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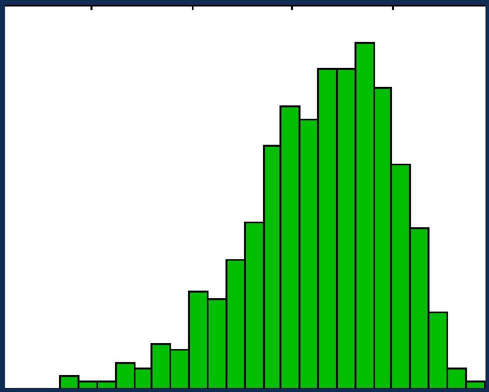

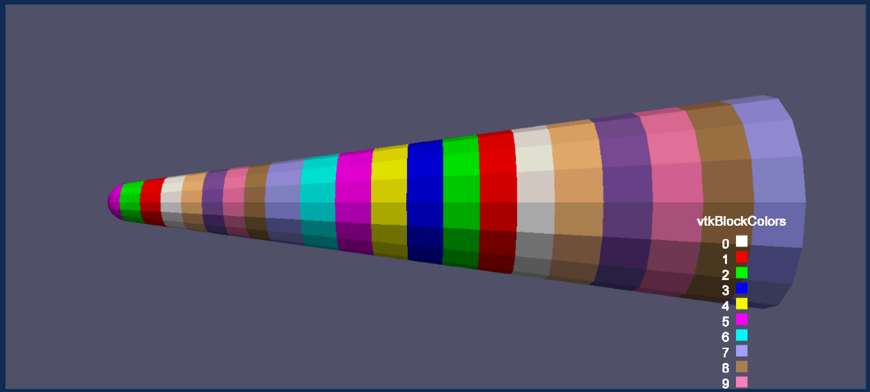

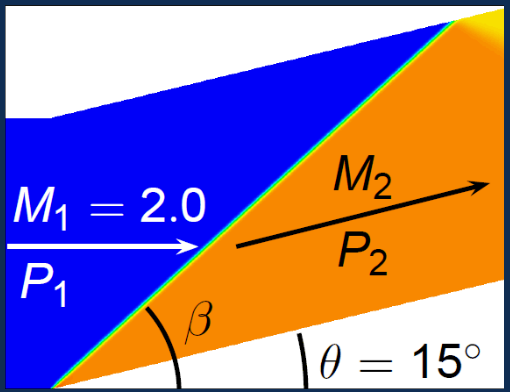

Parameterized Reduced Order Models for Enabling Design Optimization and Uncertainty Quantification

Matthew Brake, Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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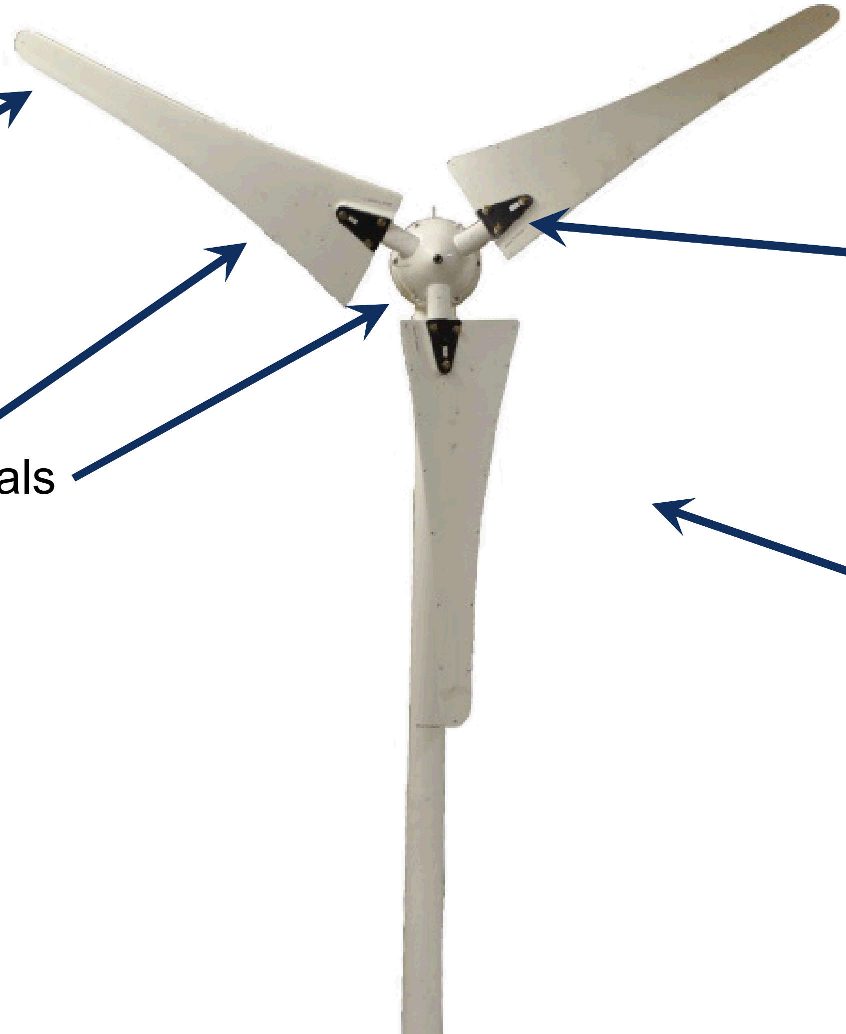
Research Overview

How can we efficiently and accurately predict the nonlinear response of a built up system?



