Model Reduction for Uncertainty Quantification and Optimization (Under Uncertainty) of Complex Systems

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Outline

• Motivation and example problems

• Model reduction

• Multifidelity optimization

• Multidisciplinary optimization decomposition methods
Decision under uncertainty (in engineering problems)

• Decision problem may take many forms
  – Design optimization
  – Control
  – Policy decision support

• Many flavors of uncertainty
  – Parameter uncertainty (uncertainty in inputs)
  – Parametric variability (uncontrolled variations in inputs, design requirements)
  – Model inadequacy
  – Discretization error/approximation error
Example: FAA Aviation Environmental Tools Suite

Uncertainty assessment of complex multidisciplinary systems to support policy-making.

Policy and Scenarios

**Environmental Design Space**
What are the aircraft design characteristics?

**APMT Economics**
What are the airline supply & consumer demand effects?

**Aviation Environmental Design Tool**
- Single Airport
- Regional
- Global Studies
- Integrated Noise, Emissions, and Fuel Burn Analyses

**APMT Impacts**
- CLIMATE IMPACTS
- AIR QUALITY IMPACTS
- NOISE IMPACTS

Cost Benefit
Aviation environmental Portfolio Management Tool (APMT)
What are the monetized benefits of decision alternatives?
Example: Effect of variability on system performance

Probabilistic analyses of large-scale (e.g. CFD) models to support design.

- Compressor blade mistuning: small variations in blade structural parameters and blade shape can have a large impact on blade row performance.

- 2D CFD model unsteady analysis for two blade passages:
  ~3 minutes per geometry.

- Monte Carlo simulation for forward uncertainty propagation:
  5000 samples ≈10 days
  50,000 samples ≈ 3.5 months

- To include uncertainty in design decisions: formulate and solve robust or stochastic optimization problems.
Example: Optimal aircraft/controller design with active gust load alleviation

Coupled multidisciplinary models, including a stochastic gust model.

- Benefits of active gust load alleviation require simultaneous design of controller and vehicle

![Diagram]

- Design variables:
  - AR, sweep, t/c, begin cruise alt, cruise \( C_L \)
  - Max gust load

- Coupling variables:
  - Geometry & size
  - Weights
  - Mission performance

- Aircraft Module:
  - Max gust load

- Gust Module:
  - Max actuator deflection
  - Max actuator rate

- LQR penalty factors
- Actuator bandwidth
Decision under uncertainty for complex systems

• Formulation is key (and often overlooked)
  – How to represent uncertainty
  – Constraints, objectives, measures of risk
  – How to communicate uncertainty

• Decomposition may be essential
  – Especially if the problem is multidisciplinary

• Cost of analysis may be prohibitive for repeated evaluations (sampling, scenarios)
  – Need surrogate models and multifidelity approaches
Surrogate modeling

- Simplified physics models
- Data-fit models
- Reduced-order models

Large-scale model → Reduced-order model (ROM)
Parameterized Dynamical Systems

In many engineering problems, objectives and constraints are described by PDEs.

Consider here the spatially discrete equations (for ease of presentation)

\[
\begin{align*}
\dot{x} &= A(p)x + B(p)u \\ 
y &= C(p)x
\end{align*}
\]

\[
\begin{align*}
\dot{x} &= f(x, p, u) \\ 
y &= g(x, p, u)
\end{align*}
\]

\[x \in \mathbb{R}^N: \text{ state vector (e.g. flow unknowns)}\]
\[u \in \mathbb{R}^{N_i}: \text{ input vector (e.g. boundary forcing)}\]
\[p \in \mathbb{R}^{N_p}: \text{ parameter vector (e.g. geometry)}\]
\[y \in \mathbb{R}^{N_o}: \text{ output vector (e.g. forces, moments)}\]
Example: CFD Systems

\[
\begin{align*}
\dot{x} &= A(p)x + B(p)u \\
y &= C(p)x
\end{align*}
\]

\[
\begin{align*}
\dot{x} &= f(x, p, u) \\
y &= g(x, p, u)
\end{align*}
\]

