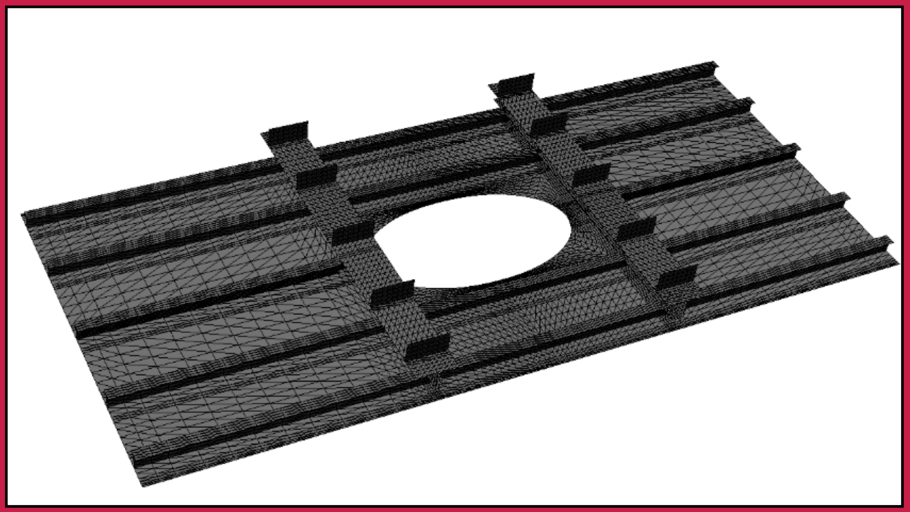
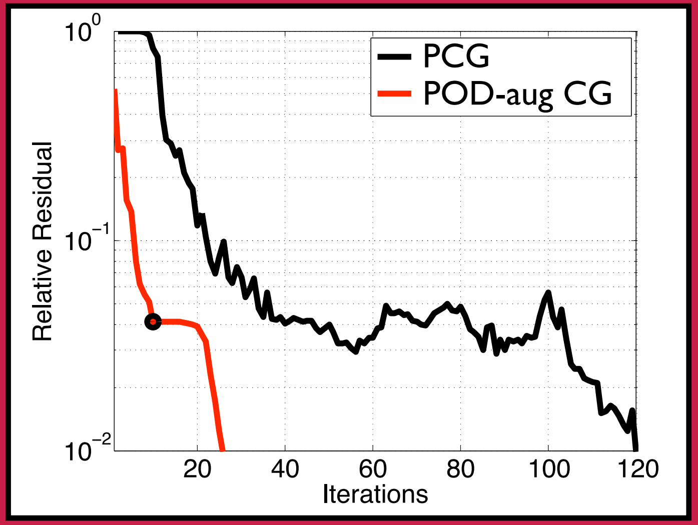
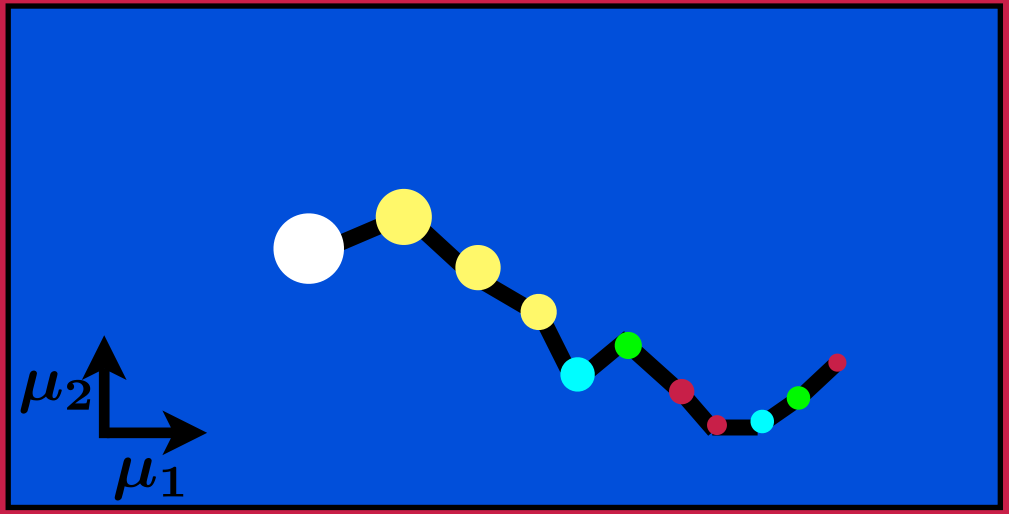
A Proper Orthogonal Decomposition-Based Augmented Conjugate Gradient Algorithm for Nearby Problems







