Design Computation under Uncertainty via Rapid Simulation

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Part I

Introduction
Brief Bio

1. BS at Pusan National University, Feb 2001
2. MS at KAIST, Aug 2002 (Discontinued)
3. MS at Georgia Tech (Prof. D Mavris), Dec 2004
4. PhD at Georgia Tech (Prof. D Mavris), Aug 2010
5. Postdoctoral Fellow at Georgia Tech (Prof. D Mavris), Feb 2011
7. Assistant Professor at PNU, Mar 2014
Research Interest and Technology

Interest
Design computation under uncertainty via rapid simulation

Technology

1 Rapid Simulation
- Reduced order method: versatile but not assurable
- Reduced basis method: rigorous but limited

2 Uncertainty Quantification
- Statistical inference: expectation-maximization (EM), variational Bayesian Inference, etc.
- Computational statistics: Monte Carlo simulation (MCS), MCMC (Markov chain Monte Carlo), etc.
- Optimization under uncertainty: reliability-based design optimization, etc.
Research Order/Basis Concept

A PDE solution lies in a low dimensional space/manifold for the parameter variation of interest.

(1) Vector Space

(2) Topology

Computational Strategy

Achieve affordable supercomputing by exerting computational effort upfront to swiftly run simulation whenever necessary

1. Offline: model construction
2. Online: model evaluation

Target Applications: real-time, many query contexts
Research Order/Basis Methods

Reduced order/basis methods approximate $u$ such that

$$u(x; \theta) \approx \sum_{i=1}^{N} c_j(\theta) \Phi_j(x),$$

and can be categorized depending on how $c_j$ is obtained:

1. Solve a reduced PDE
   - It is popular in the simulation community.
   - It requires a source-level access.

2. Use interpolation/regression
   - It works with commercial tools.
   - It may require more effort than the first approach.

Issue with Approximation

- Reduced order methods cannot guarantee the accuracy of approximate solutions in general.
- However, reduced basis methods can by virtue of a \textit{posteriori} error estimation.
Part II

Research with Reduced Order Methods

2 Theoretical Comparison of Deterministic and Probabilistic Basis Extraction Methods

3 PIV Data Restoration with a Low-Dimensional Flow Structure

4 Reduced Order Modeling of Numerical Propulsion System Simulation
Deterministic vs. Probabilistic Perspectives
Effective Data Representation

1. Gappy proper orthogonal decomposition (POD)
   - Deal with missing data with the gappy norm
   - Evaluate orthogonal basis $V$ by POD

2. Probabilistic principal component analysis (PPCA)
   - Estimate probability parameters and missing data as well by an expectation-maximization (EM) algorithm
   - Evaluate nonorthogonal basis $W$ by statistical inference

$p(t_j; \mu, W, \sigma^2)?
Theoretical Comparison
Unifying Least-Squares Perspective

For an incomplete snapshot ensemble, both methods solve

$$\min \| \mathbf{y}_j - \Phi \mathbf{c}_j \|_\alpha^2 \quad \text{w.r.t.} \quad \Phi \text{ and } \mathbf{c}_j.$$ 

<table>
<thead>
<tr>
<th>Problem</th>
<th>Gappy POD</th>
<th>EM-PCA w/o $\sigma^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\min | \mathbf{y}_j - \mathbf{V} \mathbf{b}_j |_n^2$</td>
<td>$\min | \mathbf{y}_j - \mathbf{W} \mathbf{x}<em>j |</em>{L^2}$</td>
</tr>
<tr>
<td></td>
<td>w.r.t. $\mathbf{b}_j$</td>
<td>w.r.t. $\mathbf{x}_j$ and $\mathbf{W}$</td>
</tr>
<tr>
<td>Basis $\Phi$</td>
<td>Orthogonal basis by POD $\mathbf{V}$</td>
<td>Nonorthogonal basis by M-step $\mathbf{W} = \mathbf{Y} \mathbf{X}^T (\mathbf{X} \mathbf{X}^T)^{-1}$</td>
</tr>
<tr>
<td>Norm $\alpha$</td>
<td>gappy norm $n$</td>
<td>$L^2$ norm</td>
</tr>
<tr>
<td>Coeff. $\mathbf{c}_j$</td>
<td>Weighted Least-Squares $\mathbf{b}_j = (\mathbf{V}^T \mathbf{N}_j \mathbf{V})^{-1} (\mathbf{N}_j \mathbf{V})^T \mathbf{y}_j$</td>
<td>Ordinary Least-Squares (E-step) $\mathbf{x}_j = (\mathbf{W}^T \mathbf{W})^{-1} \mathbf{W}^T \mathbf{y}_j$</td>
</tr>
</tbody>
</table>

