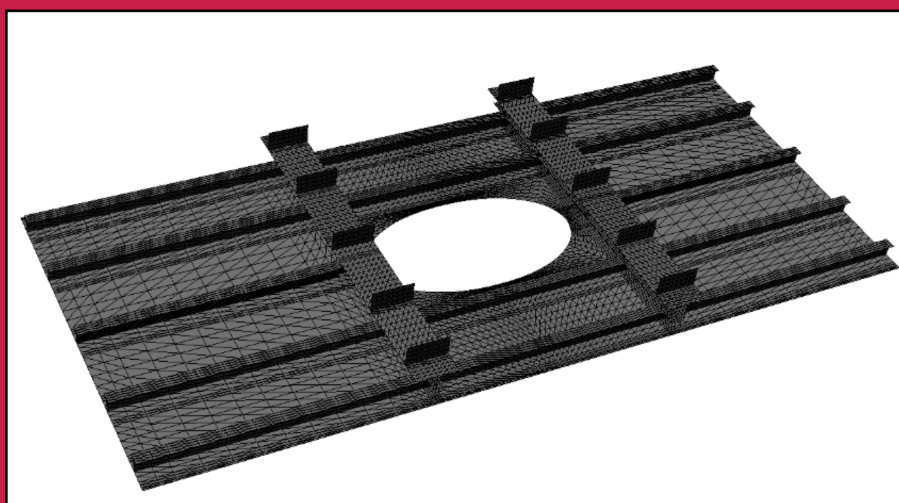
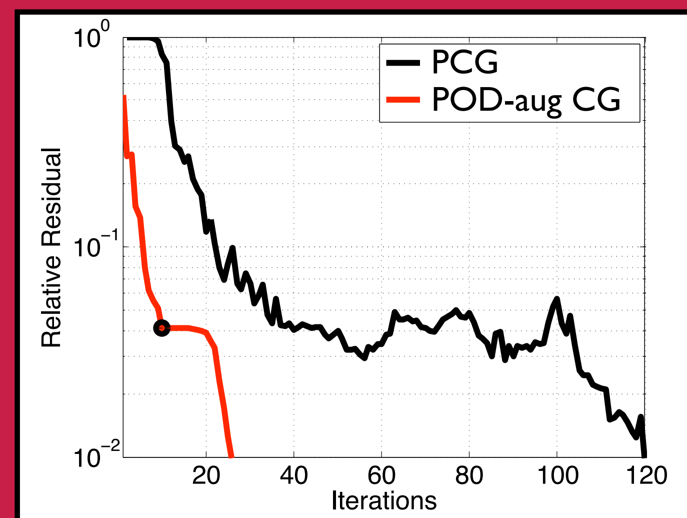
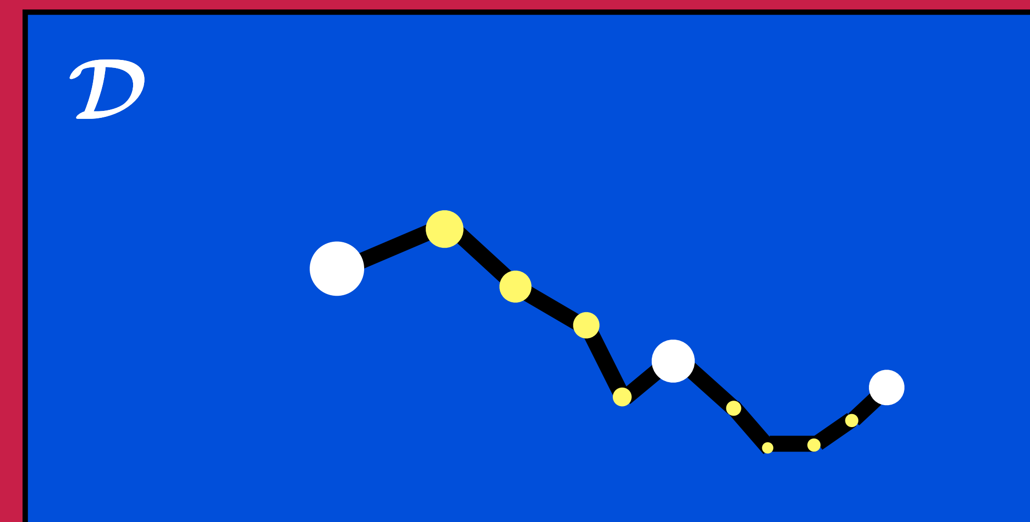
A POD-Based Iterative Solver for Fast Structural Optimization







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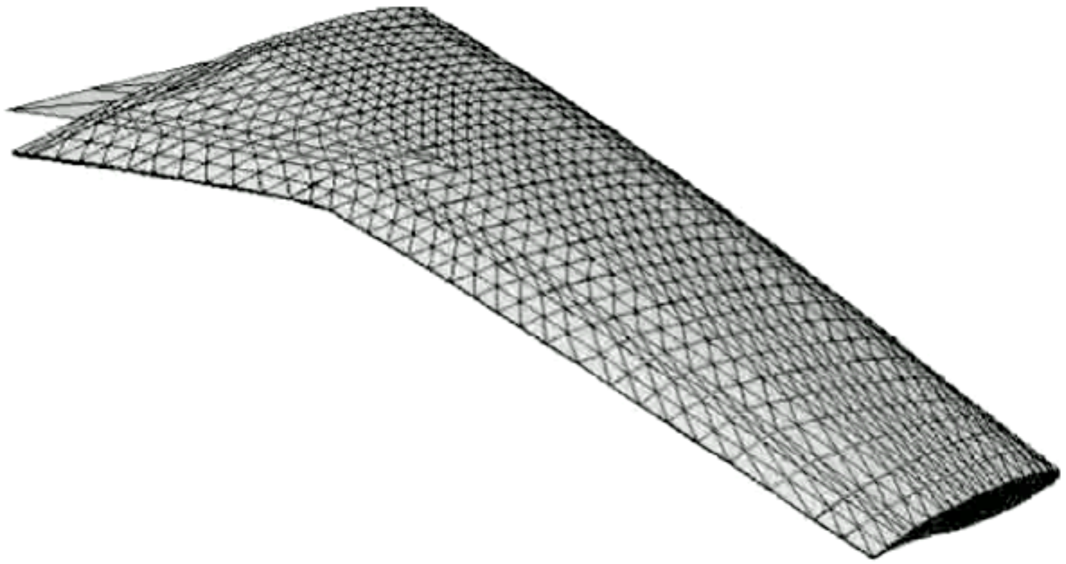
Motivation