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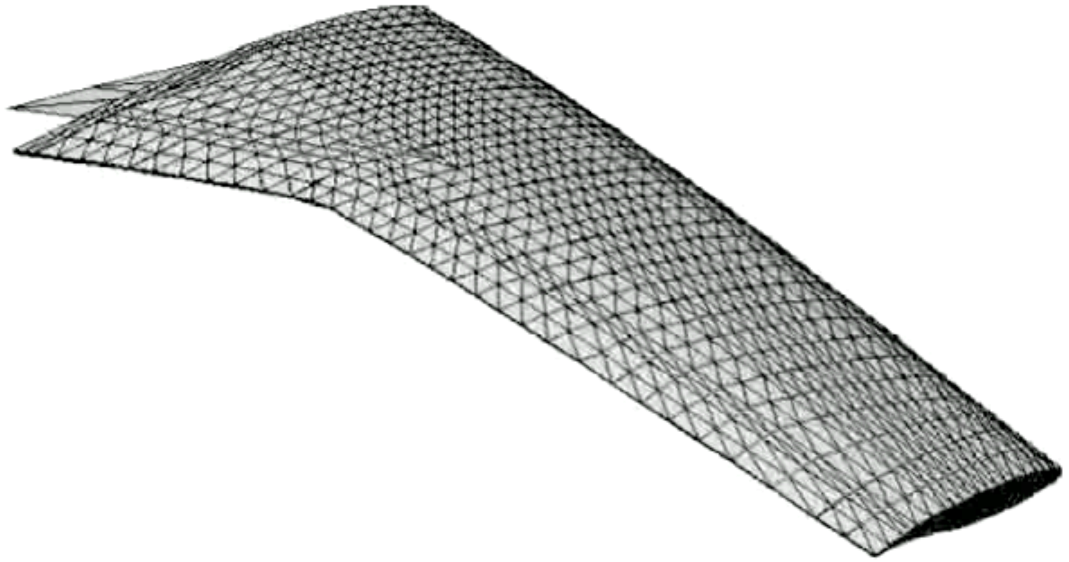
Motivation

- **Objective**: efficiently compute sufficiently accurate solutions to a sequence of linear systems with "nearby" SPD matrices
  - Applications: structural optimization, nonlinear analysis



Aero-structural optimization of ARW-2 wing

(courtesy Manuel Barcelos)

  - "Sufficiently accurate": satisfy solver tolerances $10^{-12} \leq \tau \leq 10^{-1}$
  - **Idea**: accelerate PCG convergence using a proper orthogonal decomposition (POD) basis built from previous solutions
    - ➡ POD is known to generate accurate approximations!

Nearby problems

- For $i = 1, \ldots, n_{\mathrm{LHS}}$ and $j = 1, \ldots, n_{\mathrm{RHS}}$, solve

$$\boldsymbol{A}^{(i)} \boldsymbol{x}^{(ij)} = \boldsymbol{b}^{(ij)}$$

  - $\boldsymbol{A}^{(i)} \in \mathbb{R}^{N \times N}$ sparse, SPD, and "close"
  - Parameterized variant: $\boldsymbol{A}(\boldsymbol{\mu}^{(i)})\boldsymbol{x}^{(j)}(\boldsymbol{\mu}^{(i)}) = \boldsymbol{b}^{(j)}(\boldsymbol{\mu}^{(i)})$

- Solve each system by preconditioned conjugate gradient (PCG)

$$\tilde{\boldsymbol{x}}^{(ij)} = \arg\min_{\boldsymbol{v} \in \boldsymbol{\mathcal{S}}} \|\boldsymbol{x}^{(ij)} - \boldsymbol{v}\|_{\boldsymbol{A}^{(i)}}$$

