Accounting for Variability in Design of Large-Scale Systems: A Reduced-Order Modeling Approach

Karen Willcox
Aerospace Computational Design Laboratory
Department of Aeronautics and Astronautics
Massachusetts Institute of Technology

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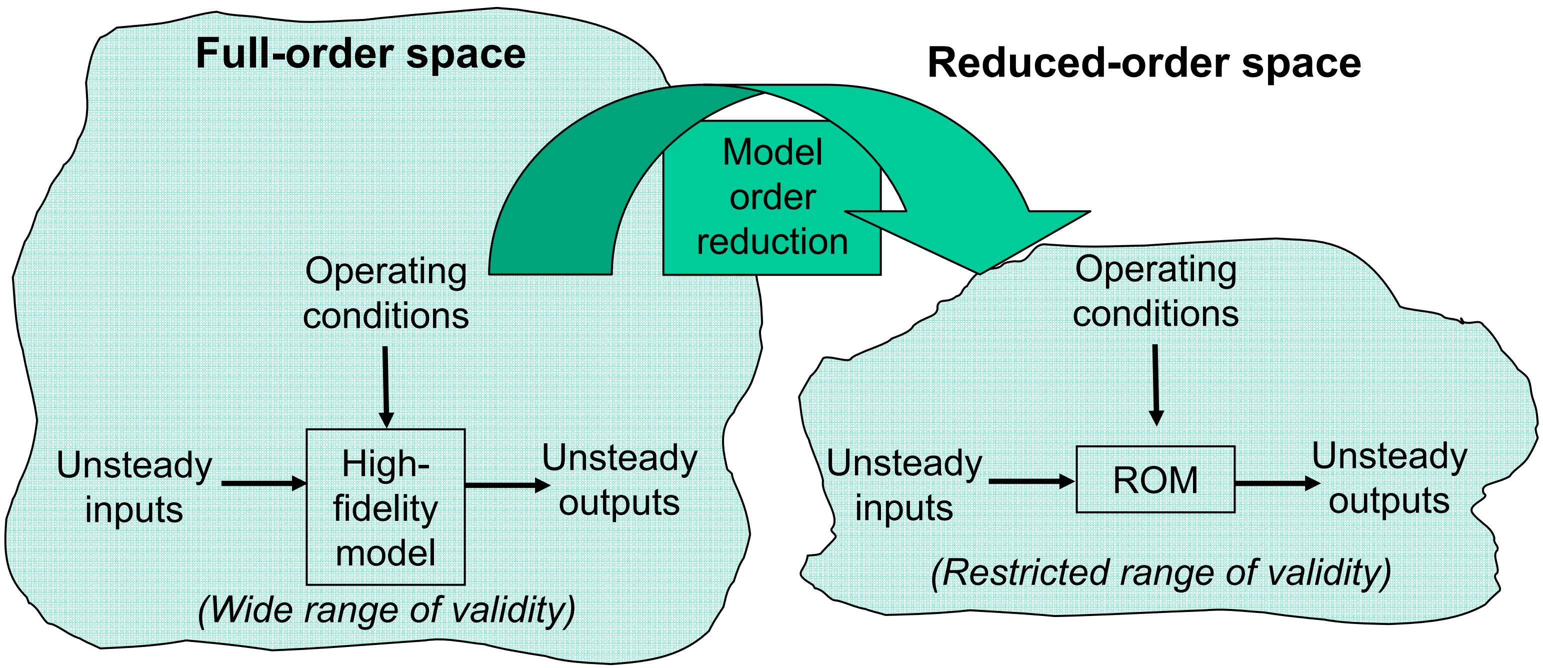
Outline

- Model reduction overview
  - Projection framework
  - Proper orthogonal decomposition (POD)
- Towards robust design and optimization (T. Bui-Thanh)
  - Including variability in reduced-order models
  - Example: design of bladed disks
- An optimization approach to model reduction (B. van Bloemen Waanders, B. Bader, O. Ghattas)

Model Order Reduction

Systematic model order reduction to replicate high-fidelity results over a restricted range of inputs.



→ Reduction level is several orders of magnitude

e.g. 2-D Euler : from ~10^4 states to ~10^1.

Why Model Reduction?

When is the high-fidelity dynamical system model too expensive?

- Multidisciplinary applications
  - Aeroelasticity (fluid/structure)
  - Flow control
- Real-time applications
- Design and optimization
- Probabilistic computations

Key idea: trade upfront computational work (offline phase) for a fast model (online phase).

Dynamical Systems

$$\begin{aligned} \dot{\mathbf{x}} &= A\mathbf{x} + B\mathbf{u} \\ \mathbf{y} &= C\mathbf{x} \end{aligned}$$

$$\begin{aligned} \dot{\mathbf{x}} &= f(\mathbf{x}, \mathbf{u}) \\ \mathbf{y} &= g(\mathbf{x}) \end{aligned}$$

$\mathbf{x} \in \mathbf{R}^n$: state vector

$\mathbf{u} \in \mathbf{R}^p$: input vector

$\mathbf{y} \in \mathbf{R}^q$: output vector

CFD Dynamical Systems

$$\begin{aligned} \dot{\mathbf{x}} &= A\mathbf{x} + B\mathbf{u} \\ \mathbf{y} &= C\mathbf{x} \end{aligned}$$

$$\begin{aligned} \dot{\mathbf{x}} &= f(\mathbf{x}, \mathbf{u}) \\ \mathbf{y} &= g(\mathbf{x}) \end{aligned}$$

- $\mathbf{x}(t)$: vector of n flow unknowns
  e.g. 2D Euler, N grid points, $n = 4N$

  $$\mathbf{x} = [\rho_1\ (\rho u)_1\ (\rho v)_1\ e_1\ \rho_2 \cdots\cdots \rho_N\ (\rho u)_N\ (\rho v)_N\ e_N]^T$$