- Structural design optimization via computer simulation
  - Widely used in industry
  - Often very expensive due to repeated simulation



Aero-structural optimization of ARW-2 wing
(courtesy Manuel Barcelos)

- We propose an adaptive model
  - Accurately and inexpensively approximates performance
  - Leads to fast design optimization

Motivation

- Design optimization:

maximize	Performance
by changing	Design variables
subject to	Constraints

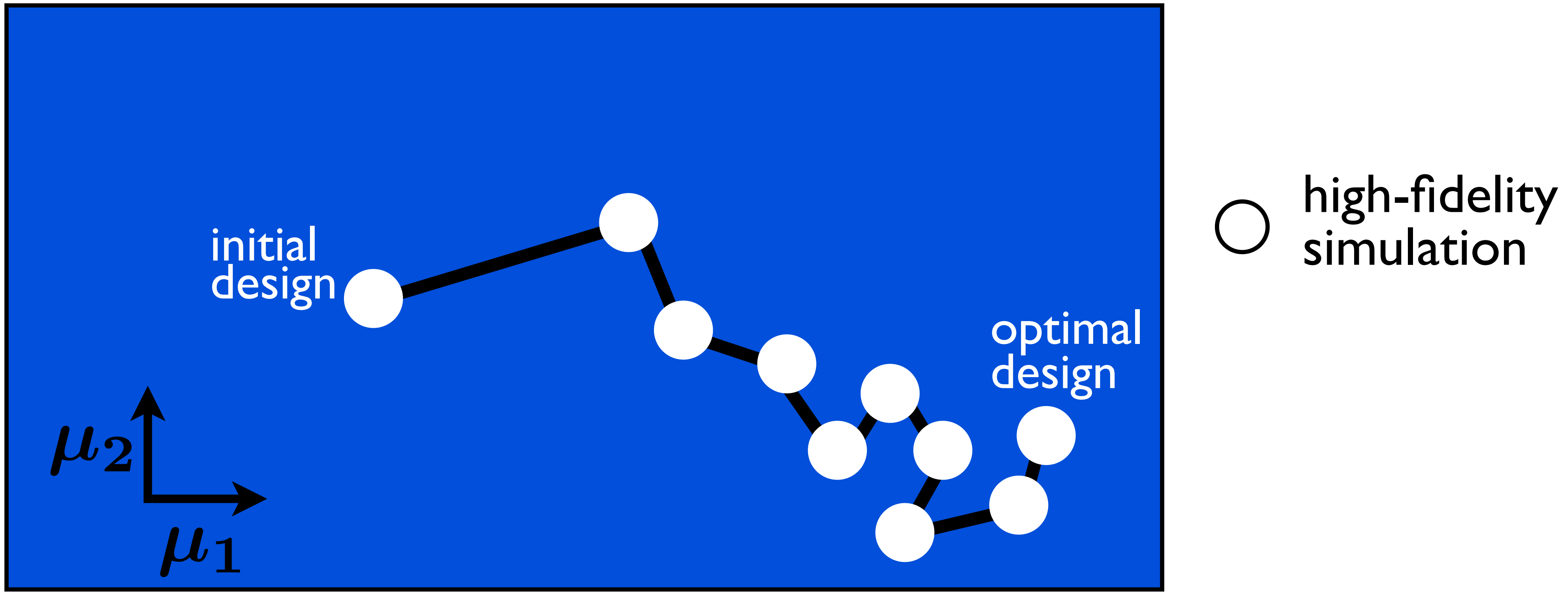
- Simulation-based design optimization:

maximize	$J(u,\mu)$
by changing	μ
subject to	$c(u,\mu)=0,\ d(u,\mu)\geq 0$
	$\boxed{K(\mu)u=f(\mu)}$

$K(\mu)$ stiffness matrix, u displacement, $f(\mu)$ load vector

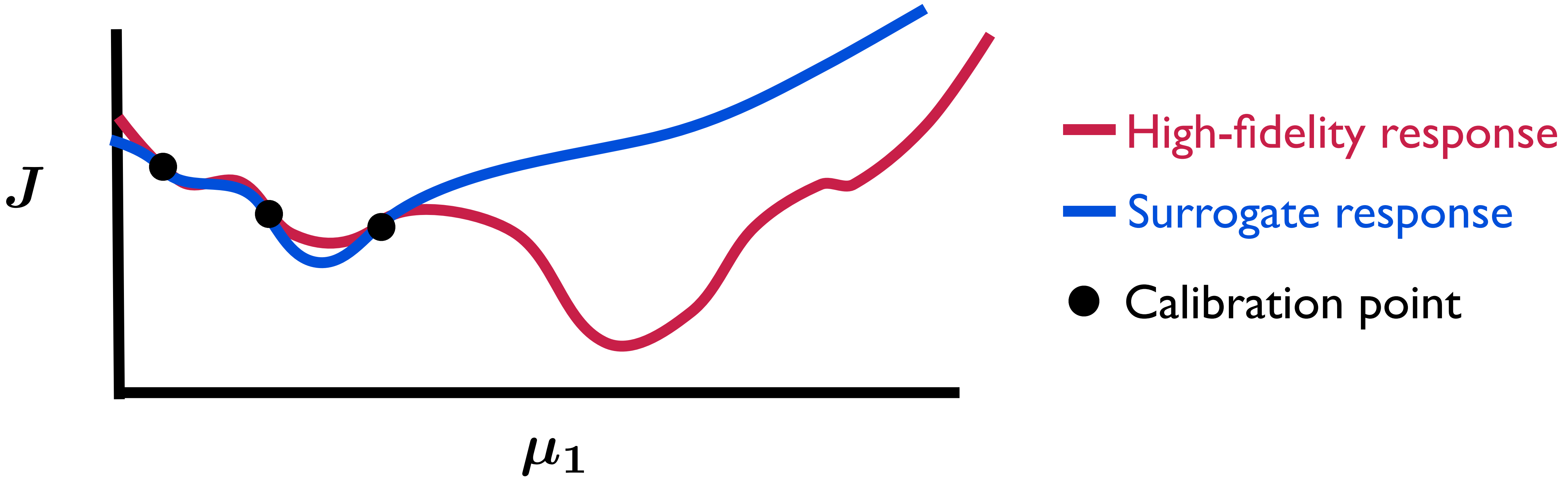
$\longrightarrow$ High-fidelity finite element model of the structure.