  - $\boldsymbol{\mathcal{S}} = \mathcal{K}_k$: k-dimensional Krylov subspace of $\mathbb{R}^N$
  - Current PCG acceleration approach: augmented CG methods

Augmented conjugate gradient methods

$$\mathcal{S} = \mathcal{K}_k + \mathcal{Y}$$

- Choices of $\mathcal{Y}$

  1. Previous search directions
  - Multi-RHS [O'Leary, 1980; Saad, 1987; Farhat *et al.*, 1994; Erhel, *et al.*, 2000]
  - Multi-LHS [Rey, 1994; Roux, 1995; Farhat, 1995; Farhat *et al.*, 2000, Risler *et al.*, 2000]
  - ➡ Large dimension: not feasible outside the context of DD

  2. Approximated extreme eigenvectors: deflation
  - Multi-RHS [Chapman *et al.*, 1997; Saad *et al.*, 2000]
  - Multi-LHS [Rey *et al.*, 1998; Parks *et al.*, 2007]
  - ➡ Effective only when a few eigenvalues hamper convergence

- Goals: 1) Feasible/general method to accelerate convergence

  2) Compatible with the augmented CG approach

→ Use POD and its optimal compression property to achieve this!

Proper orthogonal decomposition

- Given snapshots $\{w_m\}_{m=1}^{n_w}$, weights $\{\gamma_m\}_{m=1}^{n_w}$, and Θ-norm, the POD basis of dimension $n \ll N$ is $\Phi(n) \equiv [\phi_1, \ldots, \phi_n]$.

$$\mathrm{span}\{\phi_i, 1 \le i \le n\} = \arg \min_{\mathcal{S} \in \mathcal{G}(n,N)} \sum_{m=1}^{n_w} \| \left(I - \Pi_{\mathcal{S}}^{\Theta}\right) \gamma_m w_m \|_{\Theta}^2$$

  - $\Pi_{\mathcal{S}}^{\Theta}$: Θ-orthogonal projection onto $\mathcal{S}$
  - $\mathcal{G}(n, N)$: set of n-dimensional subspaces of $\mathbb{R}^N$

- Strategy: min. error for nearby target problem $\bar{A}\bar{x}^{(j)} = \bar{b}^{(j)}$

1. $\{w_m\}_{m=1}^{n_w}$: previous solutions & derivatives [Carlberg and Farhat, 2008]
2. $\{\gamma_m\}_{m=1}^{n_w}$: estimate the solution for the target problem

$$\bar{x}^{(j)} \approx \bar{x}_{\mathrm{est}}^{(j)} = \sum_{m=1}^{n_w} \gamma_m w_m$$

3. Θ: Coefficient matrix for the target problem $\bar{A}$

POD bases and key properties

- Compute one POD basis for each RHS $j = 1, \ldots, n_{\mathrm{RHS}}$

$$\boldsymbol{\Phi}_j(n) \equiv \left[\boldsymbol{\phi}_1^{(j)}, \ldots, \boldsymbol{\phi}_n^{(j)}\right]$$

- Key properties

1. Optimal ordering

   - First n POD basis vectors span optimal n-dimensional space

2. $\bar{A}$ -orthonormality

$$\boldsymbol{\Phi}_j(n)^T \bar{\boldsymbol{A}} \boldsymbol{\Phi}_j(n) = \boldsymbol{I}$$

$\rightarrow \boldsymbol{\Phi}_j(n)^T \boldsymbol{A}^{(i)} \boldsymbol{\Phi}_j(n) \approx \boldsymbol{I}$ for $\boldsymbol{A}^{(i)}$ near $\bar{\boldsymbol{A}}$

POD-based augmented CG algorithm

$$\mathcal{S} = \mathcal{K}_k + \mathrm{Range}\left(\Phi_j\left(n\right)\right)$$

1. Directly solve n_1-dimensional reduced equations (n_1 small)

$$\Phi_j(n_1)^T A^{(i)} \Phi_j(n_1)\hat{x} = \Phi_j(n_1)^T b^{(ij)}$$

$$\tilde{x}_1^{(ij)} = \Phi_j(n_1)\hat{x}$$

- Accurate (Property 1) and low cost (n_1 small)