- \(x(t)\): vector of \(N\) flow unknowns
  - e.g. 2D Euler, \(P\) grid points, \(N = 4P\)
  - \(x = [\rho_1 \ (\rho u)_1 \ (\rho v)_1 \ e_1 \ \rho_2 \cdots \cdots \rho_P \ (\rho u)_P \ (\rho v)_P \ e_P]^T\)

- \(p\): input parameters
  - e.g. shape parameters, PDE coefficients

- \(u(t)\): forcing inputs
  - e.g. flow disturbances, wing motion

- \(y(t)\): outputs
  - e.g. flow characteristic, lift force
Projection-Based State-Reduced Models

- Approximate state by a linear combination of basis vectors
  \[ \mathbf{x} \approx \sum_{i=1}^{n} \mathbf{V}_i \mathbf{x}_{r_i} \]

  - Define right basis, \( \mathbf{V} \)
    \[ \begin{bmatrix} \mathbf{V} \\ \mathbf{x}_{r} \end{bmatrix} \]
    \[ \begin{bmatrix} \mathbf{N} \times 1 \\ \mathbf{1} \end{bmatrix} \]

- Project equations onto reduced-order subspace
  - Define left basis, \( \mathbf{W} \)
    \[ \mathbf{W}^T \mathbf{V} = \mathbf{I} \]
    (Often use \( \mathbf{W} = \mathbf{V} \))
Projection-Based State-Reduced Models

\[ \begin{align*}
\dot{x} &= A(p)x + B(p)u \\
y &= C(p)x
\end{align*} \]

\[ \begin{align*}
x &\approx Vx_r \\
r &= V\dot{x}_r - AVx_r - Bu \\
y_r &= CVx_r
\end{align*} \]

\[ W^T r = 0 \]

\[ \begin{align*}
A_r(p) &= W^T A(p)V \\
B_r(p) &= W^T B(p) \\
C_r(p) &= C(p)V \\
\dot{x}_r &= A_r(p)x_r + B_r(p)u \\
y_r &= C_r(p)x_r
\end{align*} \]

\[ x \in \mathbb{R}^N: \text{ state vector} \quad x_r \in \mathbb{R}^n: \text{ reduced state vector} \]

\[ p \in \mathbb{R}^{N_p}: \text{ parameter vector} \quad V \in \mathbb{R}^{N \times n}: \text{ reduced basis} \]

\[ u \in \mathbb{R}^{N_i}: \text{ input vector} \quad V \in \mathbb{R}^{N \times n}: \text{ reduced basis} \]

\[ y \in \mathbb{R}^{N_o}: \text{ output vector} \]
Reducing the Parameter Space

- Even with reduction in state, parameter dimension may be too large for optimization, control, statistical sampling
  - Distributed parameters may be represented with thousands of dof
- Define a parameter basis and approximate the parameter:

\[ p \approx P p_r \]

\[
\begin{align*}
\mathbf{x} & \in \mathbb{R}^N: \text{state vector} \\
\mathbf{p} & \in \mathbb{R}^{N_p}: \text{parameter vector} \\
\mathbf{u} & \in \mathbb{R}^{N_i}: \text{input vector} \\
\mathbf{y} & \in \mathbb{R}^{N_o}: \text{output vector} \\
\mathbf{x}_r & \in \mathbb{R}^n: \text{reduced state vector} \\
\mathbf{p}_r & \in \mathbb{R}^{n_p}: \text{reduced parameter vector} \\
\mathbf{V} & \in \mathbb{R}^{N \times n}: \text{reduced state basis} \\
\mathbf{P} & \in \mathbb{R}^{N_p \times n_p}: \text{reduced parameter basis}
\end{align*}
\]
Reducing the Parameter Space