Consequently, the coefficient of gappy POD is different for every missing snapshot requiring new evaluation.
PIV Data Restoration

Particle Image Velocimetry (PIV)

Experimental flow visualization technique for instantaneous velocity measurements

- Poor image contrast for irregular illumination
- Low and inconsistent seeding density
- Ill-prepared experimental setup

Figure: Experimental Setup for PIV

Research Problem  Impaired measurements to repair

Current Approach  Interpolation with neighboring points

1 http://www.fhwa.dot.gov/engineering/hydraulics/research/mddot.cfm
**Restored PIV Data**

962th Snapshot

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**Accuracy**  Both deterministic and probabilistic formulations are comparable.

**Efficiency**  The probabilistic formulation is more efficient than the deterministic formulation by a factor of over 10.
Reduced Order Modeling of NPSS

**Table : Engine Cycle and Scaling Parameters**

<table>
<thead>
<tr>
<th>Extraction ratio</th>
<th>FPR</th>
<th>HPCPR</th>
<th>LPCPR</th>
<th>MaxT4 [°R]</th>
<th>T_{SLS} [lbf]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min.</td>
<td>1</td>
<td>1.5</td>
<td>18</td>
<td>1.2</td>
<td>3200</td>
</tr>
<tr>
<td>Max.</td>
<td>1.2</td>
<td>1.7</td>
<td>22</td>
<td>1.6</td>
<td>3600</td>
</tr>
</tbody>
</table>

- High bypass, two-spool, separate flow
- Engine operating points: Mach number (0.0 ∼ 0.9), altitude (0.0 ∼ 43,000 ft.), and power code (50 ∼ 21)
- Two 924 × 500 data sets for training and test

**Figure : GE90-115B²**

²http://lyle.smu.edu/propulsion/Pages/variations.htm
Prediction Test Results

Worst Coefficient of Determination ($R^2$) Cases

(1) Gross thrust of the 324th test engine deck: $R^2 = 0.9999291$

(2) Ram drag of the 289th test engine deck: $R^2 = 0.9999515$
Reduced Order NPSS in Action

Truss-Braced-Wing (TBW) Design Environment

Joint NASA research project of Georgia Tech and Virginia Tech

Figure: ModelCenter® Design Environment
Part III

Research with Reduced Basis Methods

5 Structural Integrity Assessment under Operational Uncertainty

6 Heat Transfer Education with Real-Time High-Fidelity Simulation

7 Rapid yet Rigorous Failure Analysis
Structural Integrity Assessment

Target Application
Unmanned systems with sensors attached/embedded

Current Approach
Estimate material properties treating operational conditions are known *a priori.*

Research Problem
Operational conditions

Research Proposition
Instead of material property estimates, we employ structural response predictions by propagating system parameter estimates through a simulation.

(1) System parameters
(2) Material property
(3) Response prediction
Model Problem

Solid Isotropic Cantilever Beam under Tip Loads

- Configuration: 10m-long with a unit cross section
- System parameters $\theta = (E, \nu, f_1, f_2, f_3) \in \mathbb{R}^5$
  - Material properties: 6061 aluminum alloy $(E, \nu) = (0.689 \times 10^2 \text{ [GPa]}, 0.33)$
  - Operating conditions: vertical load dominant $(f_1, f_2, f_3) = (-0.05, 0.4, -0.05) \times 10 \text{ [MN]}$
- Measurements $y_o \in \mathbb{R}^{16}$: average $x_2$ displacements on the side corrupted by measurement noise
- Predictions $y^t_p \in \mathbb{R}^2$: average $x_2$ and $x_3$ displacements at the tip
- Reduction: $N = 14,757 \text{ (65 sec)} \rightarrow N = 18 \text{ (0.0035 sec)}$
Error and Noise Comparison

The Virtue of *A Posteriori* Error Estimation

![Graph showing comparison of true and estimated CRB model errors with measurement noise.](image)

**Observations**

1. True RB model error is always bounded by estimated CRB model error obtained by *a posteriori* error analysis.

2. Estimated RB model error becomes smaller than measurement noise as the basis size increases.
Comparative Study on Eigenvector Space

Young’s Modulus Loss Rate: 0% ~ 10%

(1) Operational Uncertainty 1%
(2) Operational Uncertainty 5%

Finding

Response predictions are more discernible than material property estimates as operational uncertainty become large.
Engineering Physics Education