- Current Approach #1
  - Embed high-fidelity model within a numerical optimization algorithm



→ Prohibitively expensive for large-scale structures

- Current Approach #2
  - Optimize with a surrogate model
    1. Mimics the high-fidelity model
    2. Inexpensive to evaluate

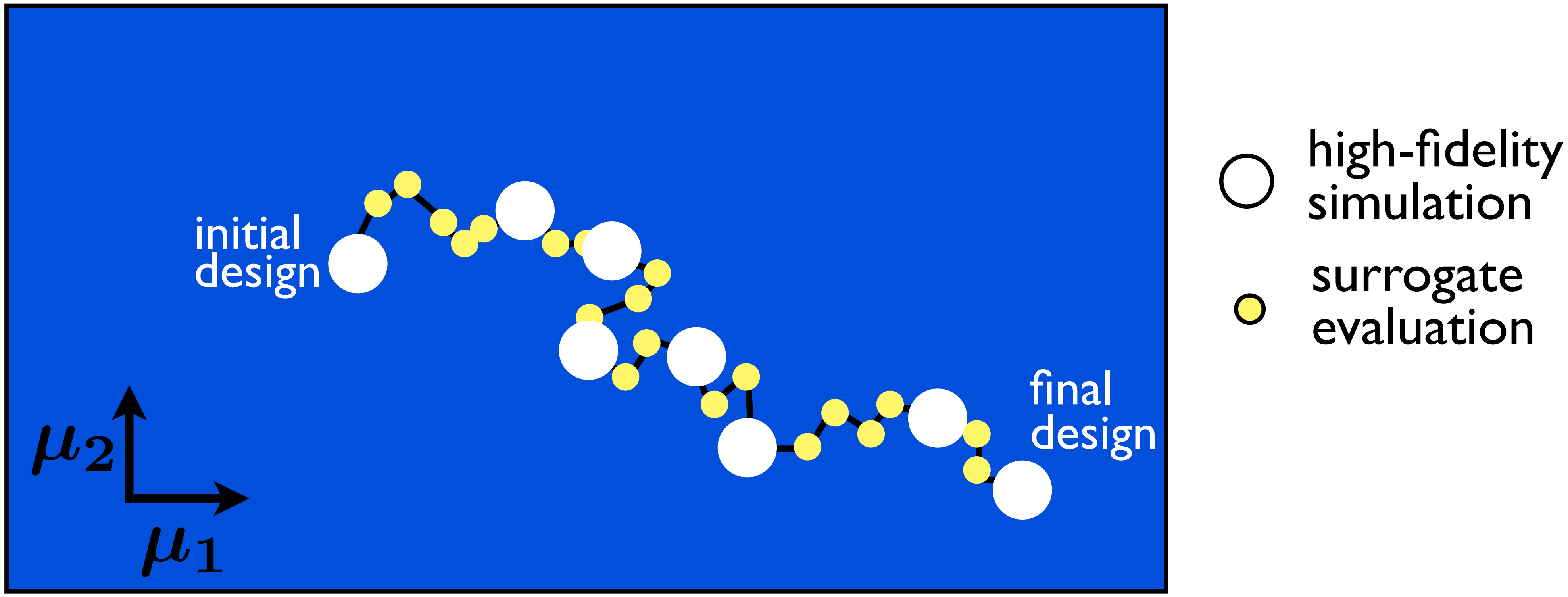


  - Inaccurate away from calibration points

SBO Problem

- Trust-region model management (Alexandrov *et al.*, 1998)

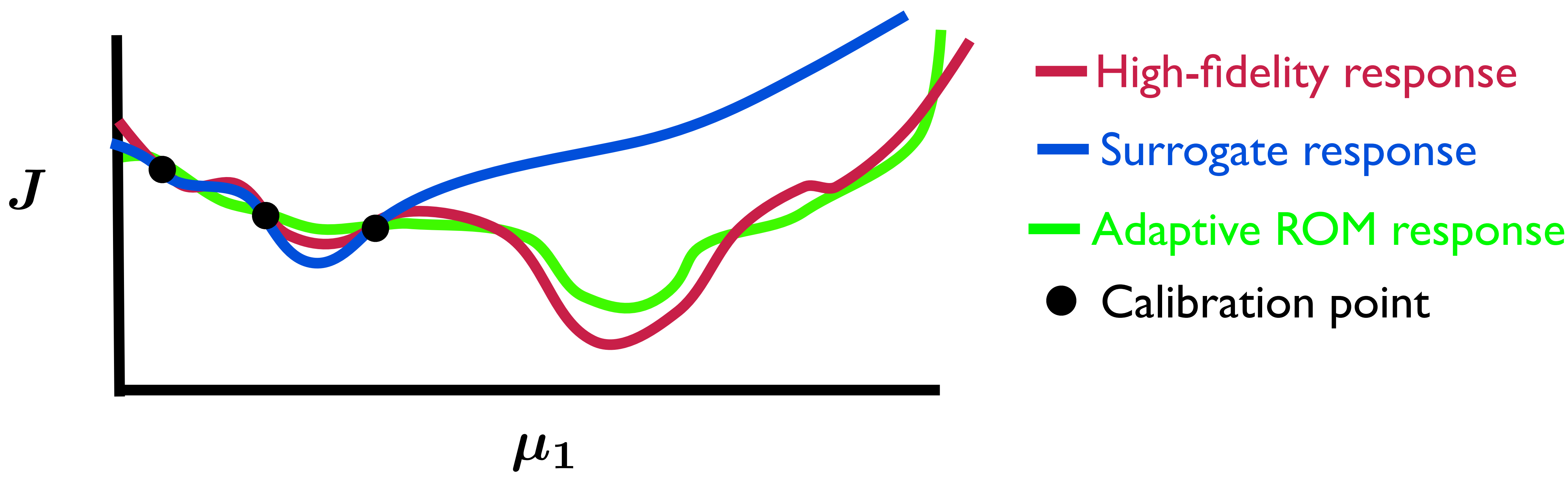
1. Calibrate surrogate by high-fidelity simulation
2. Optimize within a trust region using the surrogate
3. Grow/shrink trust region depending on surrogate accuracy