\(x \in \mathbb{R}^N\): state vector \\
\(p \in \mathbb{R}^{N_p}\): parameter vector \\
\(u \in \mathbb{R}^{N_i}\): input vector \\
\(y \in \mathbb{R}^{N_o}\): output vector \\
\(x_r \in \mathbb{R}^n\): reduced state vector \\
\(p_r \in \mathbb{R}^{n_p}\): reduced parameter vector \\
\(V \in \mathbb{R}^{N \times n}\): reduced state basis \\
\(P \in \mathbb{R}^{N_p \times n_p}\): reduced parameter basis

\[\begin{align*}
\dot{x} &= A x(p) + B u(p) \\
y &= C x(p)
\end{align*}\]

\[\begin{align*}
x &\approx V x_r \\
p &\approx P p_r
\end{align*}\]

\[\begin{align*}
\dot{x}_r &= A_r(p_r) x_r + B_r(p_r) u \\
y_r &= C_r(p_r) x_r
\end{align*}\]

\[\begin{align*}
A_r(p_r) &= W^T A(P p_r) V, \\
B_r(p_r) &= W^T B(P p_r), \\
C_r(p_r) &= C(P p_r) V
\end{align*}\]
State Basis Example: 
Proper Orthogonal Decomposition (POD)

(aka Karhunen-Loève expansions, Principal Components Analysis, 
Empirical Orthogonal Eigenfunctions, …)

• Consider $K$ snapshots $x_1, x_2, \ldots, x_K \in \mathcal{R}^N$
  (solutions at selected times or parameter values)

• Form the snapshot matrix $X = [x_1 \ x_2 \ \ldots \ \ x_K]$

• Choose the $n$ basis vectors $V = [V_1 \ V_2 \ \cdots \ V_n]$ to be left singular vectors of the snapshot matrix, with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq \sigma_{n+1} \geq \cdots \geq \sigma_K$

• This is the optimal projection in a least squares sense:

$$\min_V \sum_{i=1}^{K} ||x_i - VV^T x_i||^2_2 = \sum_{i=n+1}^{K} \sigma_i^2$$
Parameter and State Reduction

• How to determine the parameter basis $\mathbf{P}$?
  – While sampling states to form the state basis $\mathbf{V}$, also collect “snapshots” of $\mathbf{p}$
  – Apply POD/SVD to compute the parameter basis $\mathbf{P}$

• Choosing the right snapshots is critical
  – For both the state and the parameter basis
  – Especially for model reduction application to design, optimization, inverse problems
  – Especially challenging when parameter dimension is large

• Greedy algorithm
  (Veroy, Prud’homme, Rovas & Patera, 2003; Grepl & Patera, 2005)
  – Adaptive heuristic to choose “good” sample points for a state basis
  – Sample the location in parameter space of maximum error between full and reduced-order model outputs
Sampling: Model-Constrained Optimization

- Formulate the greedy task of finding the parameter sample points as a model-constrained optimization problem
  - Adaptive sampling (sequence of optimization problems)

- Sampling is driven by error, which includes effects of state and parameter approximations

- Linear problem with initial-condition parameters: explicit solution via eigenvalue problem
  \[ \begin{align*}
  \dot{x} &= A(p)x + B(p)u \\
  y &= C(p)x \\
  \dot{x}_r &= V^T A(Pp)Vx_r + V^T B(Pp)u \\
  y_r &= C(Pp)Vx_r \\
  p_l &\leq p \leq p_u 
  \end{align*} \]

- Nonlinear parametric dependence: solve with tailored PDE-constrained optimization algorithm
  (Bui-Thanh, Willcox, Ghattas; SIAM J. Sci. Comp., 2008)

- Simultaneous reduction in state and parameter: “regularized greedy formulation” reflects prior information
Parametric Inputs (Steady): Thermal Fin Design
Choosing the right snapshots is key

- Model-constrained optimization sampling approach for parametric input spaces
  - Application to thermal fin design problem with 21 parameter input space
  - Finite element model: 17,899 states
  - Reduced model has 3-4 orders magnitude lower error compared to Latin hypercube, log-random, and other sampling methods