- $\mathbf{u}(t)$: inputs
  e.g. flow disturbances, wing motion

- $\mathbf{y}(t)$: outputs
  e.g. flow characteristic, lift force

Reduced-Order Projection

$$\mathbf{x}(t) = \sum_{i=1}^{m} V_i \alpha_i(t)$$

$$\mathbf{x}(t) = V \mathbf{x}_r(t)$$

$$n \times 1 \left\{ \begin{bmatrix} x \end{bmatrix} \right. = \begin{bmatrix} \quad V \quad \end{bmatrix} \left. \begin{bmatrix} x_r \end{bmatrix} \right\} m \times 1$$

$$W^T V = I$$

Reduced-Order Dynamical Systems

$$n \times 1 \left\{ \begin{bmatrix} x \end{bmatrix} = \begin{bmatrix} & V & \end{bmatrix} \begin{bmatrix} x_r \end{bmatrix} \right\} m \times 1 \qquad W^T V = I$$

$$\dot{x} = f(x,u) \qquad \xrightarrow{x = V x_r} \qquad \dot{x}_r = W^T f(V x_r, u)$$
$$y = g(x,u) \qquad\qquad\qquad y_r = W^T g(V x_r, u)$$

$$\dot{x} = Ax + Bu \qquad \xrightarrow{x = V x_r} \qquad \dot{x}_r = A_r x_r + B_r u$$
$$y = Cx \qquad\qquad\qquad y_r = C_r x_r$$

$$A_r = W^T A V, \quad B_r = W^T B, \quad C_r = CV$$

Reduced-Order Basis

- Determine the projection $\mathbf{x} = V\mathbf{x}_r$
  where V contains m basis vectors

$$V = [\mathbf{v}_1 \ \mathbf{v}_2 \cdots \mathbf{v}_m]$$

  so that $m \ll n$ and system dynamics are captured accurately: $\mathbf{y}_r \approx \mathbf{y}$

- Most, but not all, reduction techniques use projection framework

Proper Orthogonal Decomposition

- Consider *M* snapshots $x_1, x_2, \ldots, x_M \in \mathcal{R}^n$ (instantaneous state solutions)
- Construct kernel $K \in \mathcal{R}^{n \times n}$

$$K = \sum_{j=1}^{M} x_j x_j^T$$

n×n eigenvalue problem

- $V = [v_1, v_2, v_3, \ldots]$ are eigenvectors of K with $\lambda_1 \geq \lambda_2 \geq \lambda_3 \ldots$
- If V_P contains the first P eigenvectors, then $Q_P = V_P V_P^T$ is the optimal projection in a least squares sense:

$$\min_{Q_P} \sum_{i=1}^{M} \left\| x_i - Q_P x_i \right\|_2^2 = \sum_{i=P+1}^{N} \lambda_i$$

- Note: optimality and error bound applies to the reconstruction of sampled data, not to the ROM.

Method of Snapshots

Sirovich: the eigenvectors of the kernel are linear combinations of the snapshots:

$$v_i = \sum_{j=1}^{M} \alpha_j^i x_j$$

The eigenvalue problem becomes:

$$R\alpha^i = \lambda_i \alpha^i \qquad \alpha^i = \begin{bmatrix} \alpha_1^i \\ \alpha_2^i \\ \vdots \end{bmatrix}$$

M×*M* eigenvalue problem

where *R* is the *M*×*M* correlation matrix:

$$R_{ij} = x_i^T x_j$$

Time-Domain POD Algorithm

Reduction procedure:

1. Simulate the high-order CFD system to get *M* snapshots $\mathbf{x}_j$, j=1,2,…,M
2. Construct the correlation matrix $R_{ij} = \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j$
3. Calculate the eigenvectors α^i and eigenvalues λ_i of R
4. Construct the basis functions

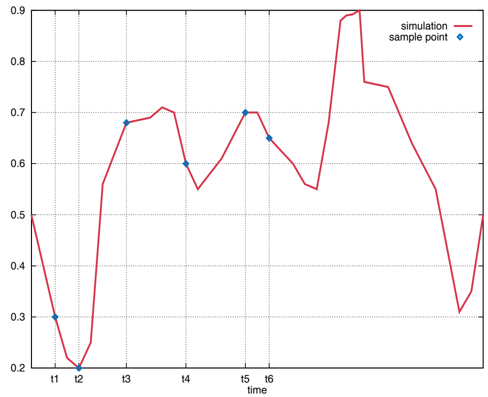
$$v_i = \sum_{j=1}^{M} \alpha_j^i x_j$$

5. Select the most energetic basis functions using λ_i
6. Project the governing equations onto the reduced basis

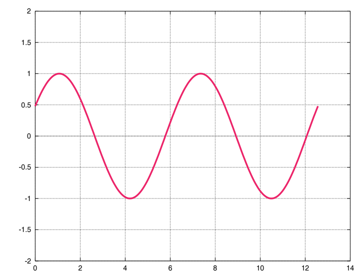
Most expensive step is the CFD simulation.

Frequency Domain

For linear systems, response can be decomposed into temporal harmonics:



$$= \sum$$



For $u = \bar{u}e^{j\omega t}$, $X = \bar{X}e^{i\omega t}$ and $y = \bar{y}e^{i\omega t}$

$$\boxed{\begin{aligned} \bar{X} &= [j\omega I - A]^{-1} B\bar{u} \\ \bar{y} &= C\bar{X} \end{aligned}}$$

Frequency Domain POD

- Difficulty in choosing appropriate time simulation to obtain snapshots
- Instead, pick a set of sample frequencies ω_k
- Solve frequency domain equations at each frequency to obtain complex snapshots

$$\bar{X}(\omega_k) = [j\omega_k I - A]^{-1} B$$

$$K = \frac{1}{M} \sum_{k=1}^{M} \bar{X}(\omega_k) \bar{X}^*(\omega_k)$$

A Different View of POD

- POD often thought of in least squares context
  - POD basis vector provides least squares fit to snapshot data
- **Balanced truncation** provides different insight
  - Concepts of **controllability** and **observability**