Variability/Uncertainty

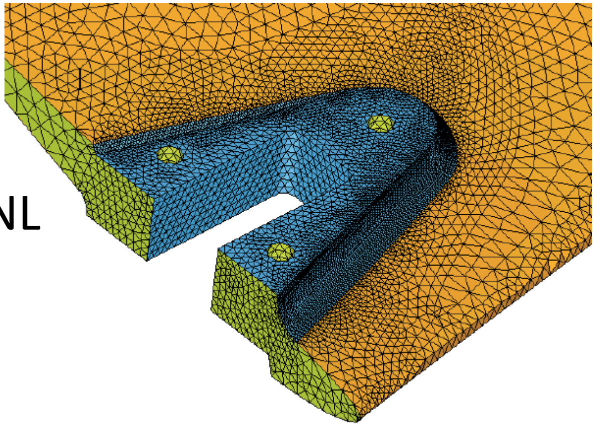
Interfaces

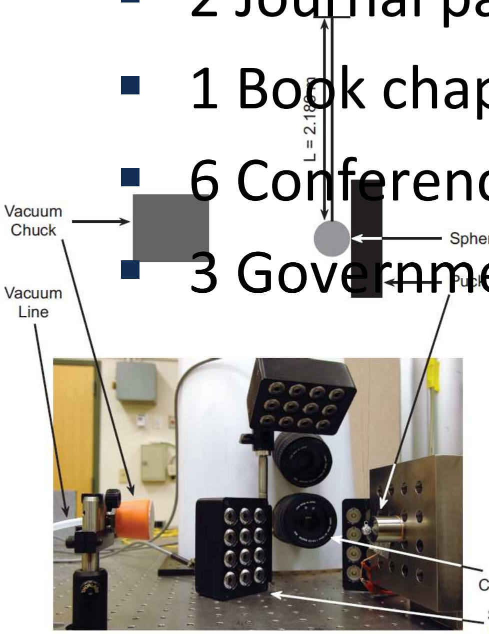
Nonlinear Materials and Composites

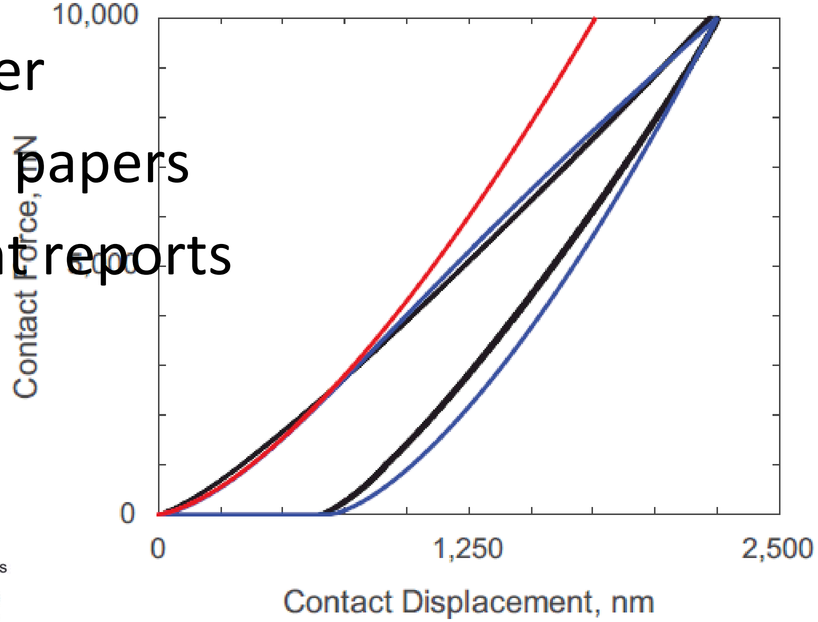
Large Models Necessitated

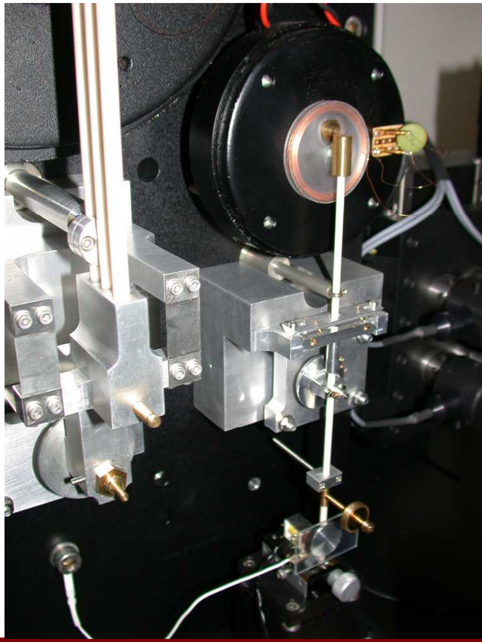
Nonlinearities Due to Interfaces

- Normal contact
  - Can go into the plastic regime
  - Extensive macro- and micro- scale study at SNL
  - Constitutive model developed to incorporate strain hardening and oblique, frictional interactions
- 4 year long research effort spanning:
  - Experimental validation
  - Theoretical Development
  - Numerical implementation into commercial codes
- 2 Journal papers
- 1 Book chapter
- 6 Conference papers
- 3 Government reports





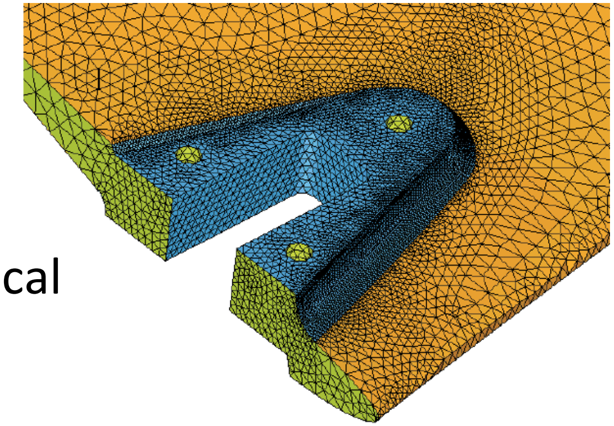


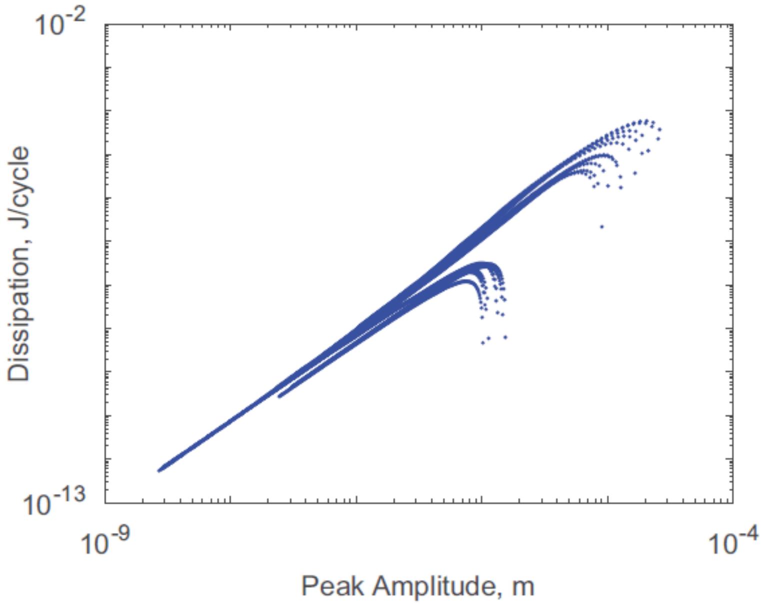


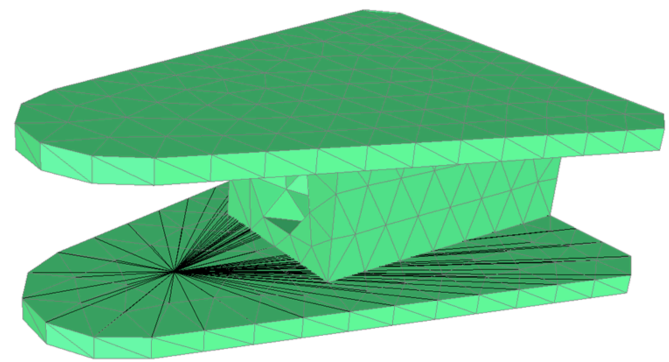
Nonlinearities Due to Interfaces

- Frictional contact
  - Coulomb's law breaks down for microslip interactions
  - Introduces a strong nonlinearity into numerical modeling
  - Often incorporated as a hysteretic model

- Constitutive modeling effort: RIPP joint
  - Analytical model
  - Already adopted by over 12 institutions
  - Journal article under review
  - In second year of research program