Current Approach

Analytical model + illustration of real physical phenomena

Pros
1. Delineate dominant physical phenomena
2. Reveal significant non-dimensional quantities

Cons
1. Rely on simplifying assumptions
2. Lose connection to real world problems

Proposition

Analytical model + simulation of real physical phenomena

Pros
1. Learn the validity of an analytical model
2. Fill the gap between analytical models and real physical phenomena by active learning
3. Develop a problem solving capability

Enabling Technology

Reduced basis methods for real-time high-fidelity simulation with affordable computational resources
MATLAB GUI Software

T-Shaped Fin

(1) Lumped Model

(2) RB Model

CPU Heat Sink System

(3) RB Model
Failure Analysis for Reliability

Reliability is a major concern to high-consequence systems, such as aerospace systems.

Figure: Consideration of Uncertainty in Design

Research Problem
Failure analysis demands both accuracy and efficiency.

Proposition
We capitalize on reduced basis methods to achieve both accuracy and efficiency.

Figure: Consideration of Uncertainty in Design

Note: The diagram illustrates the distinction between robustness and reliability in terms of the probability density function. Robust design is concerned with the event distribution near the mean of the distribution, while reliability-based design is concerned with the event distribution in the tails of the distribution. Robust design seeks to ensure that the system performs well under everyday fluctuations, whereas reliability-based design focuses on ensuring that the system can handle extreme events or failures.
Demonstration

Failure Analysis of the T-Shaped Fin

Results of Monte Carlo simulation (MCS) and MCS with importance sampling (IS)

\[
\frac{1}{\hat{\sigma}_F} \text{Biot number} = \begin{cases} 
0.05 & \text{if } \mu_1, \text{thermal conductivity} \\
0.5 & \text{if } \mu_1, \text{thermal conductivity} > 10
\end{cases}
\]

<table>
<thead>
<tr>
<th>Method</th>
<th>( \mathbb{E}[\hat{\theta}_F] )</th>
<th>( \text{Var}(\hat{\theta}_F) )</th>
<th>Sample size</th>
<th>Run time w/ RB</th>
<th>Run time w/o RB</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCS</td>
<td>0.0729</td>
<td>6.7580e-08</td>
<td>1e+06</td>
<td>2.78 hours</td>
<td>208.33 days</td>
</tr>
<tr>
<td>MCS w/ IS</td>
<td>0.0729</td>
<td>8.6222e-08</td>
<td>1e+05</td>
<td>0.28 hours</td>
<td>20.83 days</td>
</tr>
</tbody>
</table>

\(^a\) Run time is extrapolated based on a single evaluation.
Part IV

Summary
Future Research 1
Reduced Order Modeling with Probabilistic Basis Extraction

1. Experimental flow data repair (ex. PIV data)
2. Flow data assimilation
3. Reduced order modeling of fluid dynamics
Future Research 2

Lego RB Method: Component-Based System Modeling

(1) Component Library

(2) System

Advantages over the Current RB Methods

- Easier to deal with many parameters
- More flexible for topological changes
Future Research 2

Lego RB Method: Component-Based System Modeling

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Future Research 2

Lego RB Method: Component-Based System Modeling

Advantages over the Current RB Methods

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Future Research 3
Real-time, In Situ Design and Analysis App

(1) rbAPPmit by Huynh, Knezevic, and Patera

(2) Los Montes Simple Span Bridge in El Salvador

Possible Applications

1. Engineering for developing countries (Bridges to Prosperity)
2. Simulation-based real-time, in situ monitoring and control
Potential of Reduced Basis Methods

- Reduced basis methods work best for linear PDEs (elliptic and parabolic)
- For nonlinear PDEs, we can apply the empirical interpolation method (EIM)

Various Physics Phenomena

1. Potential flow in fluid dynamics
2. Convection-diffusion equation in fluid dynamics
3. Linear elasticity in structural analysis
4. Linear heat conduction in heat transfer
5. Maxwell’s equations in electromagnetics
6. Helmholtz equation in linear acoustics
7. ...and more!

Applications that can best benefit from reduced basis methods are those in the context of real-time, many query contexts.
Closing Remarks

Summary
Reduced order/basis technology can benefit various engineering problems across diverse disciplines.

Design Computation under Uncertainty

1. Reduced order method
2. Reduced basis methods
3. Computational statistics

Target Application
Real-time control and monitoring problems
Many-query optimization and statistical analysis
Thank you for your attention!

Questions?
References

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