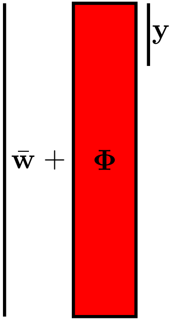
Bottleneck

$$\frac{\partial \mathbf{R}_r}{\partial \mathbf{y}}(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{y}}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})\boldsymbol{\Phi}$$



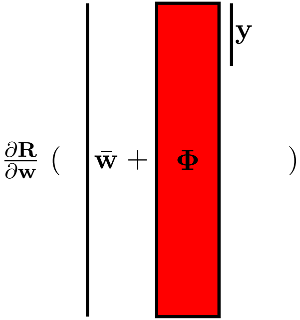
Bottleneck

$$\frac{\partial \mathbf{R}_r}{\partial \mathbf{y}}(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{y}}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})\boldsymbol{\Phi}$$



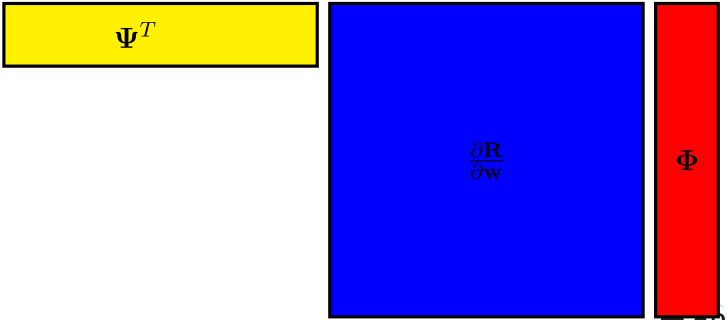
Bottleneck

$$\frac{\partial \mathbf{R}_r}{\partial \mathbf{y}}(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{y}}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})\boldsymbol{\Phi}$$



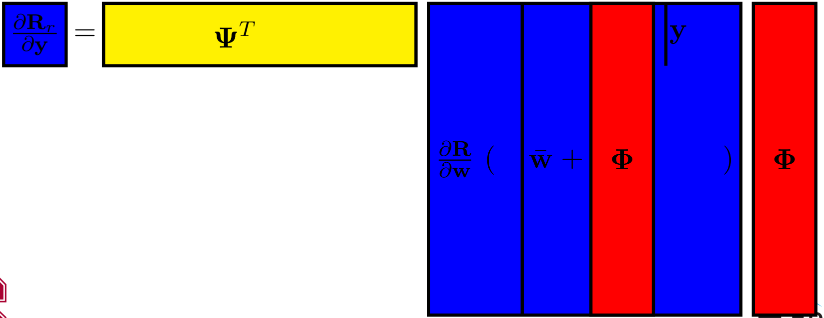
Bottleneck

$$\frac{\partial \mathbf{R}_r}{\partial \mathbf{y}}(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{y}}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})\boldsymbol{\Phi}$$



Bottleneck

$$\frac{\partial \mathbf{R}_r}{\partial \mathbf{y}}(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{y}}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})\boldsymbol{\Phi}$$



Solution: Gappy POD Approximation

- Assume nonlinear terms (residual/Jacobian) lie in low-dimensional subspace

$$\mathbf{R}(\mathbf{w}, \boldsymbol{\mu}) \approx \boldsymbol{\Phi}_R \mathbf{r}(\mathbf{w}, \boldsymbol{\mu})$$

where $\boldsymbol{\Phi} \in \mathbb{R}^{N \times n_R}$ and $\mathbf{r} : \mathbb{R}^N \times \mathbb{R}^p \to \mathbb{R}^{n_R}$ are the reduced coordinates; $n_R \ll N$

- Determine $\mathbf{R}$ by solving *gappy* least-squares problem

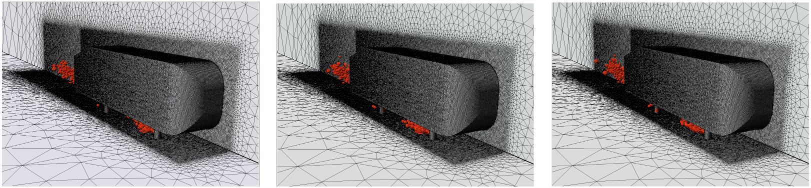
$$\mathbf{r}(\mathbf{w}, \boldsymbol{\mu}) = \arg\min_{\mathbf{a} \in \mathbb{R}^{n_r}} ||\mathbf{Z}^T \boldsymbol{\Phi}_R \mathbf{a} - \mathbf{Z}^T \mathbf{R}(\mathbf{w}, \boldsymbol{\mu})||$$