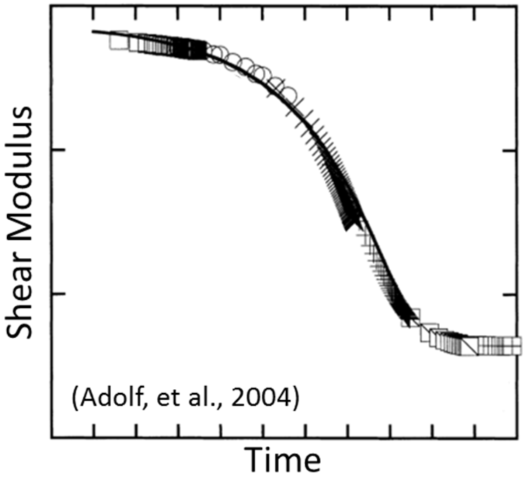


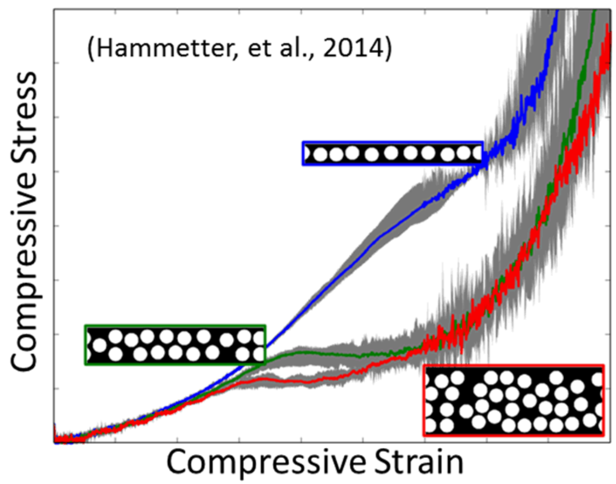


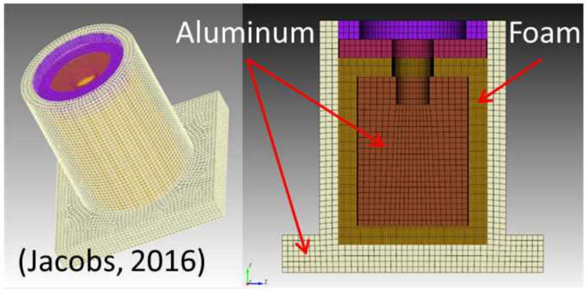


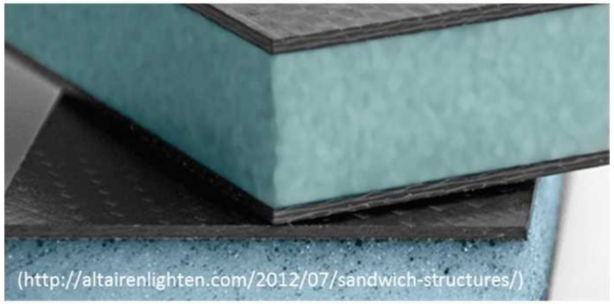
Nonlinear Materials and Composites

- Geometric nonlinearities
  - Each type of nonlinearity, to date, has required a unique formulation
  - Challenge is finding a generalized representation for nonlinear ROMs
- Composites and inelastic materials
  - Homogenization techniques (2016 NOMAD project)
  - Viscoelastic/Hyperelastic ROMs



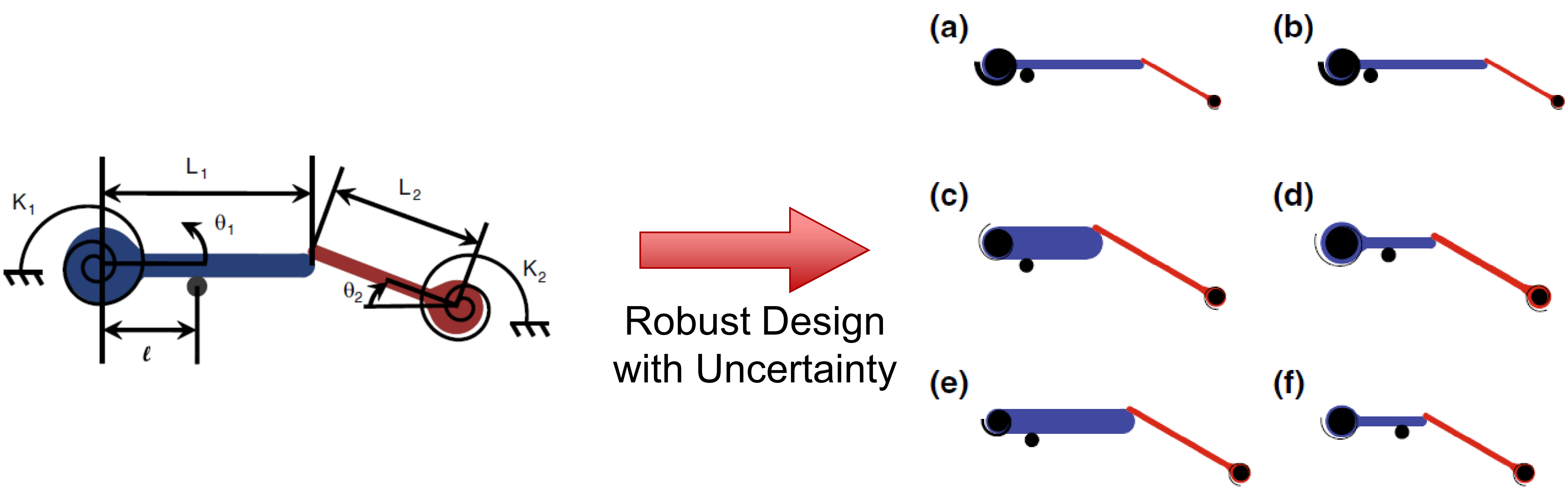






Epistemic Uncertainty

- Epistemic uncertainty – model form error (or uncertainty due to missing physics)
- Separate from aleatoric (parametric uncertainty)
- Highly prevalent in modeling of jointed structures



M.R. Brake, *Nonlinear Dynamics*, **77**, pp. 899-922, 2014

Uncertainty in Large Models

- Aleatoric (parametric) uncertainty:
  - Manufacturing tolerances –
    - Geometric variations
    - Material property variations
  - Can result in thousands of design variables
- Models of complex structures often include hundreds of thousands or millions of elements…

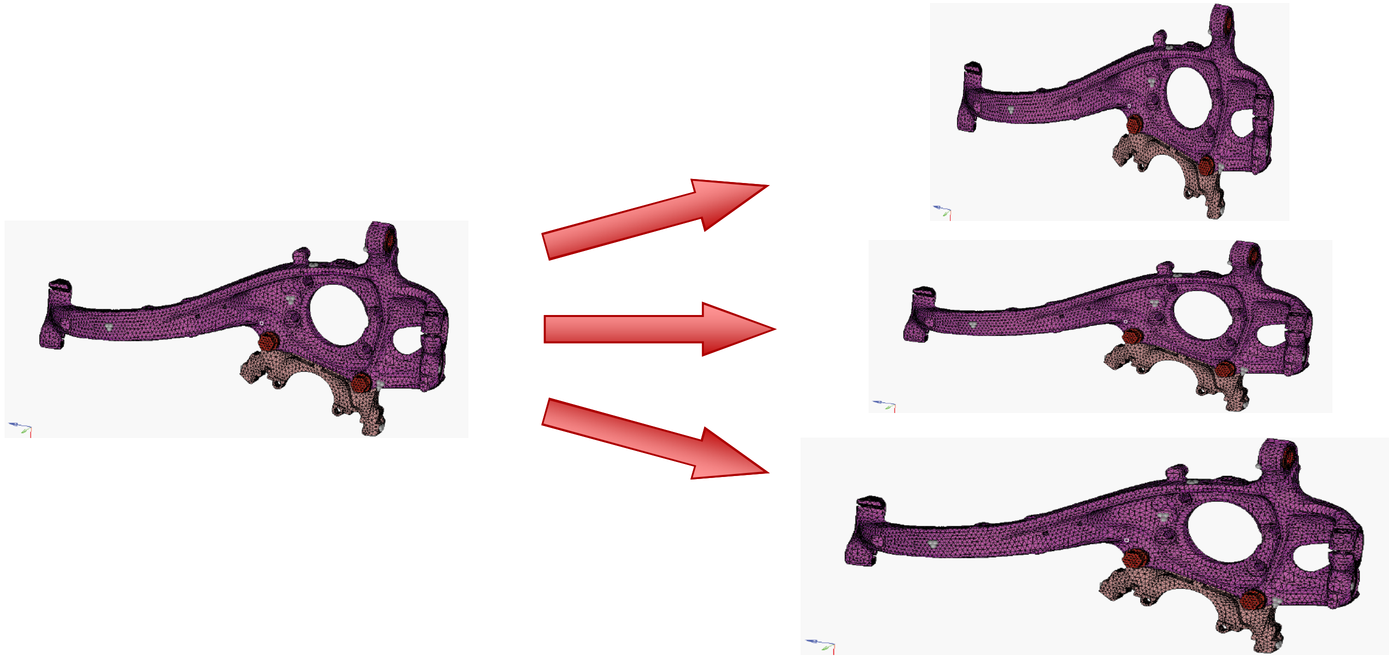
The Challenge Inherent in Modern Design for High Consequence Applications[1]