2. Iteratively solve n-dimensional reduced equations $(n > n_1)$

$$\boxed{\Phi_j(n)^T A^{(i)} \Phi_j(n)}\hat{x} = \Phi_j(n)^T \left(b^{(ij)} - A^{(i)}\tilde{x}_1^{(ij)}\right)$$

$$\tilde{x}_2^{(ij)} = \tilde{x}_1^{(ij)} + \Phi_j(n_1)\hat{x}$$

- Use augmented CG without forming reduced matrix
- More accurate (Property 1) and low cost (Property 2)

POD-augmented CG algorithm

3. Iteratively solve full state equations to specified tolerance

$$\boldsymbol{A}^{(i)}\hat{\boldsymbol{x}} = \boldsymbol{b}^{(ij)} - \boldsymbol{A}^{(i)}\tilde{\boldsymbol{x}}_2^{(ij)}$$

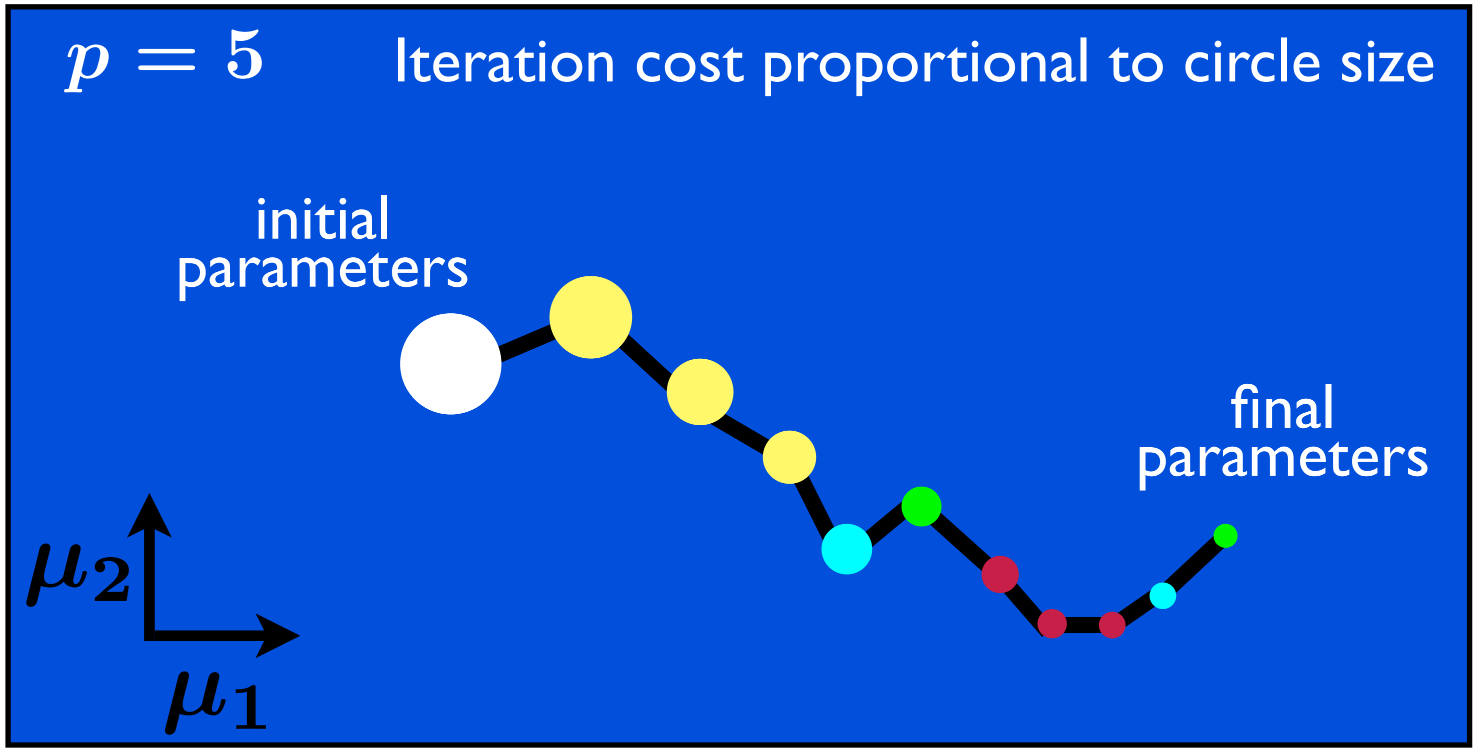
$$\tilde{\boldsymbol{x}}^{(ij)} = \tilde{\boldsymbol{x}}_2^{(ij)} + \hat{\boldsymbol{x}}$$