- Global inaccuracy of surrogate leads to many costly calibrations

Goal: directly control approximation errors → lower overall cost

- Use surrogate as acceleration tool for high-fidelity simulation
- Directly control the error (high-fidelity tolerance)
  - Global accuracy: fewer high-fidelity simulations
  - Improve accuracy as optimum is approached



- At each optimization iteration k, solve

  1) State equations $K(\mu^{(k)})u = f(\mu^{(k)})$

  2) Sensitivity equations

     - Direct S.A. For $i = 1, \ldots, n_{\text{vars}}$

$$K(\mu^{(k)})\frac{du}{d\mu_i} = \left.\frac{\partial f}{\partial \mu_i}\right|_{\mu^{(k)}} - \left.\frac{\partial K}{\partial \mu_i}\right|_{\mu^{(k)}} u$$

     or

     - Adjoint S.A. For $i = 1, \ldots, n_c + 1$

$$K(\mu^{(k)})\psi_i = \left.\frac{\partial \gamma_i}{\partial u}\right|_{\mu^{(k)}}^T \qquad \gamma_i = \begin{cases} c_i, & i = 1, \ldots, n_c \\ J, & i = n_c + 1 \end{cases}$$

Repeated analyses formulation

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

$$\boldsymbol{K}(\boldsymbol{\mu}^{(k)})\boldsymbol{u}_i = \boldsymbol{f}_i(\boldsymbol{\mu}^{(k)})$$

  - $\boldsymbol{K}(\boldsymbol{\mu}^{(k)})$ large, sparse, symmetric positive definite (SPD)

- Iteratively solve by preconditioned conjugate gradient (PCG)
  - For $m = 1, \ldots, M$ (until convergence)

$$\underset{\boldsymbol{x} \in \mathcal{K}_m}{\text{minimize}} \quad \frac{1}{2}\boldsymbol{x}^T \boldsymbol{K}(\boldsymbol{\mu}^{(k)})\boldsymbol{x} - \boldsymbol{x}^T \boldsymbol{f}_i(\boldsymbol{\mu}^{(k)})$$

  - $\mathcal{K}_m$ Krylov subspace of dimension m
  - Final solution $\tilde{\boldsymbol{u}}_i \in \mathcal{K}_M$ satisfies specified solver tolerance

- Approach: accelerate PCG convergence using ROM concepts

Adaptive ROM Approach

Solve $K(\mu^{(k)})u_i = f_i(\mu^{(k)})$ for $k = 1, \ldots, K$, $i = 1, \ldots, n_{\mathrm{RHS}}$

- Compute approximations $\tilde{u}_i$ satisfying controlled tolerance ϵ_k

$$\frac{\|f_i(\mu^{(k)}) - K(\mu^{(k)})\tilde{u}_i\|_2}{\|f_i(\mu^{(k)}\|_2} < \epsilon_k$$

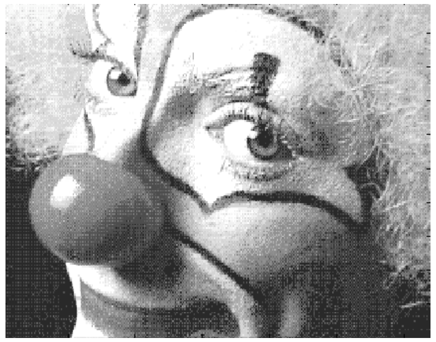
- Increase accuracy ($\epsilon_k \longrightarrow 0$) as the optimum is approached
- Approximations lie in the sum of two subspaces

$$\tilde{u}_i \in \mathcal{P} + \mathcal{K}_M$$

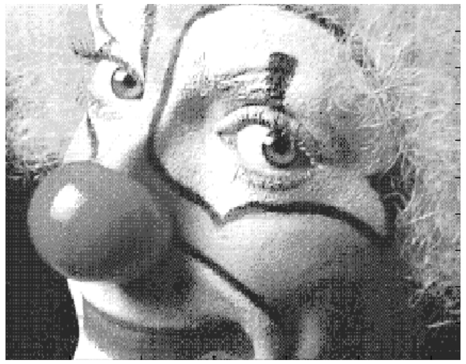
  - $\mathcal{P}$ proper orthogonal decomposition (POD) subspace
- Compute $\tilde{u}_i$ very efficiently by a novel augmented conjugate gradient (CG) iterative method

Proper Orthogonal Decomposition

- Optimal representation of "snapshot" data



Original: rank 200



POD rank 50 approximation

POD rank 10 approximation

Proper Orthogonal Decomposition

- Optimal representation of "snapshot" data
- Here, approximately minimize the projection error of the solution at a target configuration $\bar{\boldsymbol{\mu}}$ near $\boldsymbol{\mu}^{(k)}$

1. Snapshots $\{\boldsymbol{w}_j\}_{j=1}^{n_w}$: components of solution $\boldsymbol{u}(\bar{\boldsymbol{\mu}})$
    - Solution at previous configurations
    - Sensitivity derivatives (Carlberg and Farhat, 2008)
2. Weights $\{\gamma_j\}_{j=1}^{n_w}$: estimate the solution

$$\boldsymbol{u}(\bar{\boldsymbol{\mu}}) \approx \boldsymbol{u}_{\mathrm{est}}(\bar{\boldsymbol{\mu}}) = \sum_{j=1}^{n_w} \gamma_j \boldsymbol{w}_j$$

    - Radial basis functions & Taylor expansion coefficients
3. POD norm: $\|\boldsymbol{x}\|_{\boldsymbol{K}(\bar{\boldsymbol{\mu}})} \equiv \sqrt{\boldsymbol{x}^T \boldsymbol{K}(\bar{\boldsymbol{\mu}}) \boldsymbol{x}}$