- High fidelity FEA leads to desire for FEA modeling/verification
  - Contrast with approach taken in the 50s…
- Uncertainties omnipresent
  - Environmental specifications, manufacturing tolerances, defects, epistemic sources, etc.
- Result: robust design requirements
  - Can require thousands of perturbed models
- Rough estimate of time to robustly design a single component at SNL:
  - 10 years of human effort, plus 3 years of a dedicated super computer using high fidelity FEA…
- Need for an efficient, automated process…

[1]: High consequence – systems where consequences of failure are non-trivial, such as airplanes or automobiles

Enabling Technologies for UQ

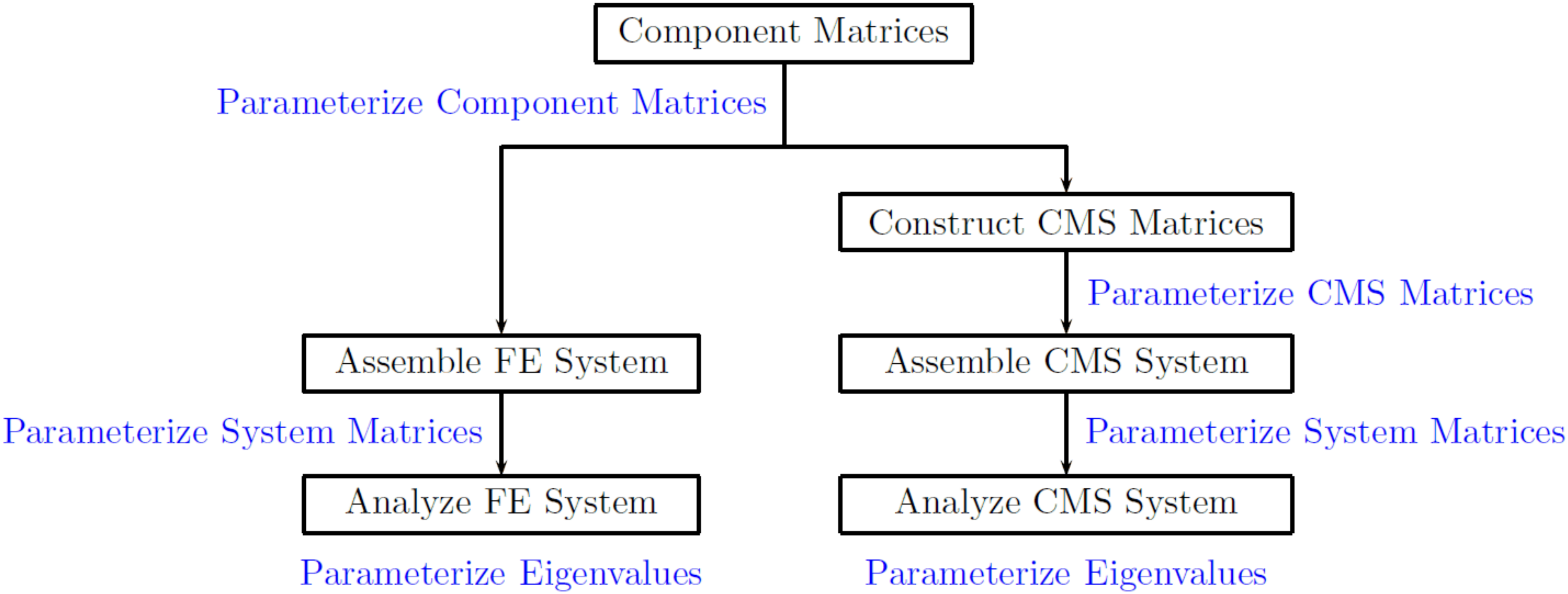
- Given needs for UQ (and optimization), what theoretical basis will enable it?
  - Fast simulations
  - Ability to incorporate variations without remeshing
  - Confidence in accuracy
- One solution: Parameterized Reduced Order Models (PROMs)



Outline

- Context
- Finite difference implementation of methodology
- Hyper dual number basis
- Extension to large, FE systems

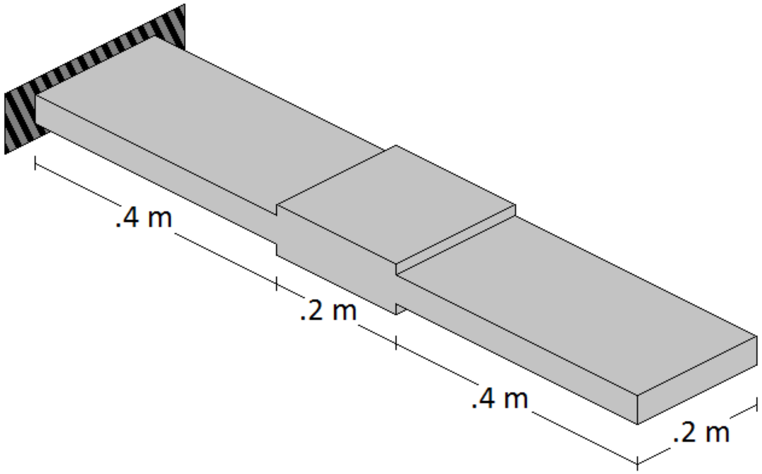
Possible Parameterizations



- What is the optimal path for parameterization?
- How many terms should be taken in the expansions?
- Existing research focused on parameterizing the CMS matrices

Candidate System

- Simple system considered since there is an analytical answer



- Length: 1 meter
- Thickness: 50 millimeters
- Width: 200 millimeters
- Material: 6061 Aluminum (E = 68.9 GPa, rho = 2700 kg/m^3)
- Feature: Middle of beam, 0.2 meters long
- Boundary conditions: Clamped-Free and Pinned-Pinned

Overview of Method (Details to follow…)

- Given a linear subsystem expressed as

$$[M]\{\ddot{u}\} + [K]\{u\} = \{0\}$$

- The CB model and eigenvalues of the nominal system are readily available
- These quantities are then parameterized in terms of the variables of interest using

$$f(a+h) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \ldots \frac{f^{(n)}(a)}{n!}(x-a)^n$$

- Challenge in specifying derivatives

Calculation of Derivatives

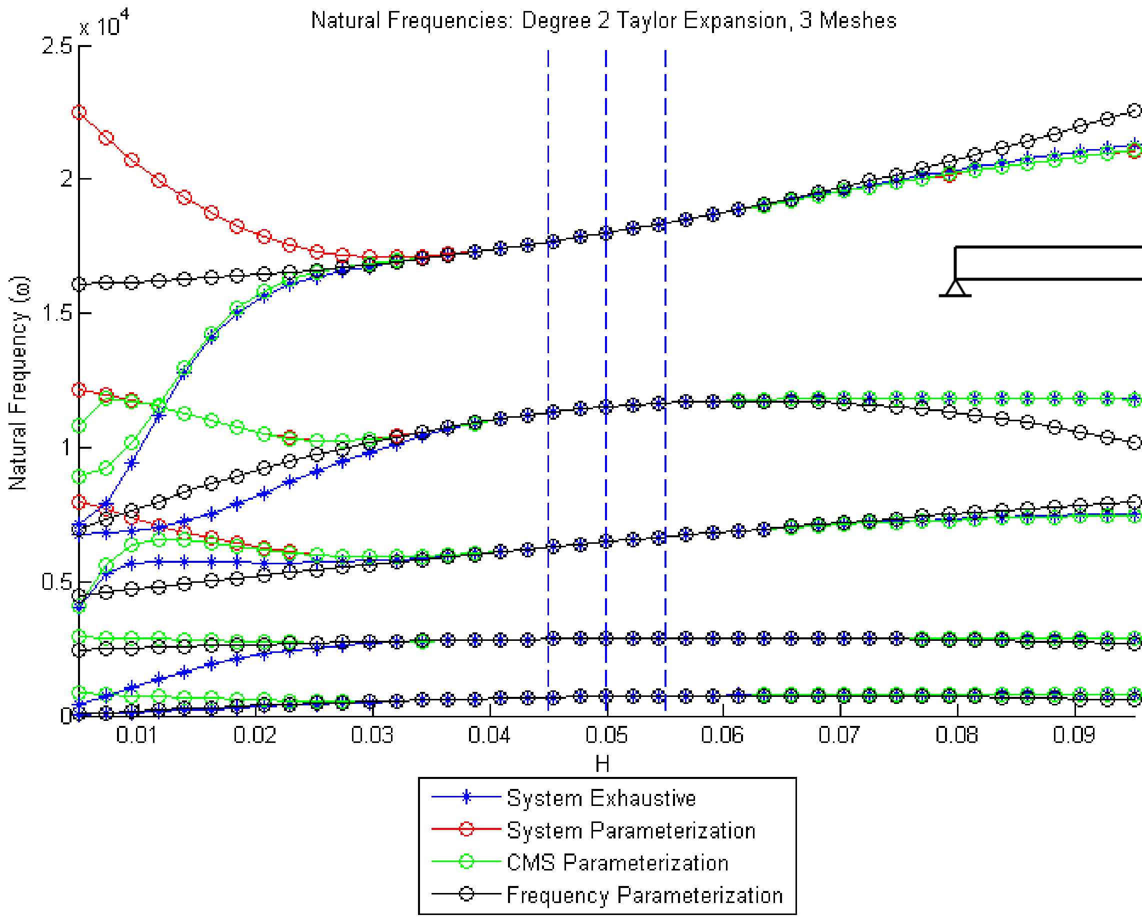
- First approach: finite difference approximations.
- Calculated using Taylor series expansions