![Graph showing comparison of maximum output error vs. number of reduced basis vectors for different sampling methods. The graph includes lines for Model-constrained, LHS, LogRandom, CVT, and URandom, with Model-constrained having the lowest error.]
Model Reduction for Probabilistic Analysis: Blade Shape Variations

\[ \frac{\partial w}{\partial t} + \nabla \cdot \mathcal{F}(w) = 0 \]

\[ w = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}, \quad \mathcal{F}^x = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ \rho u H \end{pmatrix}, \quad \mathcal{F}^y = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho v H \end{pmatrix} \]

- Subsonic rotor blade, Mach 0.113
- 2D linearized Euler equations, DG CFD model
- 51,504 states per blade passage
- Small variations in blade structural parameters and blade shape can have large impact on blade row performance
- Inputs: blade plunging motion, blade shape parameters
- Output: blade lift forces

Goal: create a reduced-order model that captures input/output mapping between plunging motion input and lift force output over a range of blade geometries.
Model Reduction for Probabilistic Analysis: Blade Shape Variations

- Forced response of two blade passages to sinusoidal plunging motion (180° interblade phase angle)
- Full model: 103,008 states
- Reduced model: 201 states
- Offline cost ~3 hours
Model Reduction for Probabilistic Analysis: Blade Shape Variations

- Parameterized reduced model used to evaluate unsteady response over a range of geometry variations (same 10,000 random samples in each case)

- Full model: 103,008 states; ~3 mins per geometry
- Reduced model: 201 states, <0.1 secs per geometry

<table>
<thead>
<tr>
<th></th>
<th>Full CFD</th>
<th>Reduced CFD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model size</td>
<td>103,008</td>
<td>201</td>
</tr>
<tr>
<td>Number of nonzeros</td>
<td>2,846,056</td>
<td>40,401</td>
</tr>
<tr>
<td>Offline cost</td>
<td>-</td>
<td>2.8 hours</td>
</tr>
<tr>
<td>Online cost</td>
<td>501.1 hours</td>
<td>0.21 hours</td>
</tr>
<tr>
<td>Blade 1 WPC mean</td>
<td>-1.8572</td>
<td>-1.8573</td>
</tr>
<tr>
<td>Blade 1 WPC variance</td>
<td>2.687e-4</td>
<td>2.6819e-4</td>
</tr>
<tr>
<td>Blade 2 WPC mean</td>
<td>-1.8581</td>
<td>-1.8580</td>
</tr>
<tr>
<td>Blade 2 WPC variance</td>
<td>2.797e-4</td>
<td>2.799e-4</td>
</tr>
</tbody>
</table>
Model Reduction of Nonlinear Systems

\[
\begin{align*}
\dot{x} &= f(x, u) \\
y &= g(x)
\end{align*}
\]

\[
\begin{align*}
x &= v_{x_r} \\
\dot{x}_r &= V^T f(Vx_r, u) \\
y_r &= g(Vx_r)
\end{align*}
\]

- Nonlinear systems: standard projection approach leads to a model that is low order but still expensive to solve.

- The cost of evaluating the nonlinear term

\[
f_r(x_r, u) = V^T f(Vx_r, u)
\]

still depends on \( N \), the size of the large-scale system.

- Can achieve efficient nonlinear reduced models via interpolation: Empirical Interpolation Method

\[
\dot{x}_r = A_r x_r + E_r f_r(D_r x_r, u)
\]
• Goal: Simulation of few-million neuron system. State-of-the-art: 10K neuron system.

• Approach: construct a reduced-order model that captures input/output dynamics of a neuron type.

Math. Model: Hodgkin-Huxly Nonlinear PDE

Voltage $v_j$ in and synaptic input $I_{j,\text{syn}}$ into branch $j$

$$
\frac{a_j}{2R_t} \partial_{xx} v_j = C_m \partial_t v_j + G_N a m^3 h_j (v_j - E_Na) + G_K n^4_j (v_j - E_K) + G_l (v_j - E_l) + I_{j,\text{syn}}
$$

Kinetics of potassium ($n$) and sodium ($h, m$) channels

$$
\partial_t m_j = \alpha_m(v_j)(1 - m_j) - \beta_m(v_j)m_j,
\partial_t h_j = \alpha_h(v_j)(1 - h_j) - \beta_h(v_j)h_j,
\partial_t n_j = \alpha_n(v_j)(1 - n_j) - \beta_n(v_j)n_j.
$$
Model Reduction of Hodgkin-Huxley Fiber

- Segment of neuron with three inputs. Observe voltage at node 10.
- Highly nonlinear system.