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

$$\boldsymbol{\Phi}_i(n) \equiv \left[\phi_1^i, \ldots, \phi_n^i\right]$$

- Key properties

1. Optimal ordering
   - First n POD basis vectors span an optimal n-dimensional subspace

2. $K(\bar{\mu})$-orthonormality

$$\boldsymbol{\Phi}_i(n)^T \boldsymbol{K}(\bar{\mu}) \boldsymbol{\Phi}_i(n) = \boldsymbol{I}$$

   - $\boldsymbol{\Phi}_i(n)^T \boldsymbol{K}(\mu) \boldsymbol{\Phi}_i(n) \approx \boldsymbol{I}$ for μ near $\bar{\mu}$

- Three stages to compute approximation $\tilde{\boldsymbol{u}}_i$ at $\boldsymbol{\mu}^{(k)}$ near $\bar{\boldsymbol{\mu}}$

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

$$\boldsymbol{\Phi}_i(n_1)^T \boldsymbol{K}(\boldsymbol{\mu}^{(k)})\boldsymbol{\Phi}_i(n_1)\hat{\boldsymbol{u}} = \boldsymbol{\Phi}_i(n_1)^T \boldsymbol{f}_i(\boldsymbol{\mu}^{(k)}),$$
$$\tilde{\boldsymbol{u}}_{i,1} = \boldsymbol{\Phi}(n_1)\hat{\boldsymbol{u}}$$

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

2. Iteratively solve n_2-dimensional reduced equations ($n_2 \gg n_1$)

$$\boxed{\boldsymbol{\Phi}_i(n_2)^T \boldsymbol{K}(\boldsymbol{\mu}^{(k)})\boldsymbol{\Phi}_i(n_2)}\hat{\boldsymbol{u}} = \boldsymbol{\Phi}_i(n_2)^T \left(\boldsymbol{f}_i(\boldsymbol{\mu}^{(k)}) - \boldsymbol{K}(\boldsymbol{\mu}^{(k)})\tilde{\boldsymbol{u}}_{i,1}\right),$$
$$\tilde{\boldsymbol{u}}_{i,2} = \tilde{\boldsymbol{u}}_{i,1} + \boldsymbol{\Phi}_i(n_2)\hat{\boldsymbol{u}}$$

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

3. Iteratively solve full state equations to specified tolerance ϵ_k

$$\boldsymbol{K}(\boldsymbol{\mu}^{(k)})\hat{\boldsymbol{u}} = \boldsymbol{f}_i(\boldsymbol{\mu}^{(k)}) - \boldsymbol{K}(\boldsymbol{\mu}^{(k)})\tilde{\boldsymbol{u}}_{i,2}$$
$$\tilde{\boldsymbol{u}}_i = \tilde{\boldsymbol{u}}_{i,2} + \hat{\boldsymbol{u}}$$

- Use augmented PCG (Farhat *et al.*, 1994)
- Provides "adaptivity" to meet any specified tolerance
- Preconditioner: incomplete Cholesky, previous stiffness (Kirsch, 2002)

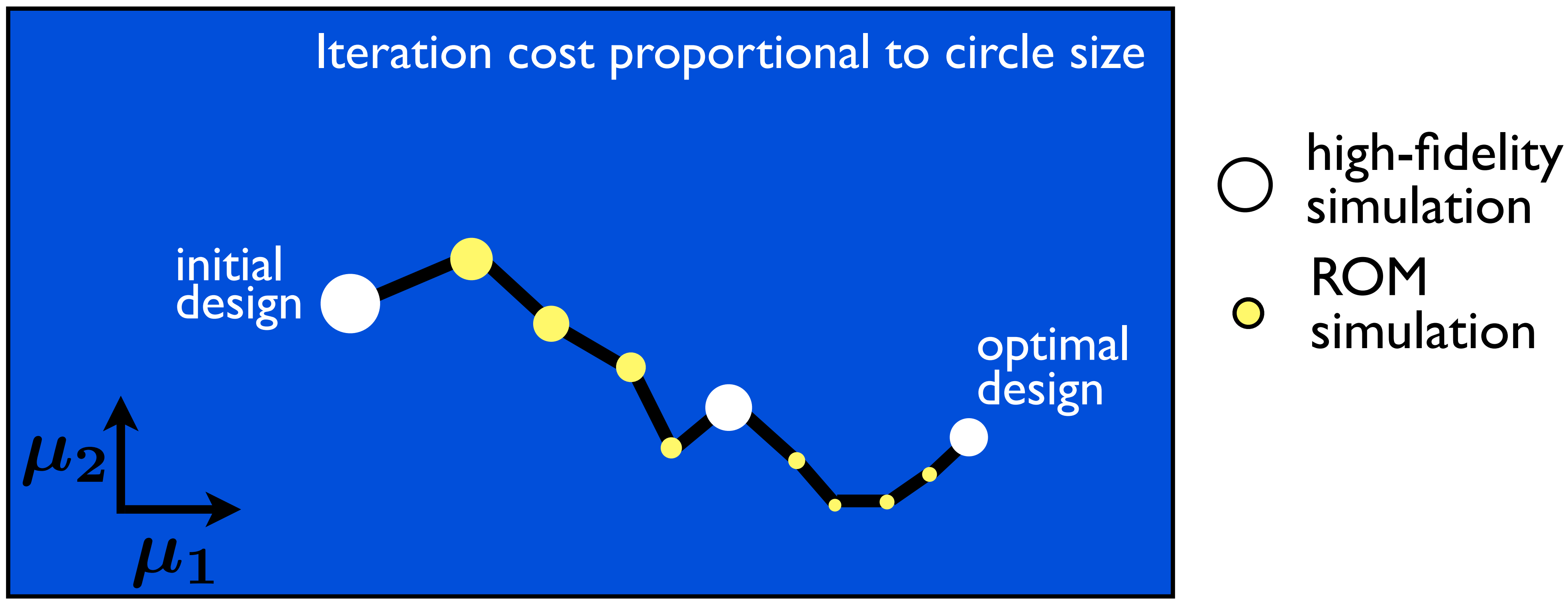
- Multiple-RHS (solving state equations + sensitivity analysis)
  - Sequentially execute Stages 1-3 for $i = 1, \ldots, n_{\mathrm{RHS}}$
  - Stage 1 approximation space includes search directions from all previous RHS