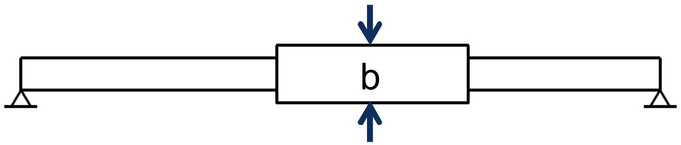
$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$$f^{(4)}(x) \approx \frac{f(x-2h) - 4f(x-h) + 6f(x) - 4f(x+h) + f(x+2h)}{h^4}$$

- Thus, derivative information can be calculated from perturbations of the system's model

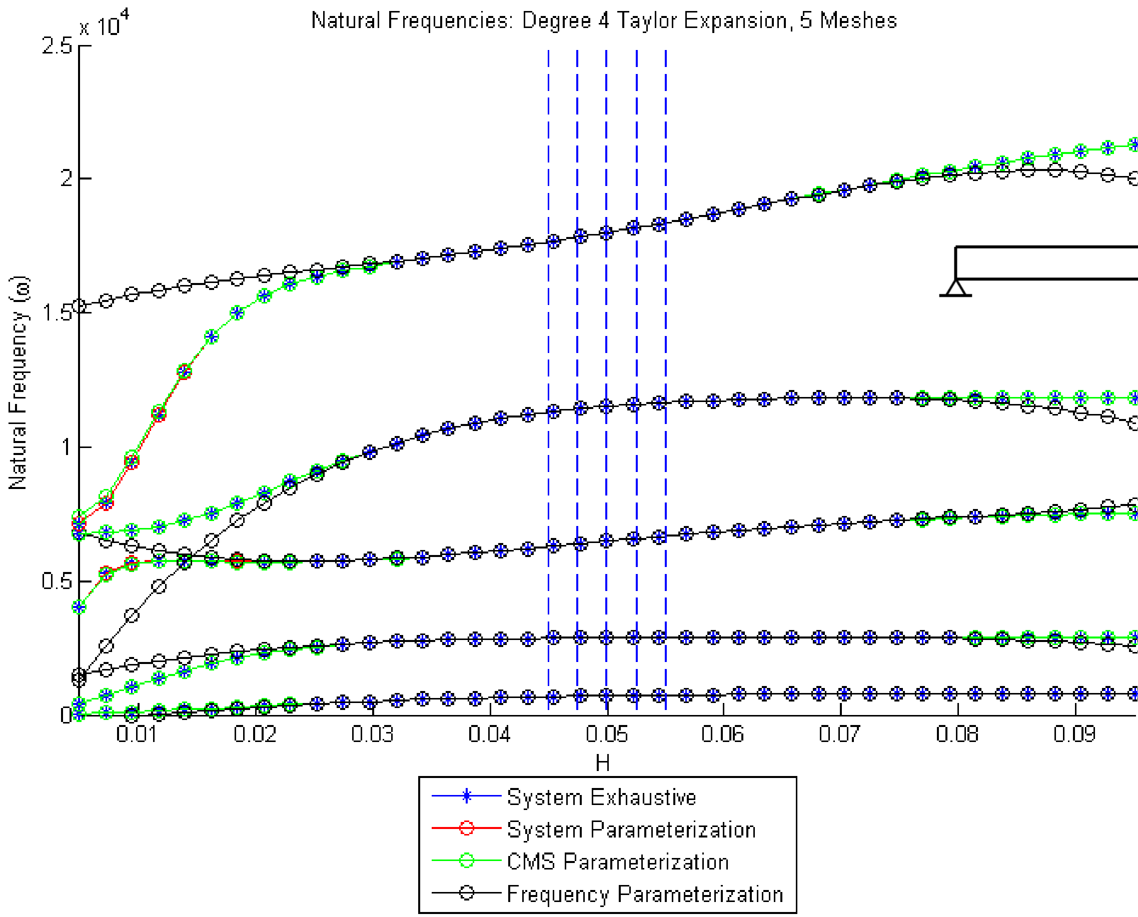
Varying Defect Thickness 2nd Order Expansion

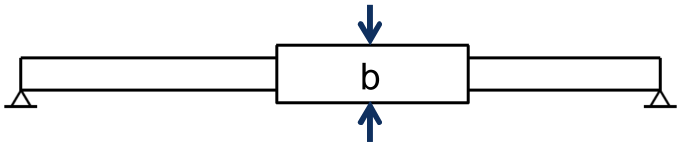




- Exhaustive and analytical solution lie atop one another
- Dashed blue lines indicates regime for calculating PROM

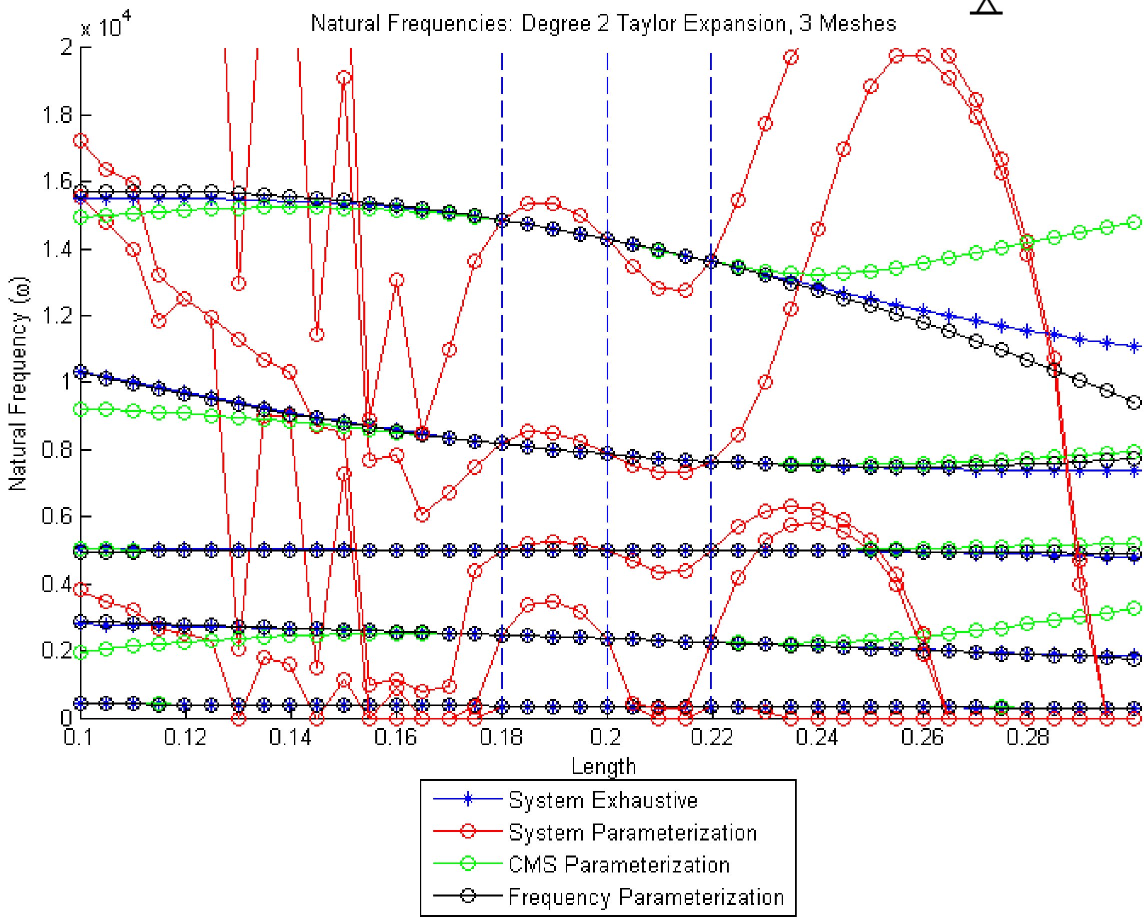
Varying Defect Thickness
4th Order Expansion