where $\mathbf{Z}$ is a restriction operator

- Analytical solution

$$\mathbf{r}(\mathbf{w}, \boldsymbol{\mu}) = \left(\mathbf{Z}^T \boldsymbol{\Phi}_R\right)^\dagger \left(\mathbf{Z}^T \mathbf{R}(\mathbf{w}, \boldsymbol{\mu})\right)$$

Gappy POD in Practice



(a) 253 sample nodes (b) 378 sample nodes (c) 505 sample nodes

Hyper-Reduced Model

Using the Gappy POD approximation, the hyper-reduced governing equations are

$$\mathbf{R}_h(\mathbf{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \boldsymbol{\Phi}_R \left(\mathbf{Z}^T \boldsymbol{\Phi}_R\right)^\dagger \left(\mathbf{Z}^T \mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})\right) = 0$$

where

$$\mathbf{E} = \boldsymbol{\Psi}^T \boldsymbol{\Phi}_R \left(\mathbf{Z}^T \boldsymbol{\Phi}_R\right)^\dagger$$

is known *offline* and can be precomputed

$$\mathbf{R}_r = \boxed{\mathbf{E}} \, \mathbf{Z}^T \mathbf{R}$$

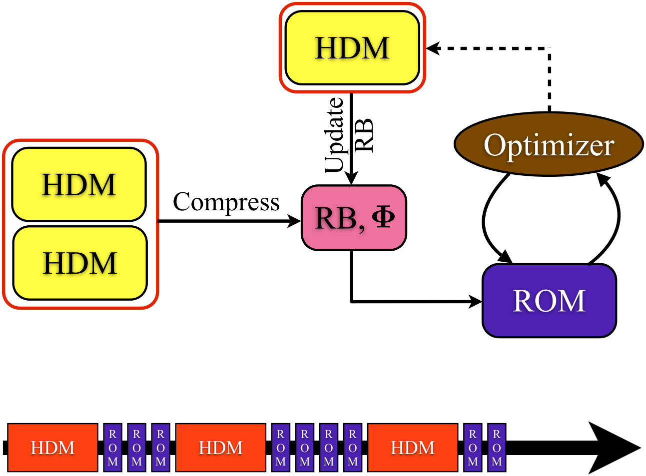
Hyper-Reduced Optimization

Using the hyper-reduced model as a surrogate for the HDM in the PDE-constrained optimization, we have the hyper-reduced optimization problem

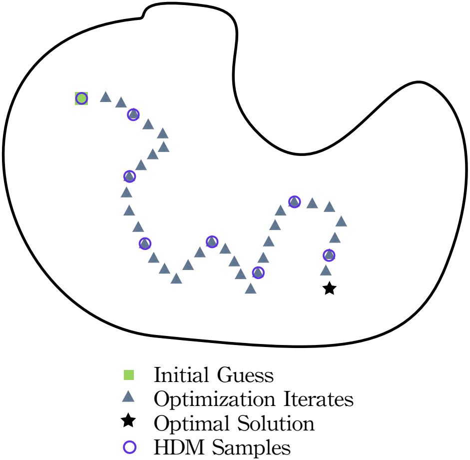
$$\begin{aligned} \underset{\mathbf{y}\in\mathbb{R}^n,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & \tilde{f}(\mathbf{y}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{R}_h(\mathbf{y}, \boldsymbol{\mu}) = 0 \end{aligned}$$

where $\mathbf{R}_h : \mathbb{R}^k \times \mathbb{R}^p \to \mathbb{R}^k$ is the hyper-reduced PDE and $\mathbf{y} \in \mathbb{R}^k$ are the reduced coordinates, where $k \ll N$.