- Maintain $\boldsymbol{A}^{(i)}$-conjugacy to old search directions using augmented PCG [Farhat *et al.*, 1994]

- Multiple-RHS $(n_{\mathrm{RHS}} > 1)$
  - Sequentially execute Stages 1-3 for $j = 1, \ldots, n_{\mathrm{RHS}}$
  - Stage 1 approximation space includes search directions from all previous RHS

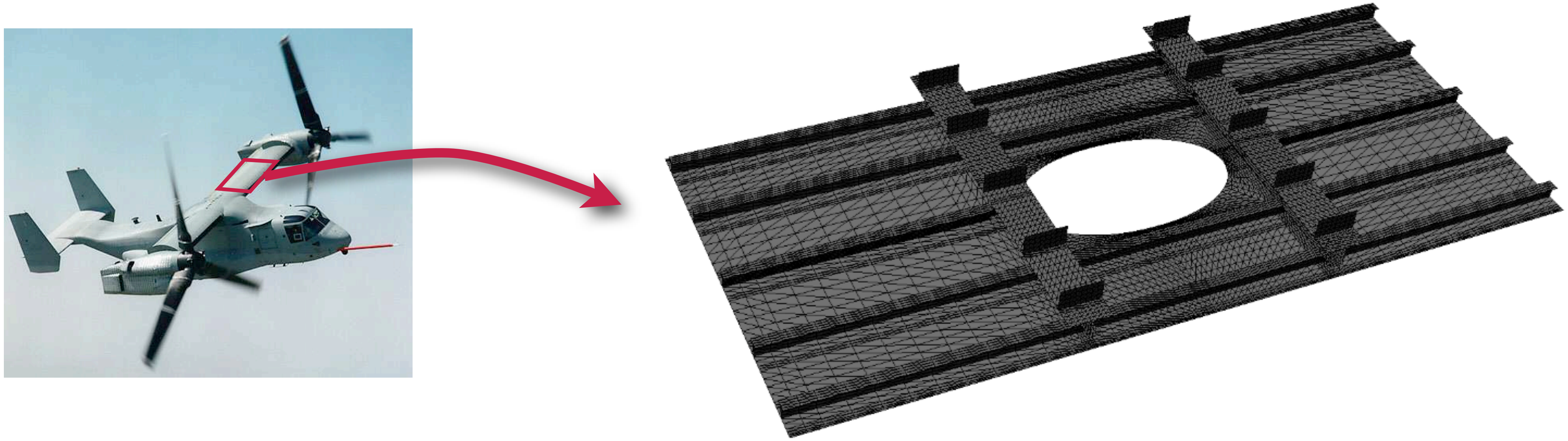
Implementation

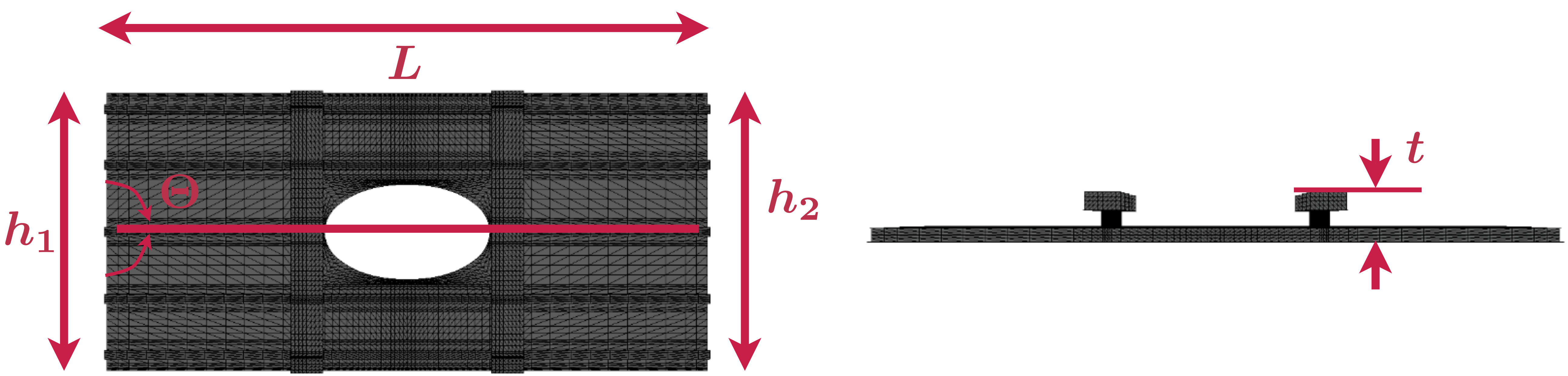
- $p =$ # LHS before recomputing POD basis (data compression)