Inputs → State → Outputs

"Controllable" modes
- easy to reach, require small control energy

"Observable" modes
- generate large output energy

Subspaces

$x(0) = 0$

$u(t) \neq 0$

$$\dot{x} = Ax + Bu$$
$$y = Cx$$

$\{x(t)\} \in$ **controllable subspace**

*The **controllable subspace** is that set of states that can be obtained with zero initial state and a given input (reachable states).*

$\{x(0)\} \in$ **observable subspace**

$u(t) = 0$

$$\dot{x} = Ax + Bu$$
$$y = Cx$$

$y(t) \neq 0$

*The **observable subspace** is that set of states which as initial conditions produce a non-zero output with no external input.*

Gramians

Controllability Gramian:

eigenvectors of W_c span the controllable subspace

$$W_c = \frac{1}{2\pi}\int_{-\infty}^{\infty} \underbrace{(j\omega I - A)^{-1}B}_{\bar{X}_\omega} B^T\left(-j\omega I - A^T\right)^{-1} d\omega$$

$(j\omega I-A)^{-1}B$ is the response to sinusoidal forcing

Observability Gramian:

eigenvectors of W_o span the observable subspace

$$W_o = \frac{1}{2\pi}\int_{-\infty}^{\infty} \underbrace{\left(j\omega I - A^T\right)^{-1}C^T}_{\bar{Z}_\omega} C(-j\omega I - A)^{-1} d\omega$$

$(j\omega I-A^T)^{-1}C^T$ is the dual response to sinusoidal forcing

POD Versus Balanced Truncation

POD Kernel:

$$K = \frac{1}{M}\sum_{j=1}^{M}\left(j\omega_j I - A\right)^{-1} BB^*\left(-j\omega_j I - A^*\right)^{-1}$$

Controllability Gramian:

$$W_c = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(j\omega I - A\right)^{-1} BB^*\left(-j\omega I - A^*\right)^{-1} d\omega$$

- POD is an approximation to the controllability Gramian with rectangular rule.
- POD basis vectors approximate the most controllable modes (over sampled frequencies).
- Can also include POD analysis of dual for observability.

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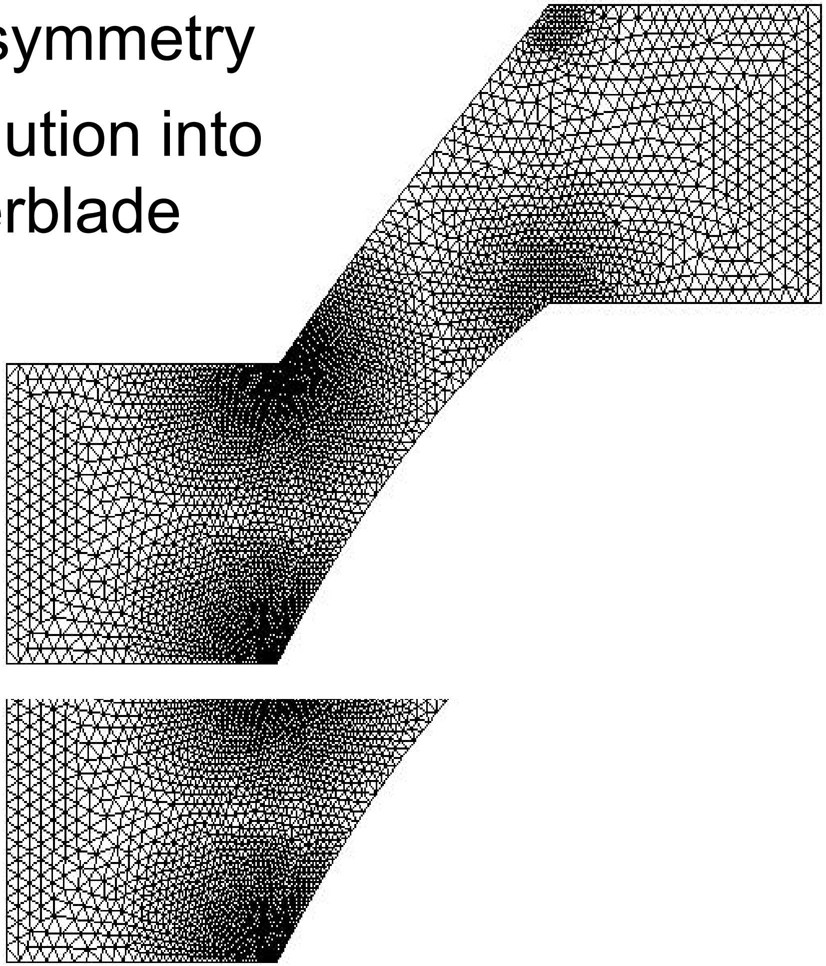
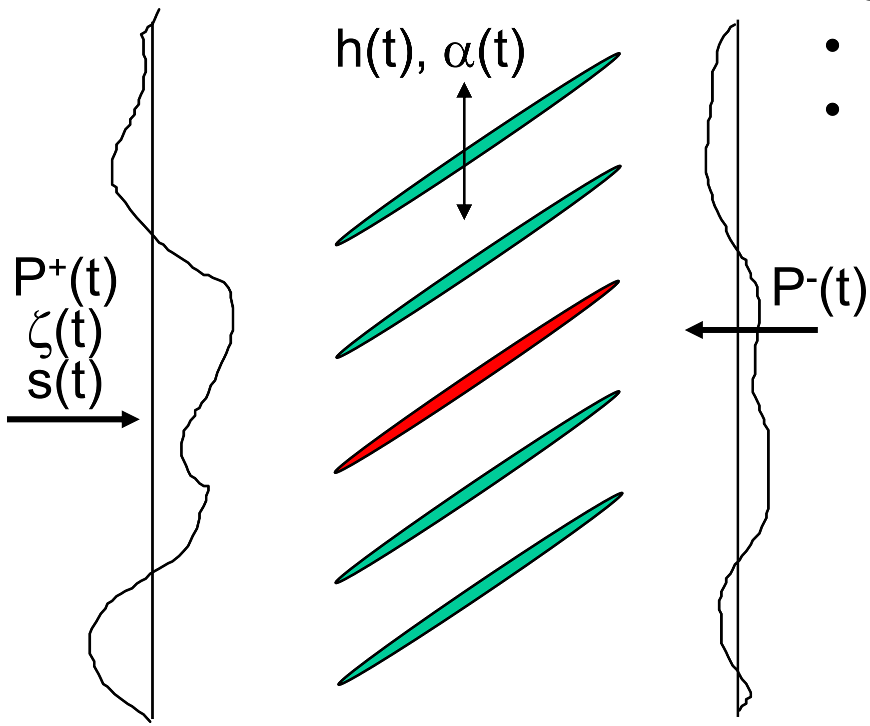
Turbomachinery Applications