- Apply ROM (POD) and EIM.
- Full system: 1198 DOF
- Reduced system: 30 DOF
- Simulation speed up: up to 100
- Excellent agreement between full and reduced order model.

Forked neuron: voltages at node 10
Model Reduction of Hodgkin-Huxley Fiber

Voltage Profile at Various Times at all Observation Nodes (Full vs. ROM)
Combustion Chamber Model

Parameter: reaction parameters \((p)\)
State: fuel concentration \((x)\)
Output: fuel concentration \((y)\)
Input: source \((u)\)

Advection-diffusion-reaction problem:
\[
\dot{w} + \mathbf{U} \cdot \nabla w - \nabla (\kappa \nabla w) + s(w; \mu) = f
\]
\[
s(w; \mu) = Aw(c - w) e^{ -\frac{E}{d-w}}
\]
\[
w = w_D \quad \text{on} \quad \Gamma_{in}
\]
\[
\nabla w \cdot \hat{n} = 0 \quad \text{on} \quad \partial \Omega \setminus \Gamma_{in}
\]

\[
\dot{x} = f(x, p, u)
\]
\[
y = Cx
\]
POD-EIM Model Reduction for Combustor

3D FEM solution: $N=8.5M$, $M=20M$. One forward solve: 13h CPU time.

DEIM ROM: $n=40$, $m=50$. One forward solve: < 0.1s CPU time.
Bayesian Uncertainty Quantification of Combustor Inverse Problem (2D)

FEM: 10,000 samples, ~110 hours
ROM: 10,000 samples, ~100 seconds

Marginal posterior histograms for Arrhenius reaction parameters computed using Markov chain Monte Carlo (MCMC).

95% credible intervals for mean estimates of Arrhenius parameters.
Bayesian Uncertainty Quantification of Combustor Inverse Problem (3D)

- Reduced model with \( n=40 \).
- MCMC with 50,000 samples in the Markov chain.

Marginal posterior histograms for Arrhenius reaction parameters.

Iso-probability contours of posterior, generated by sampling the parameter space with reduced model on a \( 256^2 \) grid.
How to achieve optimization under uncertainty for complex systems?

• Potential of surrogate models shown in forward propagation of uncertainty, statistical inverse problems (to some extent)

• In an optimization context there are many questions:
  – How to construct the surrogates
  – How to adapt the surrogates as the optimization proceeds
  – How to ensure convergence

• Draw on two ideas from deterministic MDO
  – Multifidelity optimization (exploiting coarse models)
  – Decomposition (exploiting problem structure)
Multifidelity Optimization

\[ \min_x f(x) \quad \text{s.t.} \quad g(x) \leq 0 \quad h(x) = 0 \]

- Reduced complexity of \( f(\cdot), g(\cdot), h(\cdot) \)
  - Simplified physics
  - Model reduction
  - Other surrogate models (data fit, multigrid, etc.)

- Reduced complexity of \( x \)
  - May need mapping between \( x \) and \( \hat{x} \)

Figure adapted from Choi et al. 2004
Multifidelity Optimization: Key Components

\[
\begin{align*}
\min_{x} & \quad f(x) \\
\text{s.t.} & \quad g(x) \leq 0 \\
& \quad h(x) = 0
\end{align*}
\]

\[
\begin{align*}
\min_{\hat{x}} & \quad \hat{f}^k(\hat{x}) \\
\text{s.t.} & \quad \hat{g}^k(\hat{x}) \leq 0 \\
& \quad \hat{h}^k(\hat{x}) = 0 \\
& \quad \|\hat{x} - \hat{x}^*_c\|_\infty \leq \Delta^k
\end{align*}
\]