	i	Stage 1 basis	Stage 2 basis	Compute POD?
○ (white)	1			
● (yellow)	$2 : p-1$	W		
● (cyan)	np	W		✓
● (green)	$np+1$	$\Phi(n_1)$	$\Phi(n)$	
● (red)	$np+2 : (n+1)p-1$	$[W, \Phi(n_1)]$	$[W, \Phi(n)]$	

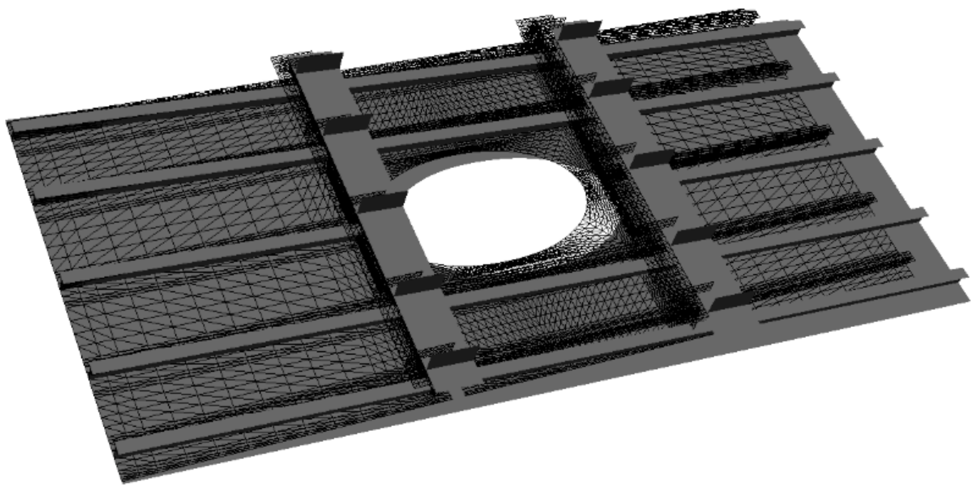
Example: V-22 Osprey wing panel



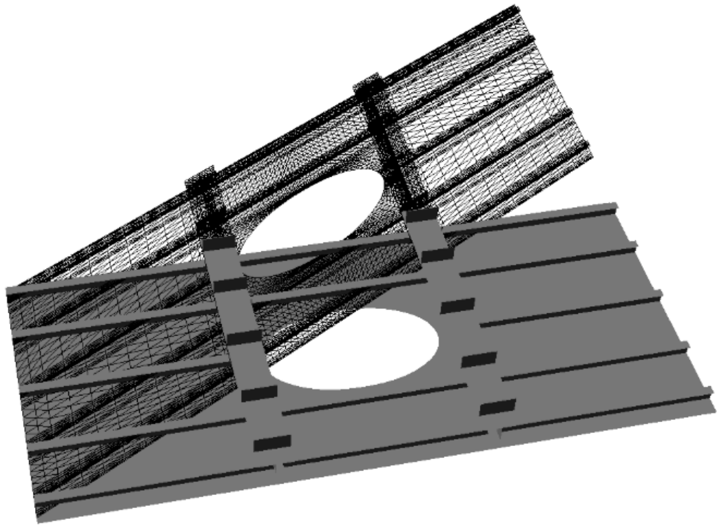


- Finite element model with 56,916 degrees of freedom
- 13 design variables (5 shape, 8 material)