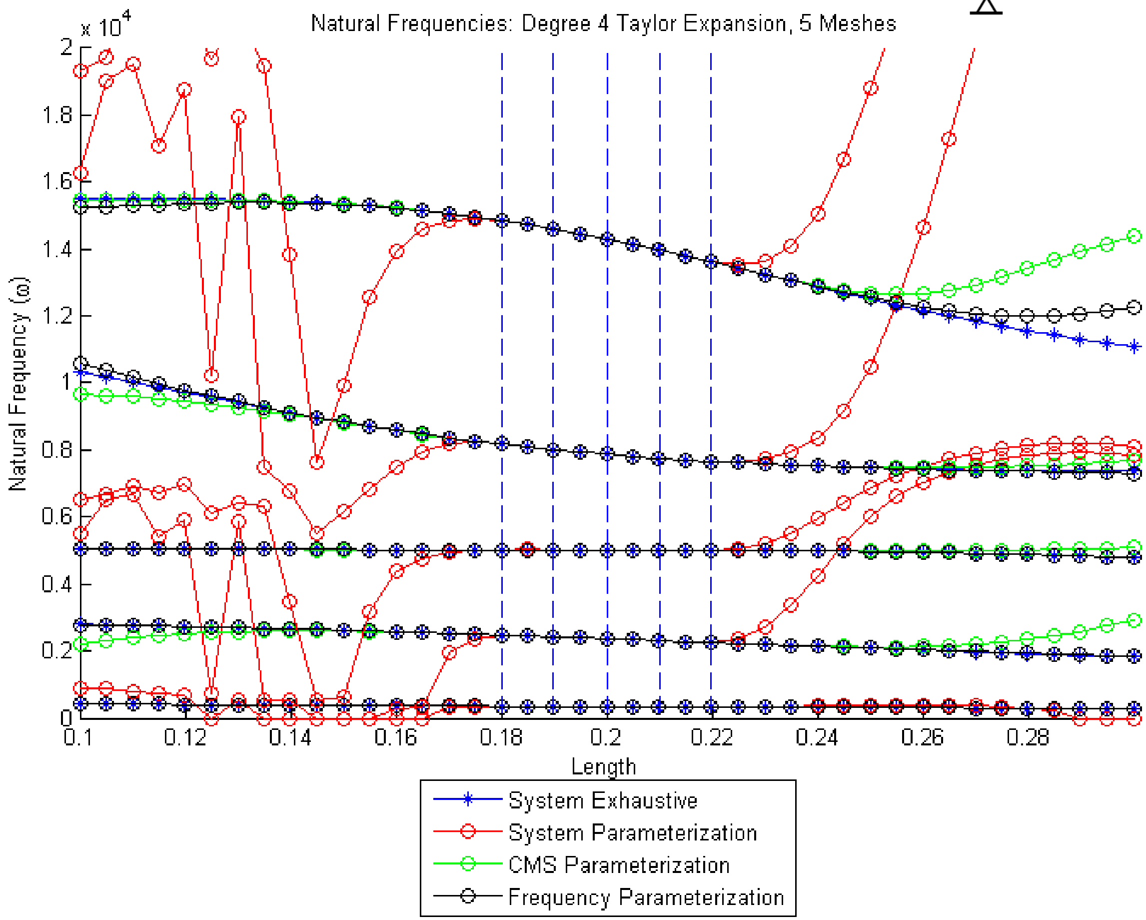
- In general, can achieve agreement well outside of the region used to calculate PROMs, but requires multiple derivatives…

Varying Defect Length
2nd Order Expansion



- In general, system parameterization least accurate for geometrical variations

Varying Defect Length
4th Order Expansion



- Though, with sufficient derivatives, even the system level PROMs are predictive over the region used to calculate them…

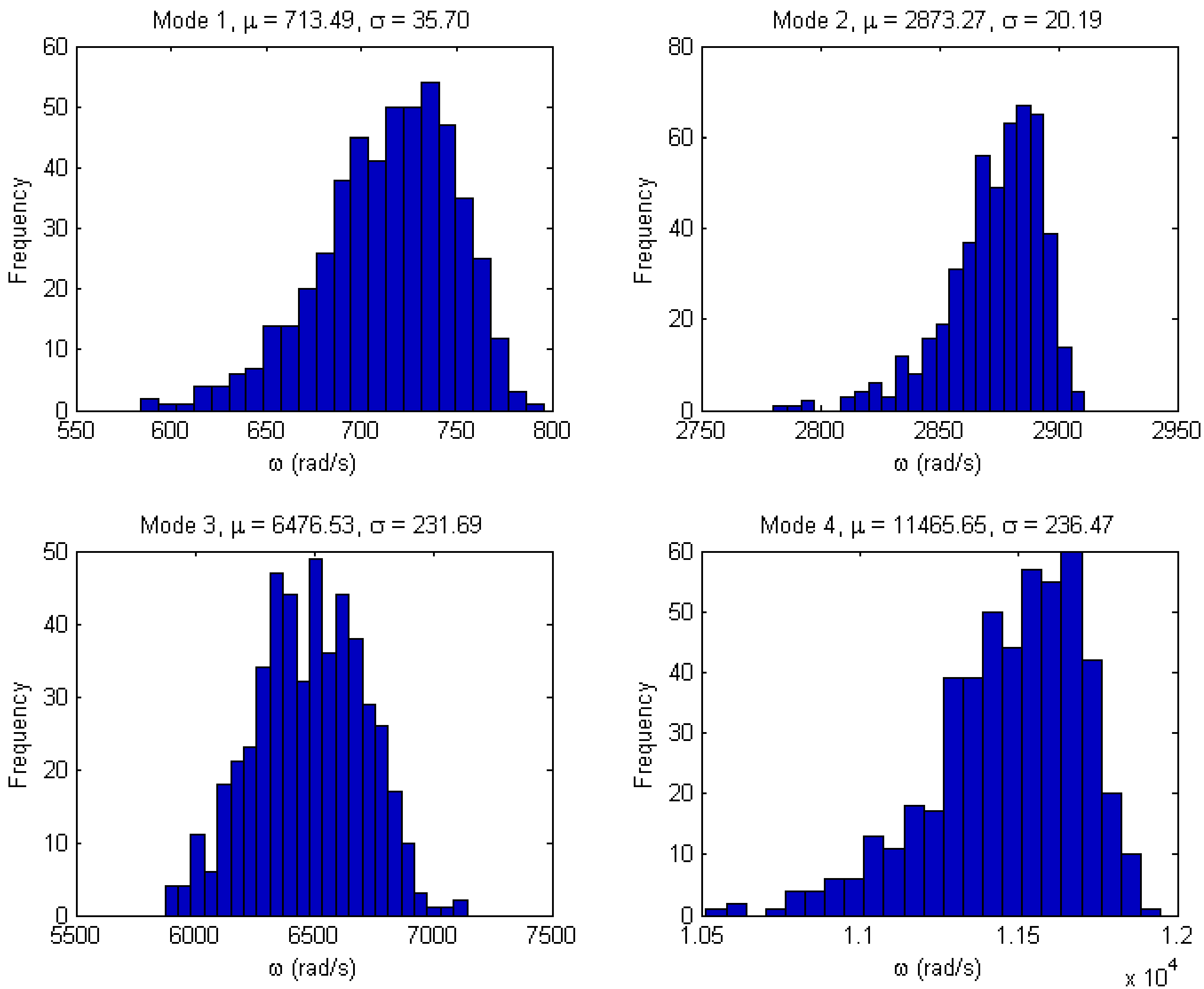
Observations on the Finite Difference Based PROMs