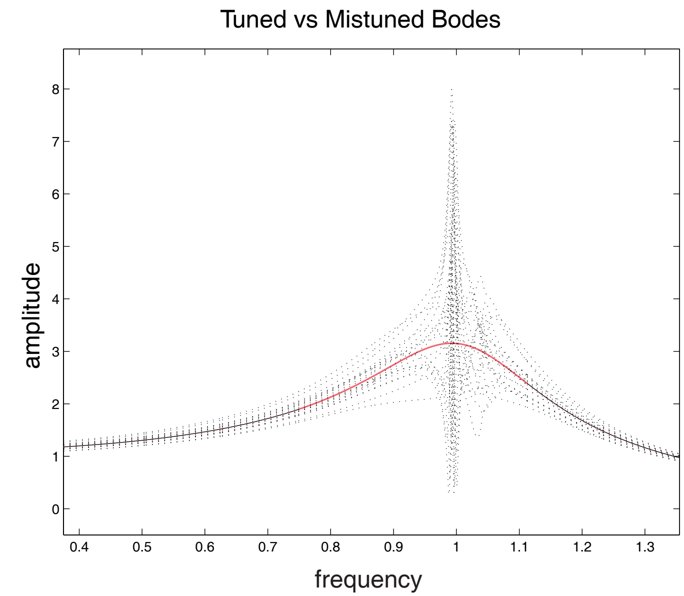
- Problems have spatial symmetry
- Decompose general solution into spatial harmonics – interblade phase angles
- Solve linearized system efficiently in frequency domain on a single passage



Effects of Variability



Variability in
- blade structural parameters
- blade shape



- Can have very large (negative) impact on forced response and a positive impact on stability
- Intentional mistuning can improve robustness
- Probabilistic design methods are a critical need

Representing Geometry Variability

- Mistuned blade geometry, g, can be expressed as (Garzon and Darmofal, 2003)

$$g = g_0 + \sum_{i=1}^{ns} \sigma_i z_i w_i$$

- g_0 : nominal blade
- w_i : POD geometry modes
- $z_i \in$ N(0,1)
- σ_i: standard deviation of the geometric data attributable to the ith mode
- ns : number of mode shapes used to represent the mistuning.

Variability in CFD Models

- CFD model dependence on geometry can now be written

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

  where $\mathbf{z} = [z_1 \;\; z_2 \ldots z_{ns}]$.

- For probabilistic calculations, too expensive to evaluate A, B, C for many geometries

Approximate Model for Variability

- Efficient approximation using interpolation at nominal conditions, g_o, and at selected interpolation points, z_i^j

$$A(z) \approx \bar{A}(z) = A_0 + \sum_{i=1}^{ns} \sum_{j=1}^{m_i} \frac{z_i \prod_{k=1,k\neq j}^{m} (z_i - z_i^k)}{z_i^j \prod_{k=1,k\neq j}^{m} (z_i^j - z_i^k)} (A_i^j - A_0)$$

- Interpretation:
  - Lagrange interpolation in each random variable z_i
  - Taylor series expansion
- Similar expressions for B, C

Approximate Model for Variability

- Approximate linearized system for arbitrary mistuning:

$$
\begin{aligned}
\dot{\mathbf{x}} &= \left(A_0 + \sum_{i=1}^{ns} \sum_{j=1}^{m_i} \alpha_i^j (A_i^j - A_0) \right) \mathbf{x} \\
&\quad + \left(B_0 + \sum_{i=1}^{ns} \sum_{j=1}^{m_i} \alpha_i^j (B_i^j - B_0) \right) \mathbf{u} \\
\mathbf{y} &= \left(C_0 + \sum_{i=1}^{ns} \sum_{j=1}^{m_i} \alpha_i^j (C_i^j - C_0) \right) \mathbf{x}
\end{aligned}
$$

where $\alpha_i^j(z_i) = \dfrac{z_i \prod_{k=1,k\neq j}^{m} (z_i - z_i^k)}{z_i^j \prod_{k=1,k\neq j}^{m} (z_i^j - z_i^k)}$

- Requires $\sum_{i=1}^{ns} m_i$ expensive linearization system evaluations (offline cost)
- Online cost to compute system for any mistuning **z** is small.