- Problem Statement: $n_{\mathrm{LHS}} = 11\,,\, n_{\mathrm{RHS}} = 14$
  - Given: 10 previously-queried designs and designs for $i = 11$:



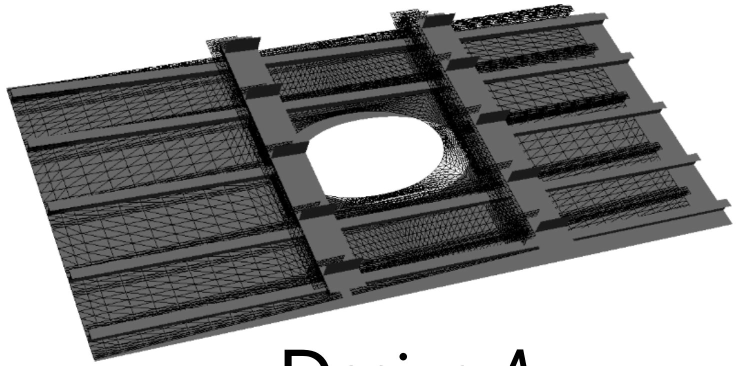
Design *A*

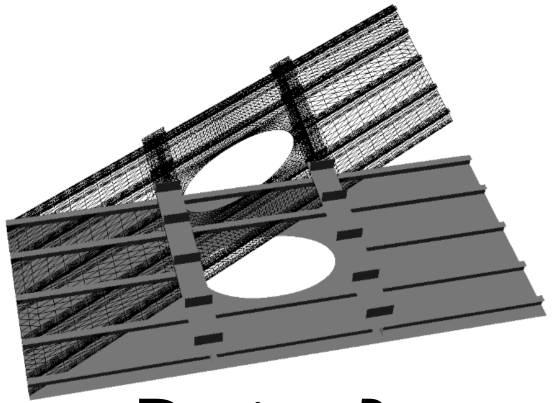


Design *B*

  - Compute: $\tilde{x}^{(11,j)},\ j = 1, \ldots, 14$ satisfying

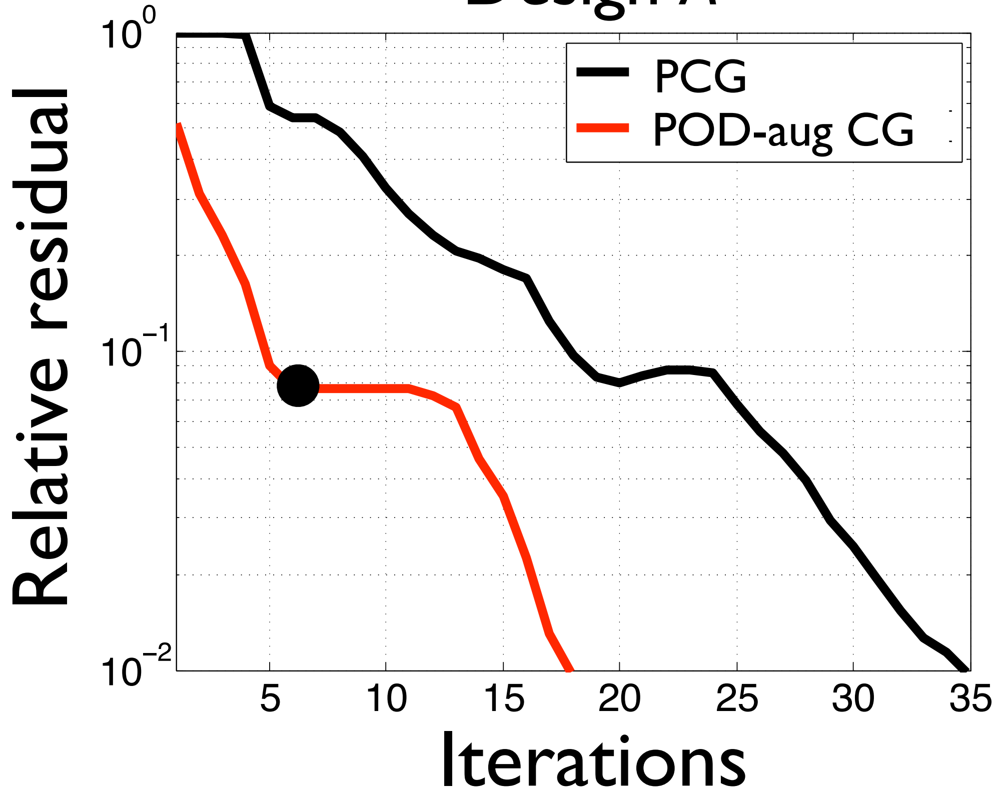
$$\frac{\|b^{(11,j)} - A^{(11)}\tilde{x}^{(11,j)}\|_2}{\|b^{(11,j)}\|_2} \leq 10^{-2}$$