- Fourth order system expansion is fairly accurate
  - Highest order term in system matrices is of third order
- System expansion is inaccurate for node shifting model variations
  - Terms with close proximity to zero; small deviations -> large error
- Reduced order model accuracy on par with eigenspace parameterization
  - Some applications only are interested in frequency characteristics, which would help guide choice in parameterization level
- PROM accuracy is good for large model variations

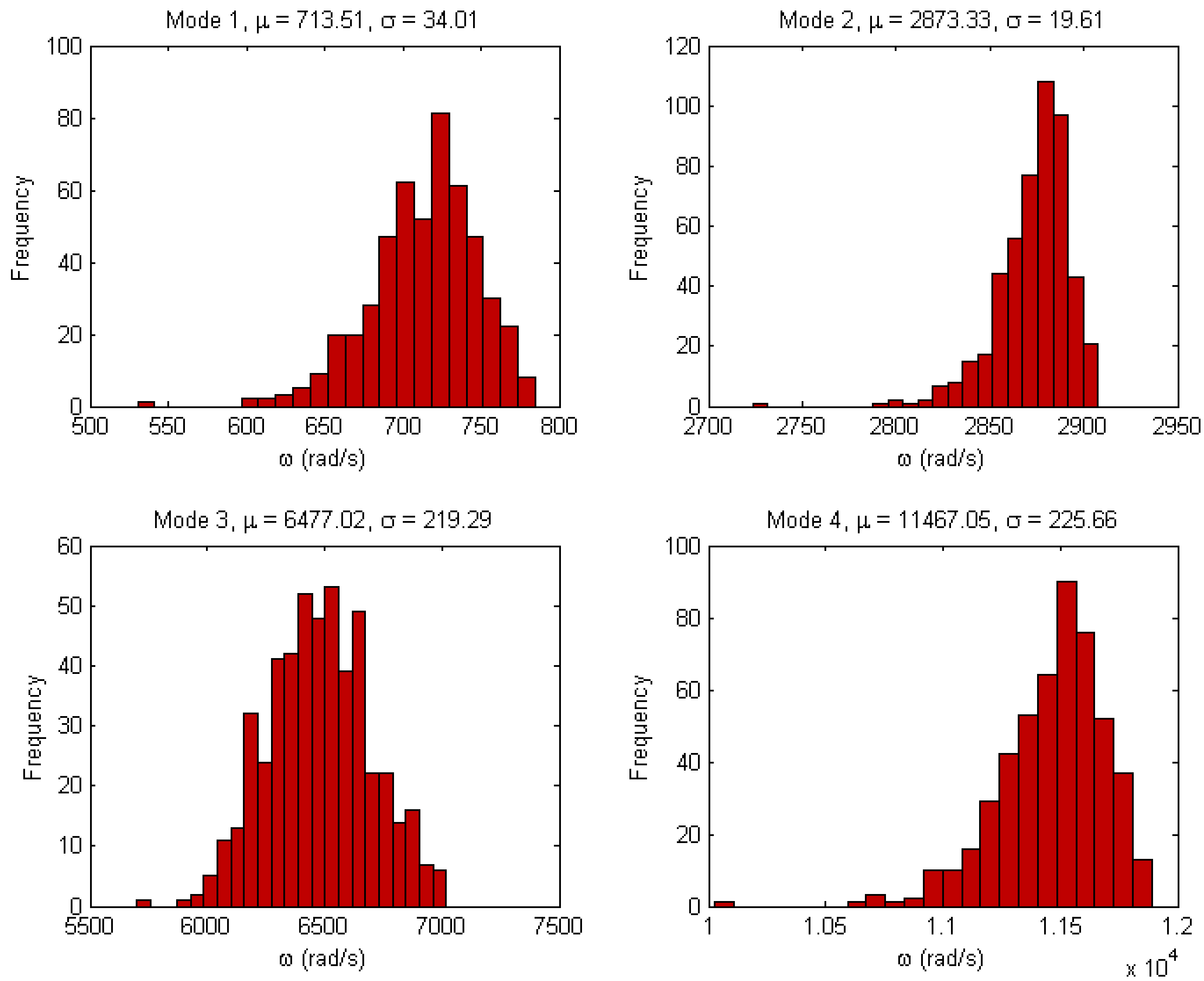
Multivariate Parameterization

- Generate multivariate expansion using N-dimensional Taylor series approximation for 5 variables simultaneously
- Specify highest order derivative (including mixed derivative terms)
- Generate Latin Hypercube Sample (LHS) based on probability distribution of parameters
- Plug samples into parameterized models and compare with true system response