Probabilistic Reduced-Order Model

- Given a reduced basis for the flow state, V, W:

$$\dot{\mathbf{x}}_r = \left(\mathcal{A}_0 + \sum_{i=1}^{ns}\sum_{j=1}^{m_i}\alpha_i^j(\mathcal{A}_i^j - \mathcal{A}_0)\right)\mathbf{x}_r + \left(\mathcal{B}_0 + \sum_{i=1}^{ns}\sum_{j=1}^{m_i}\alpha_i^j(\mathcal{B}_i^j - \mathcal{B}_0)\right)\mathbf{u}$$

$$\mathbf{y}_r = \left(\mathcal{C}_0 + \sum_{i=1}^{ns}\sum_{j=1}^{m_i}\alpha_i^j(\mathcal{C}_i^j - \mathcal{C}_0)\right)\mathbf{x}_r$$

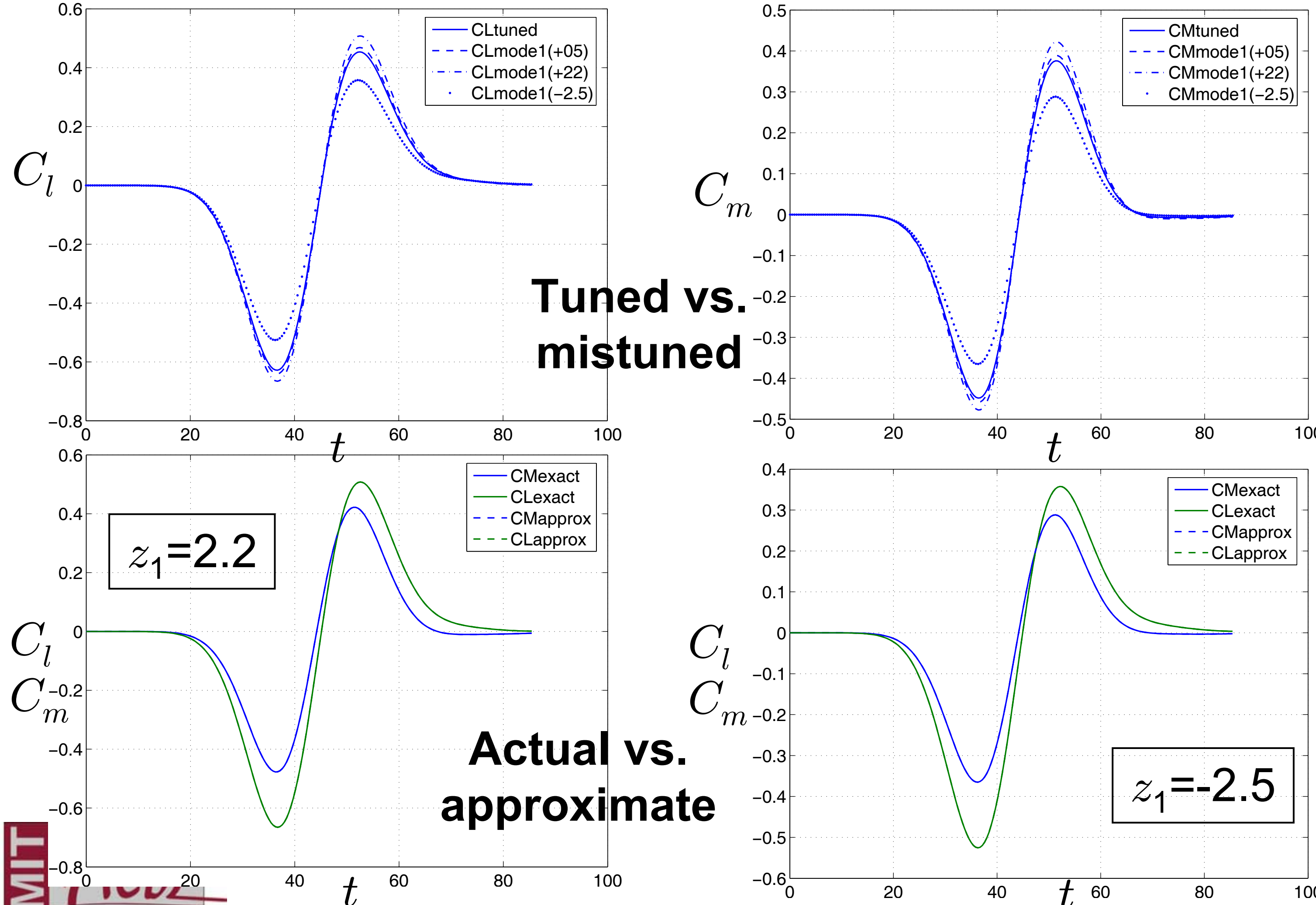
where $\mathcal{A} = W^T A V$, $\mathcal{B} = W^T B$, $\mathcal{C} = CV$

- Basis must capture both unsteady dynamics (i.e. t) and parameter variations (i.e. **z**)
- Use sampling methods proposed by Patera et al.