Optimization with POD-Krylov ROM

- Optimization procedure

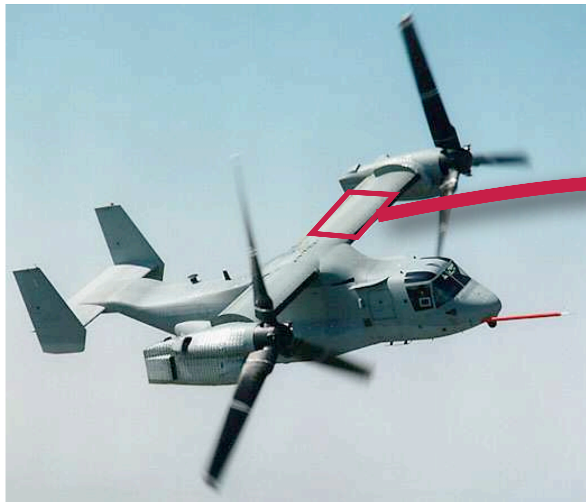
(optional)

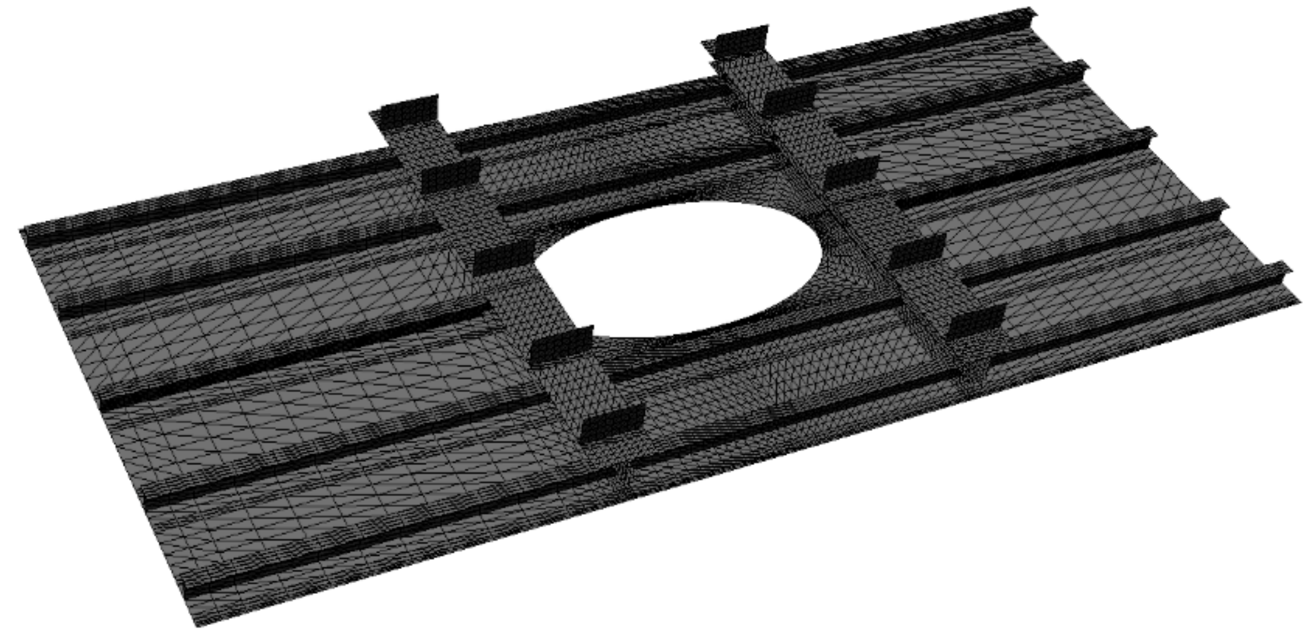
1. Calibrate ROM by high-fidelity simulation
2. Optimize using POD-Krylov ROM of desired accuracy