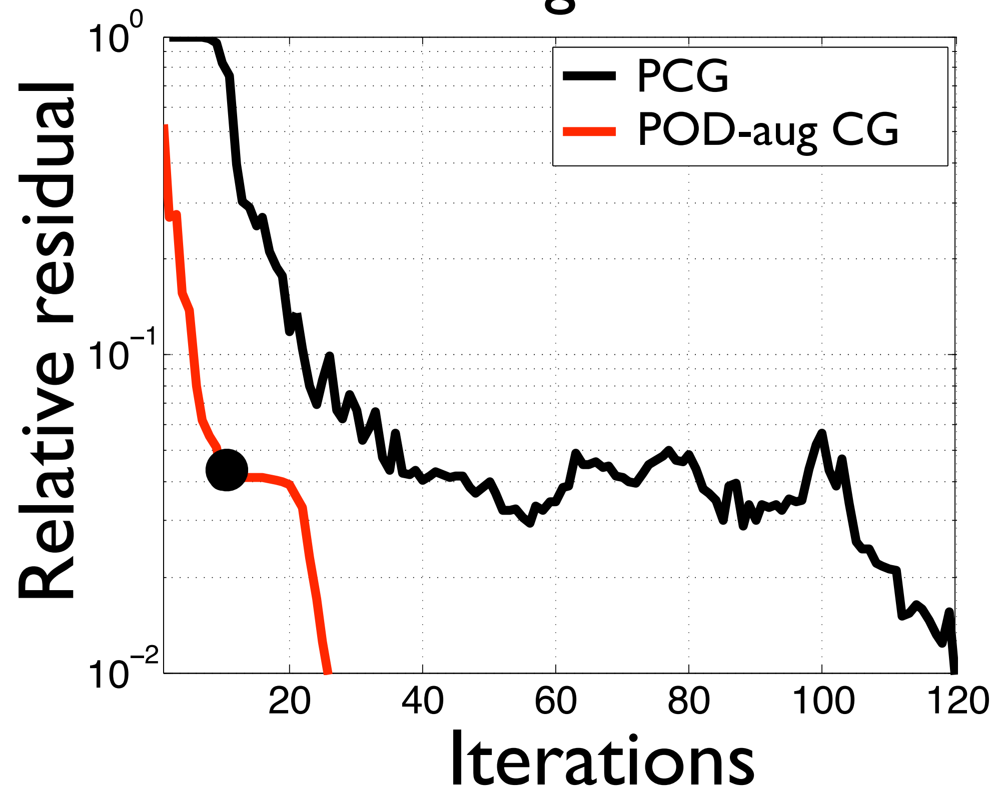




Error convergence $n_{\mathrm{RHS}} = 1$

● End of POD approximation





Simulation type	n_{RHS}	Speedup (flops), Design *A*	Speedup (flops), Design *B*
State equations	1	2.33	7.30
State equations + direct sensitivity	14	1.78	1.71

Conclusions

- A novel POD-based augmented conjugate gradient method
  - Accelerates convergence to sufficiently accurate solutions
  - Efficiency due to choice of POD snapshots, weights, and norm
  - 1.7x to 7.3x speedup over standard PCG

- Future work
  - Combine with other augmented CG approaches
    - Deflation: include approximated eigenvectors in stage 1
  - Fully implement for a repeated analyses problem
  - Extend to systems with non-SPD matrices

Thank You!

Questions?

Reference: K. Carlberg and C. Farhat, "An Adaptive POD Krylov Reduced-Order Model for Structural Optimization," 8th World Congress on Structural and Multidisciplinary Optimization, Lisbon, Portugal, June 1–5, 2009.