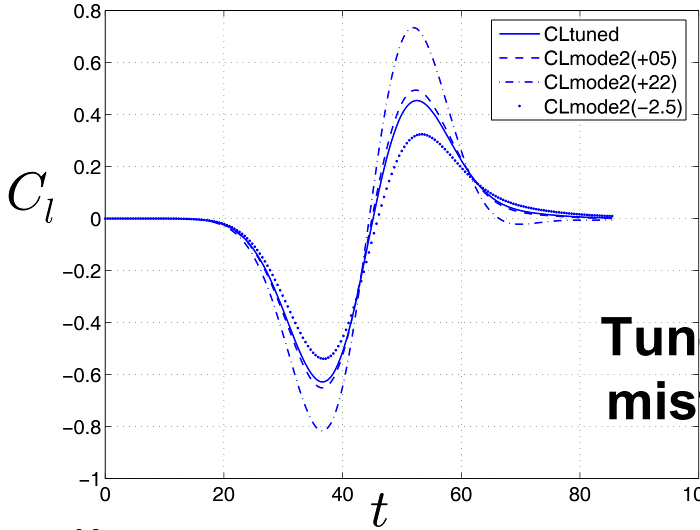
Example: Blade Shape Variability

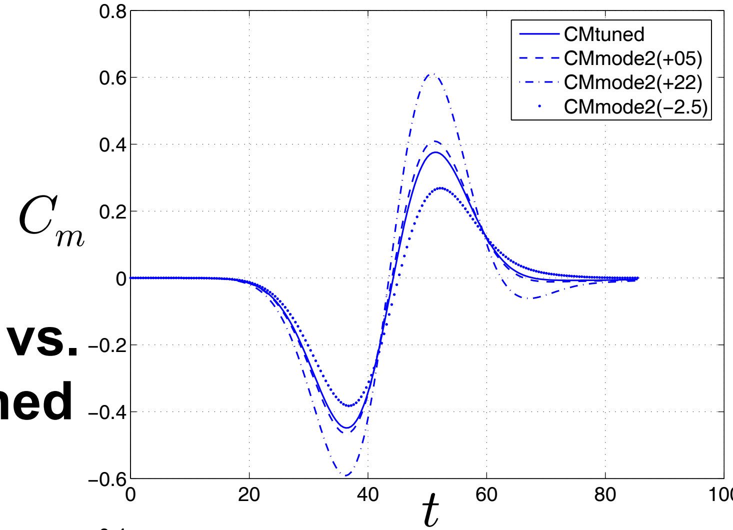
- Actual manufacturing data from Pratt & Whitney
  - 145 blades measured at 9 sections
- Preliminary analysis:
  - Blade in isolation
  - Two-dimensional analysis at mid-section
  - Rigid unsteady plunging motion
  - M=0.3
- Geometry model with 2 POD shape modes captures 82.55% of variability