Hyper-Reduced Optimization Procedure



Hyper-Reduced Optimization Schematic



Quasi-1D Euler Flow

Quasi-1D Euler equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{1}{A}\frac{\partial (A\mathbf{F})}{\partial x} = \mathbf{Q}$$

where

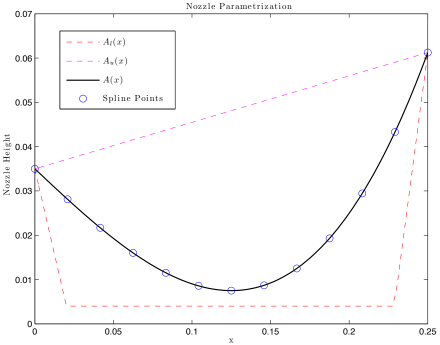
$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{bmatrix}, \qquad \mathbf{Q} = \begin{bmatrix} 0 \\ \frac{p}{A}\frac{\partial A}{\partial x} \\ 0 \end{bmatrix}$$

- Semi-discretization $\implies$ finite volumes with Roe flux and entropy corrections
- Full discretization $\implies$ Backward Euler $\rightarrow$ steady state

Nozzle Parametrization

Nozzle parametrized with *cubic splines* using 13 control points and constraints requiring

- convexity $A''(x) \geq 0$
- bounds on $A(x)$ $A_l(x) \leq A(x) \leq A_u(x)$
- bounds on $A'(x)$ at inlet/outlet $A'(x_l) \leq 0,\ A'(x_r) \geq 0$



Parameter Estimation/Inverse Design

For this problem, the goal is to determine the parameter $\boldsymbol{\mu}^*$ such that the flow achieves some optimal or desired state $\mathbf{w}^*$

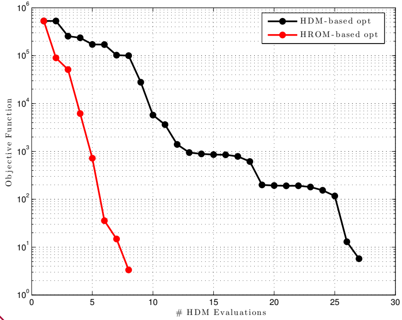
$$\begin{aligned} \underset{\mathbf{w}\in\mathbb{R}^N,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & ||\mathbf{w}(\boldsymbol{\mu}) - \mathbf{w}^*|| \\ \text{subject to} \quad & \mathbf{R}(\mathbf{w}, \boldsymbol{\mu}) = 0 \\ & \mathbf{c}(\mathbf{w}, \boldsymbol{\mu}) \leq 0 \end{aligned} \tag{2}$$

where $\mathbf{c}$ are the nozzle constraints.

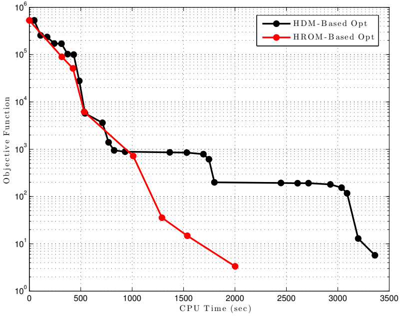
- This problem is solved using
  - the HDM as the governing equation
    - HDM-based optimization
  - the HROM as the governing equation
    - HROM-based optimization

Objective Function Convergence

(a) Convergence (# HDM Evals)

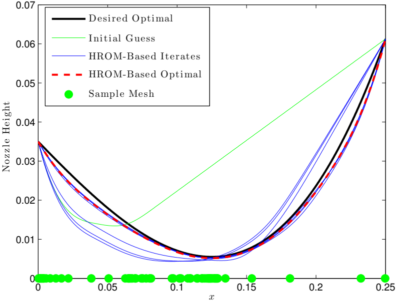


(b) Convergence (CPU Time)

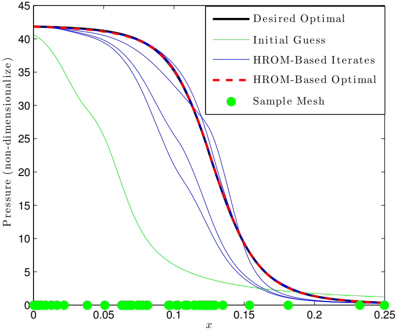


Hyper-Reduced Optimization Progression

(a) Parameter ($\boldsymbol{\mu}$) Progression



(b) Pressure Progression



Optimization Summary

	HDM-Based Opt	HROM-Based Opt
Rel. Error in μ^* (%)	1.82	5.26
Rel. Error in $\mathbf{w}^*$ (%)	0.11	0.12
# HDM Evals	27	8
# HROM Evals	0	161
CPU Time (s)	3361.51	2001.74