- Surrogate models that are updated as the optimization proceeds
- A mapping method to connect high- and low-fidelity design descriptions
- A model management framework (e.g. trust regions) to ensure convergence
Multifidelity Optimization Methods
State-of-the-art

• Bayesian model calibration methods
  – Calibrate surrogate models globally (or over a large portion of the design space)
  – Reuse information collected about the high-fidelity function at each iteration

• Trust-region methods
  – Provably convergent with appropriate conditions on the surrogate model

• Hybrid methods
  – Including methods that do not require derivatives of the high-fidelity functions
Multifidelity optimization of supersonic airfoil geometry

Biconvex airfoil in supersonic flow
- $\alpha = 2^{\circ}, M_\infty = 1.5$
- $(t/c) = 5%$

<table>
<thead>
<tr>
<th></th>
<th>Linear Panels</th>
<th>Shock Expansion</th>
<th>Cart3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_L$</td>
<td>0.1244</td>
<td>0.1278</td>
<td>0.12498</td>
</tr>
<tr>
<td>% Difference</td>
<td>0.46%</td>
<td>2.26%</td>
<td>0.00%</td>
</tr>
<tr>
<td>$C_D$</td>
<td>0.0164</td>
<td>0.0167</td>
<td>0.01666</td>
</tr>
<tr>
<td>% Difference</td>
<td>1.56%</td>
<td>0.24%</td>
<td>0.00%</td>
</tr>
</tbody>
</table>
Multifidelity objectives and constraint

- Hybrid multifidelity approach combining derivative-free trust-region method (Conn et al., 2009), radial basis function model calibration (Wild and Shoemaker, 2009), multifidelity Bayesian calibration extension (March and Willcox, 2010)

- Max Lift/Drag (multifidelity)
- subject to: Drag ≤ 0.01 (multifidelity), t/c ≥ 5% and positive thickness

<table>
<thead>
<tr>
<th></th>
<th>High-Fidelity</th>
<th>Low-Fidelity</th>
<th>SQP</th>
<th>First-Order TR</th>
<th>RBF, ξ=2</th>
<th>RBF, ξ=ξ*</th>
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</thead>
<tbody>
<tr>
<td>Objective</td>
<td>Cart3D</td>
<td>Panel Method</td>
<td>1168*</td>
<td>97 (-92%)</td>
<td>104 (-91%)</td>
<td>112 (-90%)</td>
</tr>
<tr>
<td>Constraint</td>
<td>Cart3D</td>
<td>Panel Method</td>
<td>2335*</td>
<td>97 (-96%)</td>
<td>115 (-95%)</td>
<td>128 (-94%)</td>
</tr>
</tbody>
</table>

*Cart3D optimization sensitive to scaling and finite differences
Complex systems often comprise coupled multidisciplinary models

- In deterministic optimization, there are often advantages to decomposing the problem.
- For optimization under uncertainty, decomposition will almost certainly be essential.
Multidisciplinary Feasible (MDF)

Iteration loop to resolve coupling variables at each optimization cycle

- Aircraft Module
  - Aircraft variables
  - Mission performance
  - Geometry & size, weights
  - Max gust load

- Gust Module
  - Gust variables
  - Controller variables
  - Max actuator deflection & rate

Optimizer

- Aircraft variables
- Mission performance
- Controller variables
- Max gust load
- Geometry & size, weights
Individual Discipline Feasible (IDF)

Additional design variables:
- target max gust load
- target geometry & size
- target weights

Additional constraints:
- max gust load = target
- geometry & size = target
- weights = target

Diagram:
- Aircraft Module
- Mission performance
- max actuator deflection & rate
- Gust Module
- Target geometry & size
- Target weights
Conclusions

- Surrogate models play an essential role in reducing the cost of analyses for use in uncertainty quantification and optimization.

- Achieving optimization under uncertainty of complex systems will require
  - Approaches that exploit problem structure
  - Approaches that exploit a hierarchy of models and hierarchy of UQ methods

- Problem formulation is an essential but often poorly understood aspect in engineering design under uncertainty.