Geometry Mode 1

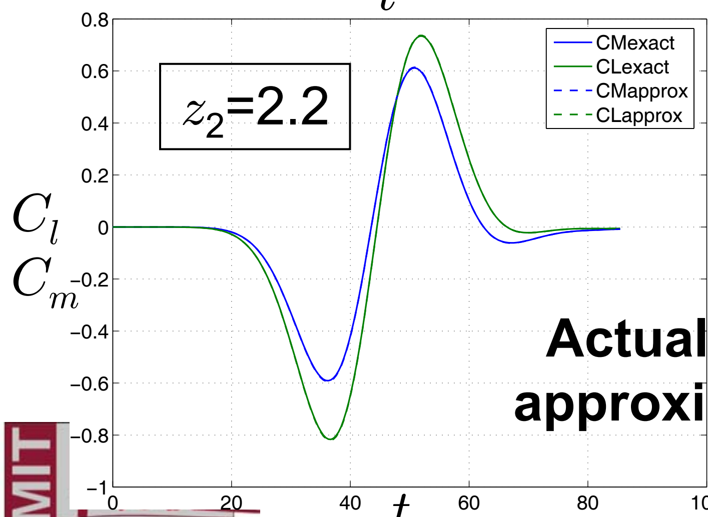


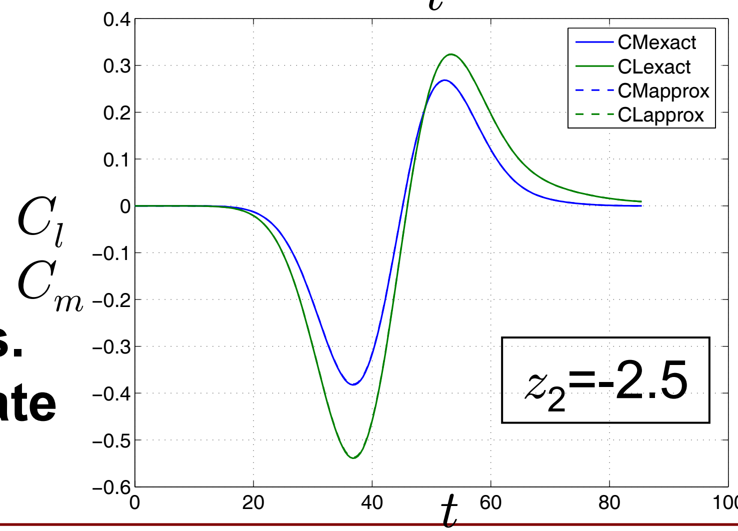
Geometry Mode 2





Tuned vs. mistuned



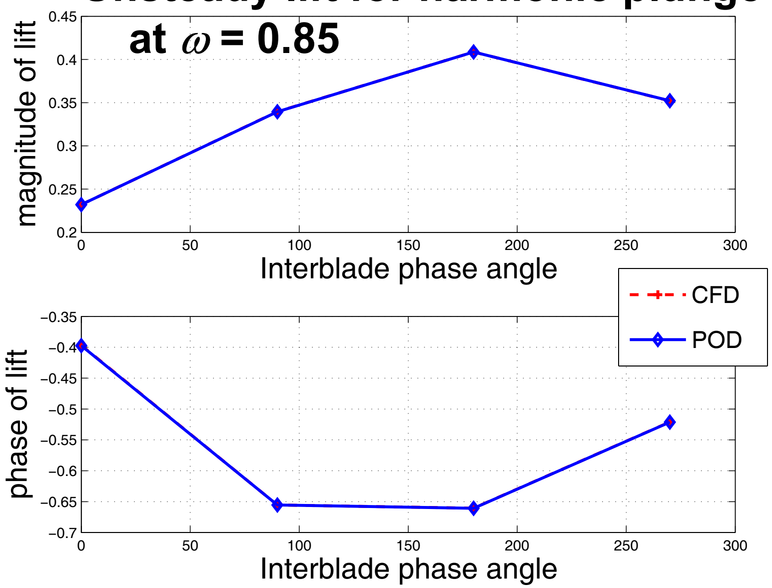


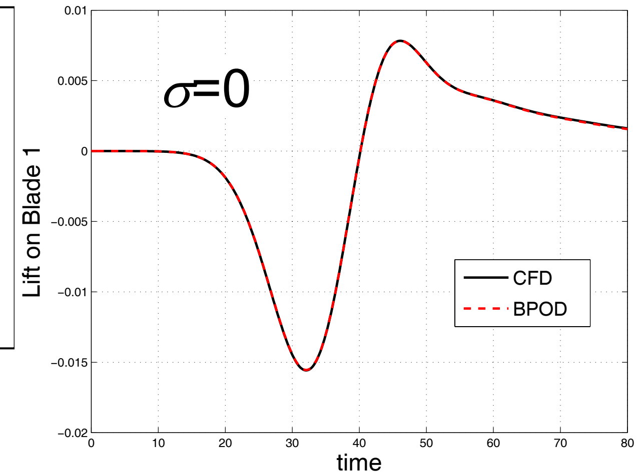
Actual vs. approximate

Tuned System ROM Results

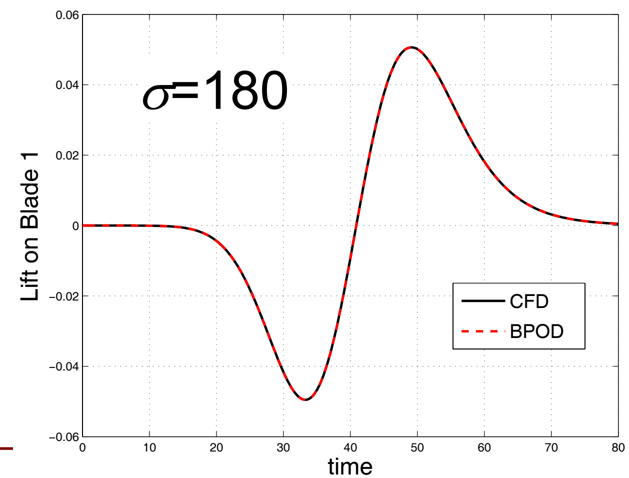
First standard configuration, 4 blades
CFD: 302,000 states
76,000 states per passage
ROM: 92 states
23 states for each IBP

Unsteady lift for harmonic plunge at ω = 0.85





Unsteady lift for pulse input in plunge



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  - Example: design of bladed disks
- An optimization approach to model reduction (B. van Bloemen Waanders, B. Bader, O. Ghattas)

Reduction via POD

- POD is a data-driven approach. Basis and ROM do not respect the governing equations.
- Reduction via POD offers no guarantees of ROM quality (accuracy/stability).
- Proposed method: pose model reduction problem as an optimization problem.

Reduction via Optimization

$$\min_{V,\mathbf{x}_r} \mathcal{G} = \frac{1}{2}\sum_{k=1}^{S}\int_0^{t_f}\left(\mathbf{y}^k - \mathbf{y}_r^k\right)^T\left(\mathbf{y}^k - \mathbf{y}_r^k\right)\,dt$$

$$+ \frac{\beta}{2}\sum_{j=1}^{m}\left(1 - \mathbf{V}_j^T\mathbf{V}_j\right)^2$$

subject to

$$\begin{aligned} V^T V \dot{\mathbf{x}}_r^k &= V^T A^k V \mathbf{x}_r^k + V^T B^k \mathbf{u}^k, \ k = 1, \ldots, S \\ V\mathbf{x}_r^k(0) &= \mathbf{x}^k(0), \ k = 1, \ldots, S \\ \mathbf{y}_r^k &= C^k V \mathbf{x}_r^k, \ k = 1, \ldots, S \end{aligned}$$

Optimization Framework: Goal-Oriented

$$\min_{V,\mathbf{x}_r} \mathcal{G} = \boxed{\frac{1}{2}\sum_{k=1}^{S}\int_0^{t_f}\left(\mathbf{y}^k - \mathbf{y}_r^k\right)^T\left(\mathbf{y}^k - \mathbf{y}_r^k\right)\; dt}$$

Error in reduced-order outputs for sample set

$$+ \frac{\beta}{2}\sum_{j=1}^{m}\left(1 - \mathbf{V}_j^T\mathbf{V}_j\right)^2$$

subject to

$$\begin{aligned}
V^T V \dot{\mathbf{x}}_r^k &= V^T A^k V \mathbf{x}_r^k + V^T B^k \mathbf{u}^k,\;\; k = 1,\ldots,S \\
V \mathbf{x}_r^k(0) &= \mathbf{x}^k(0),\;\; k = 1,\ldots,S \\
\mathbf{y}_r^k &= C^k V \mathbf{x}_r^k,\;\; k = 1,\ldots,S
\end{aligned}$$

Optimization Framework

$$\min_{V,\mathbf{x}_r} \mathcal{G} = \frac{1}{2}\sum_{k=1}^{S}\int_0^{t_f}\left(\mathbf{y}^k - \mathbf{y}_r^k\right)^T\left(\mathbf{y}^k - \mathbf{y}_r^k\right)\,dt$$

$$\boxed{+\ \frac{\beta}{2}\sum_{j=1}^{m}\left(1 - \mathbf{V}_j^T\mathbf{V}_j\right)^2}$$

Regularization term to yield basis vectors of unit length

subject to

$$\begin{aligned}
V^T V\dot{\mathbf{x}}_r^k &= V^T A^k V\mathbf{x}_r^k + V^T B\mathbf{u}^k,\ k = 1,\ldots,S \\
V\mathbf{x}_r^k(0) &= \mathbf{x}^k(0),\ k = 1,\ldots,S \\
\mathbf{y}_r^k &= C^k V\mathbf{x}_r^k,\ k = 1,\ldots,S
\end{aligned}$$

Optimization Framework: Model-Based

$$\min_{V,\mathbf{x}_r} \mathcal{G} = \frac{1}{2}\sum_{k=1}^{S}\int_0^{t_f}\left(\mathbf{y}^k - \mathbf{y}_r^k\right)^T\left(\mathbf{y}^k - \mathbf{y}_r^k\right)\,dt + \frac{\beta}{2}\sum_{j=1}^{m}\left(1 - \mathbf{V}_j^T\mathbf{V}_j\right)^2$$

Reduced output predictions from solution of governing equations

subject to

$$\begin{aligned} V^T V \dot{\mathbf{x}}_r^k &= V^T A^k V \mathbf{x}_r^k + V^T B^k \mathbf{u}^k, \;\; k = 1,\ldots,S \\ V\mathbf{x}_r^k(0) &= \mathbf{x}^k(0), \;\; k = 1,\ldots,S \\ \mathbf{y}_r^k &= C^k V \mathbf{x}_r^k, \;\; k = 1,\ldots,S \end{aligned}$$