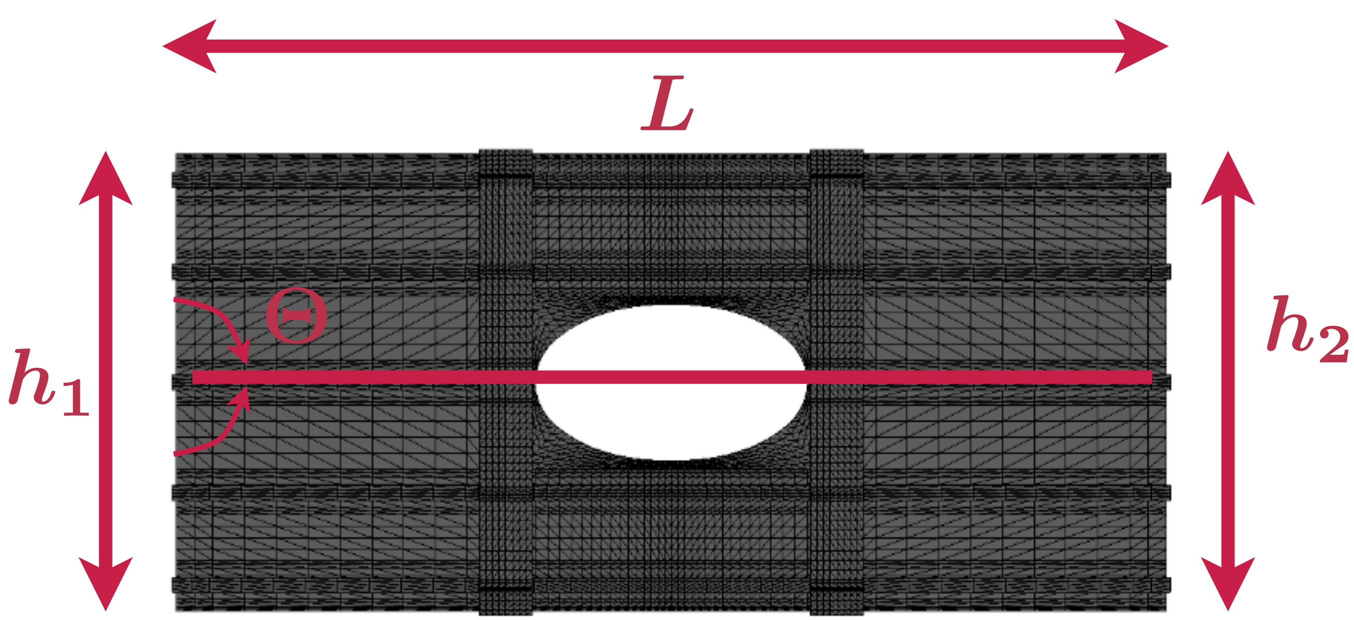


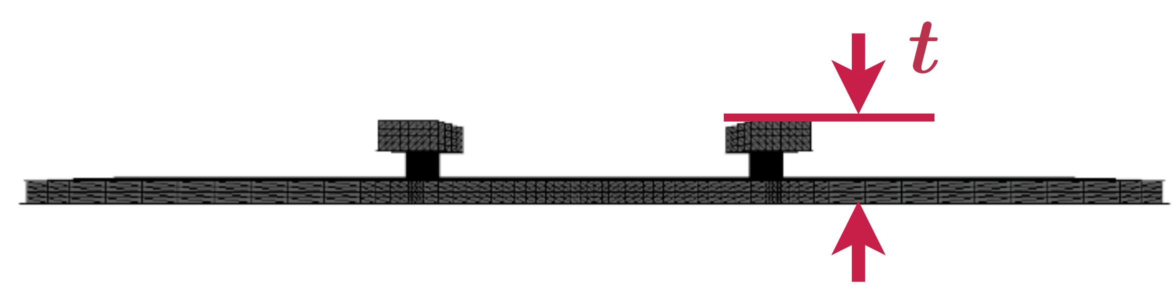
- Fewer high-fidelity simulations needed
- Accumulate snapshots → POD continually improves (cheaper)

Example: V-22 Osprey wing panel





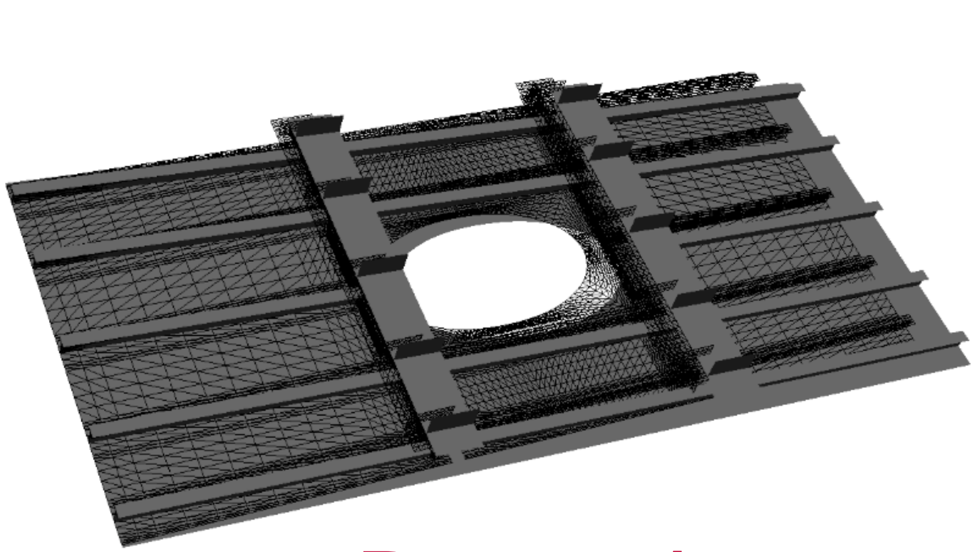




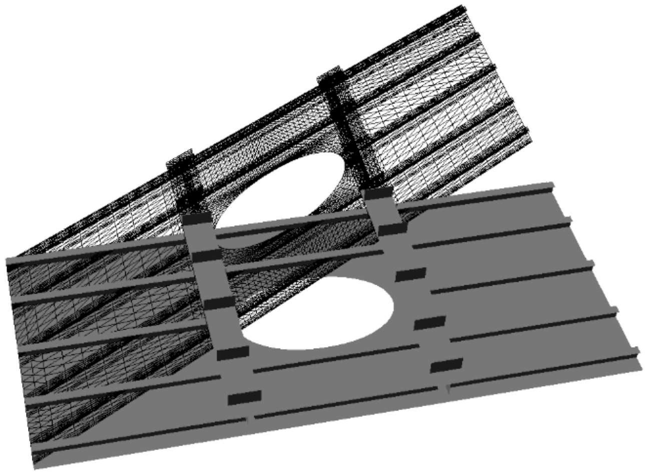
- Finite element model with 56,916 degrees of freedom
- 13 design variables (5 shape, 8 material)

Example: V-22 Osprey Wing Panel

- Problem Statement
  - Given: 10 previously-queried designs and 2 new designs



Design A



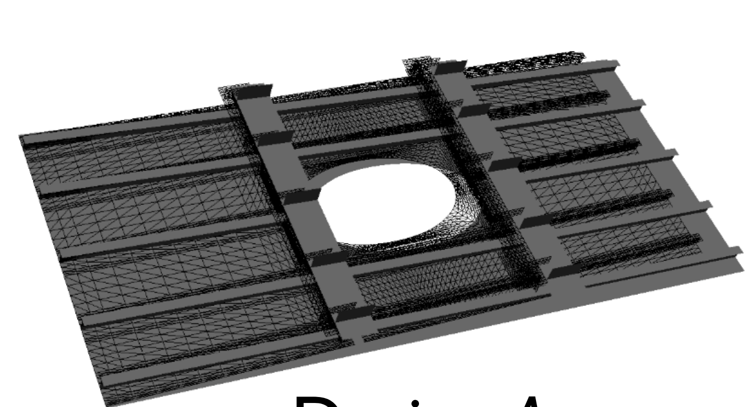
Design B

  - Compute: approximations $\tilde{u}_i, \; i = 1, \ldots, n_{\mathrm{RHS}}$ satisfying