Basis Computation

- Time integrals in objective function are replaced by a summation over a finite number of discrete time instants
  - Method requires a priori computation of a snapshot set over S parameter instances and T timesteps
- Assume the basis vectors are linear combinations of snapshots

$$\mathbf{v}_j = \sum_{i=1}^{ST} \gamma_i^j \mathbf{x}_i \quad j = 1, \ldots, m$$

  - Reduces number of unknowns from mn to mST
  - Typically $ST \ll n$

- Use POD basis as initial guess for optimizer

Optimization Framework vs. POD

$$\min_{V,\mathbf{x}_r} \mathcal{G} = \frac{1}{2}\sum_{k=1}^{S}\int_0^{t_f}\left(\mathbf{x}^k-\hat{\mathbf{x}}^k\right)^T C^{kT}C^k\left(\mathbf{x}^k-\hat{\mathbf{x}}^k\right)\,dt + \frac{\beta}{2}\sum_{j=1}^{m}\left(1-\mathbf{V}_j^T\mathbf{V}_j\right)^2$$

subject to

$$\begin{aligned} V^TV\dot{\mathbf{x}}_r^k &= V^TA^kV\mathbf{x}_r^k + V^TB^k\mathbf{u}^k,\ k=1,\dots,S \\ V\mathbf{x}_r^k(0) &= \mathbf{x}^k(0),\ k=1,\dots,S \\ \hat{\mathbf{x}}^k &= V\mathbf{x}_r^k \end{aligned}$$

$$\min_{V} \mathcal{G}_{\text{pod}} = \frac{1}{2}\sum_{k=1}^{S}\int_0^{t_f}\left(\mathbf{x}^k-\tilde{\mathbf{x}}^k\right)^T\left(\mathbf{x}^k-\tilde{\mathbf{x}}^k\right)\,dt + \frac{\beta}{2}\sum_{j=1}^{m}\left(1-\mathbf{V}_j^T\mathbf{V}_j\right)^2$$

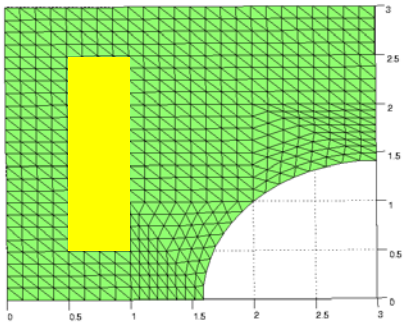
subject to $\tilde{\mathbf{x}}^k(t_j) = VV^T\mathbf{x}^k(t_j)$

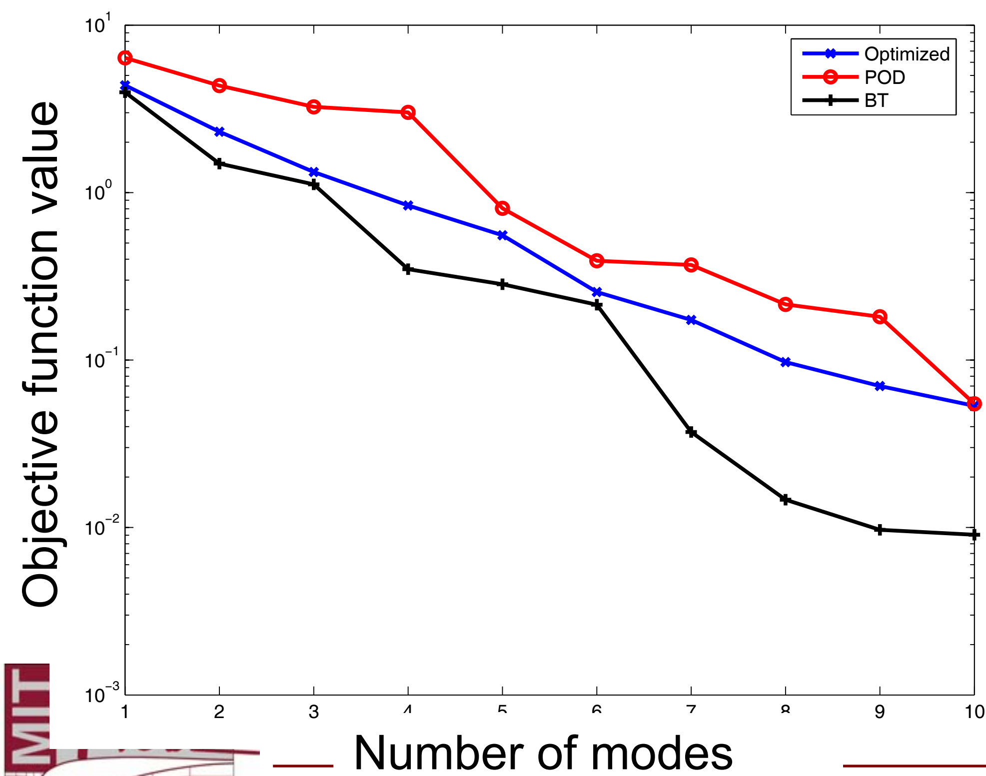
OPT: min error in *computed* data

POD: min error in *projected* data

2D Heat Conduction Example

$$
\begin{aligned}
\frac{\partial \bar{u}}{\partial t} - k\nabla^2 \bar{u} &= 0 \text{ in } \Omega \\
\bar{u} &= \bar{u}_c \text{ on } \Gamma \\
\bar{u} &= \bar{u}_0 \text{ in } \Omega \text{ for } t = 0
\end{aligned}
$$





S=5 parameter instances
T=20 time steps
n=480 states
q=47 outputs

Summary

- Model reduction methodology provides an efficient representation both for unsteady dynamics and for variability
- Formulation leads to parametric reduced-order models
  - Challenge: sampling methods to create a basis that spans high-dimensional input space
- Model reduction problem can be solved using optimization
  - An opportunity for robust optimization?
- Remaining challenge: incorporation of reduced-order models into probabilistic design and optimization