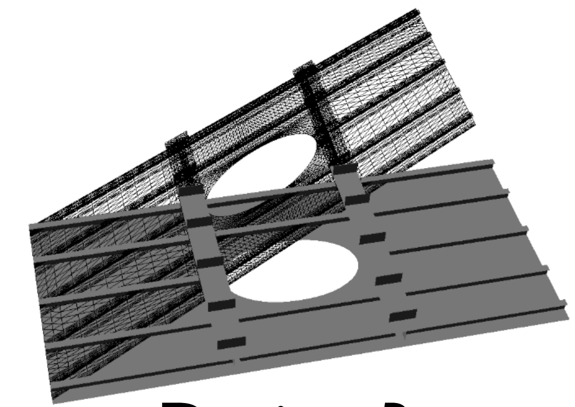
$$\frac{\|f_i(\mu) - K(\mu)\tilde{u}_i\|_2}{\|f_i(\mu)\|_2} < 10^{-2}$$

at the new designs

Results



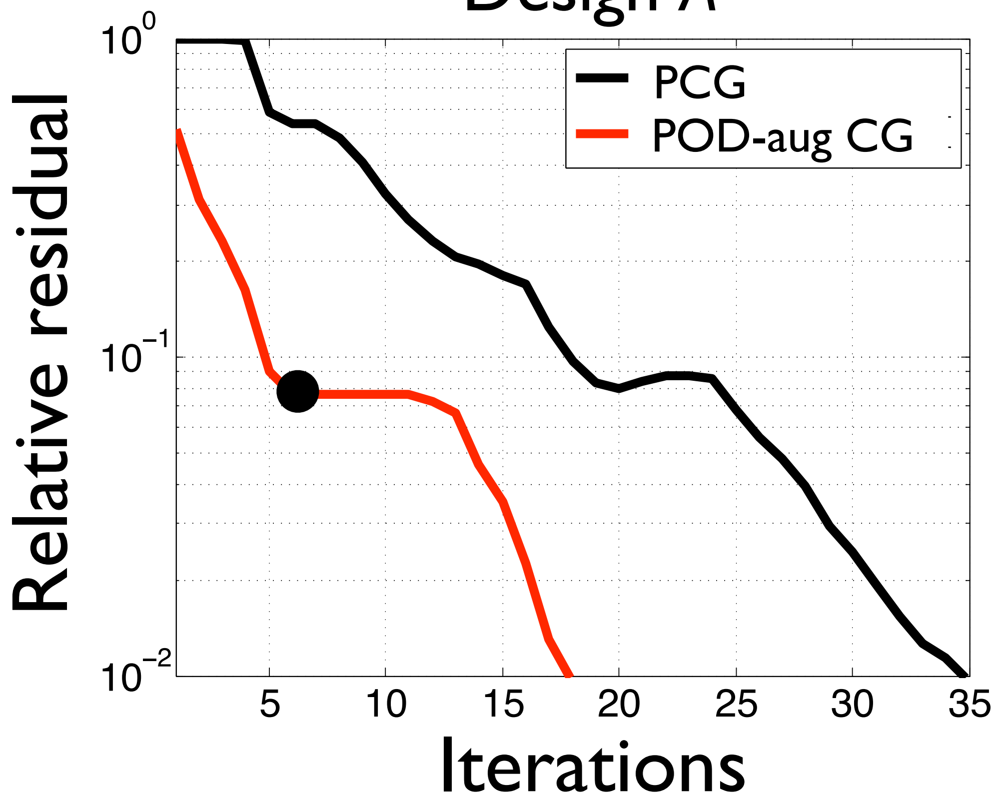
Design *A*

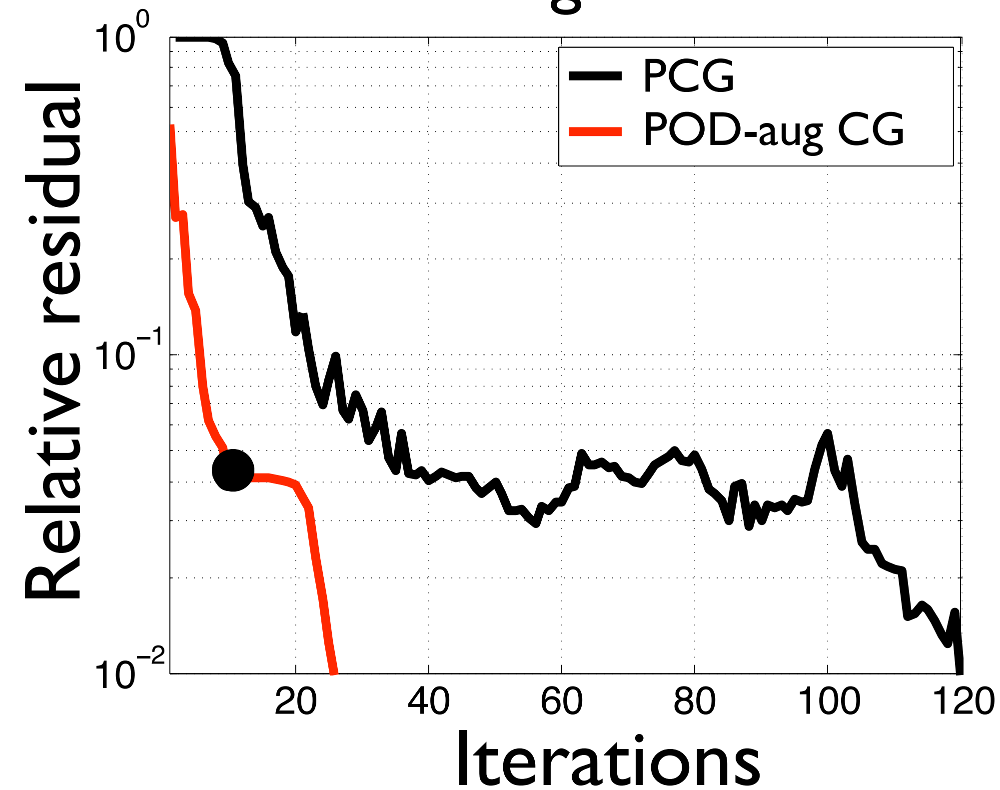


Design *B*

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 adaptive POD-Krylov reduced order model
  - Compute approximations of any desired accuracy
  - Efficiency due to choice of POD snapshots, weights, and norm
  - 1.7x to 7.3x speedup over existing iterative methods
  - Anticipate at least 3x faster structural design optimizations
- Future work
  - Implement within an optimization algorithm
  - Combine with other augmented Krylov approaches (deflation)
  - Extend to systems with non-SPD matrices and domain decomposition problems (FETI)

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.