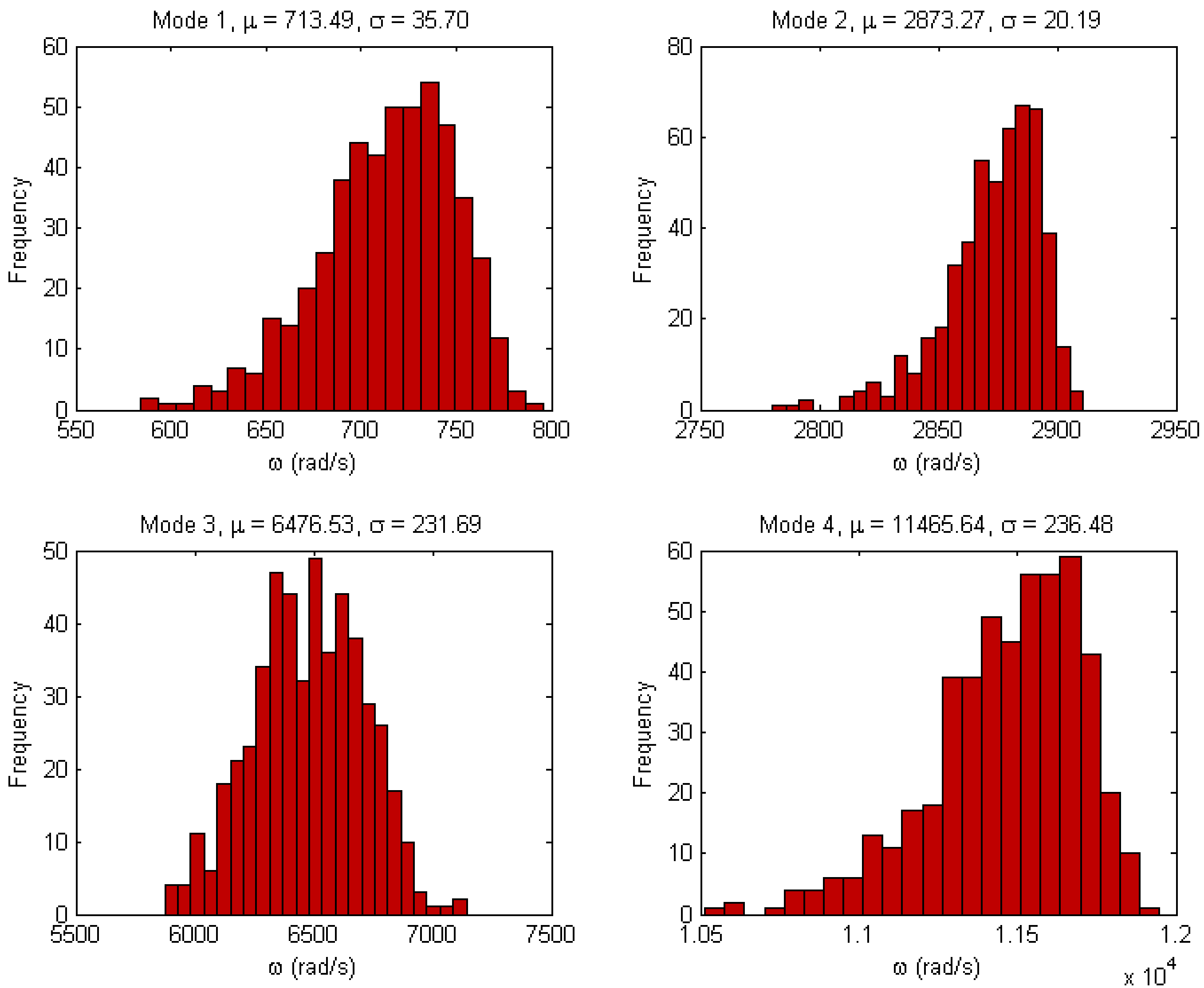
Exhaustive Sweep



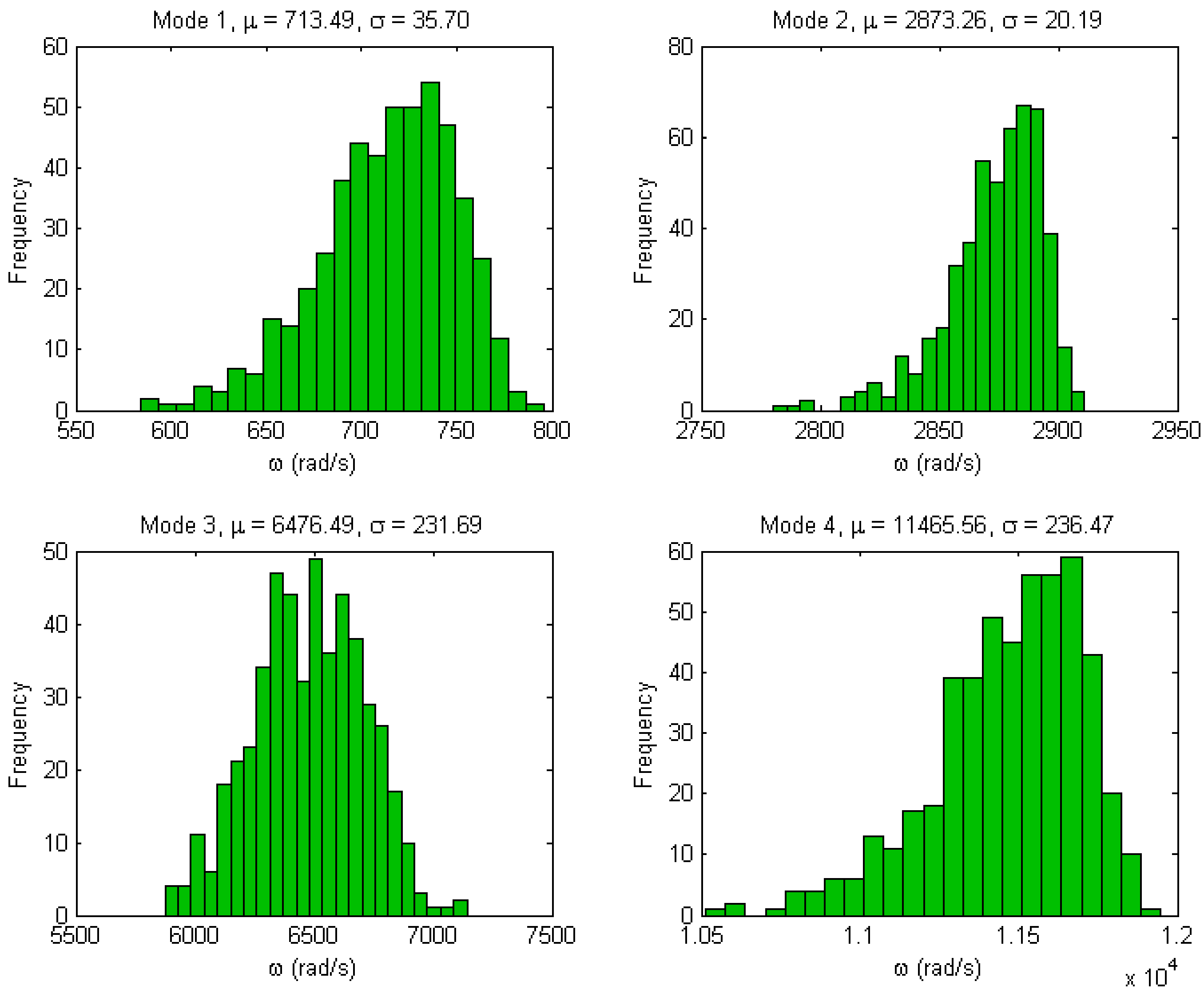
System Parameterization, 2nd Order



System Parameterization, 4th Order



ROM Parameterization, 4th Order



Observations on the Multivariate Expansions of Finite Difference Based PROMs

- Even a second order expansion is good for high component variations
  - Means and standard deviations within ~10% of exhaustive approach
  - Histograms relatively similar
  - **Uses 51 meshes**
- Fourth order expansion is almost exact
  - Means and standard deviations are well within .01% of exhaustive
  - Histograms almost indistinguishable
  - **Uses 301 meshes**

Revisiting the Derivatives

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- Recall the Taylor series expansions

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$$f^{(4)}(x) \approx \frac{f(x-2h) - 4f(x-h) + 6f(x) - 4f(x+h) + f(x+2h)}{h^4}$$

- For two dimensions, even larger expressions results
- The number of meshes needed grows geometrically with the number of free variables.
- Quickly becomes intractable for a real problem with multiple dimensions of interest…

Alternatives Exist!

- Parameterize a single element and propagate through models…
  - Book-keeping challenge…

- Replace finite difference based expansions with complex step approximations…
  - See the recent work by Millwater's group [1]…

- Alternatively, use hyper dual numbers…

[1]: A. Voorhees, H.R. Millwater, and R. Bagley, *Finite Elements in Analysis and Design*, **47**, pp. 1146-1156, 2011.

What Are Dual Numbers?

- Branch of generalized complex numbers
  - Ordinary complex numbers, $E^2 = i^2 = -1$
  - Double numbers, $E^2 = e^2 = 1$ (Clifford, 1873)
  - Dual numbers, $E^2 = \varepsilon^2 = 0$ (Study, 1903)
- The complex step approximation for a Taylor series

$$f(x+hE) = f(x) + hEf'(x) + \frac{1}{2!}h^2E^2f''(x) + \frac{1}{3!}h^3E^3f'''(x) + \cdots$$

simplifies based off of the choice for *E*…

The Complex Step Expansion

- Ordinary complex numbers ($E^2 = i^2 = -1$)

$$f(x+hi) = \underbrace{\left(f(x) - \frac{1}{2!}h^2 f''(x) + \cdots\right)}_{\text{Real}} + h\underbrace{\left(f'(x) - \frac{1}{3!}h^3 E^3 f'''(x) + \cdots\right)}_{\text{Imaginary}} i$$

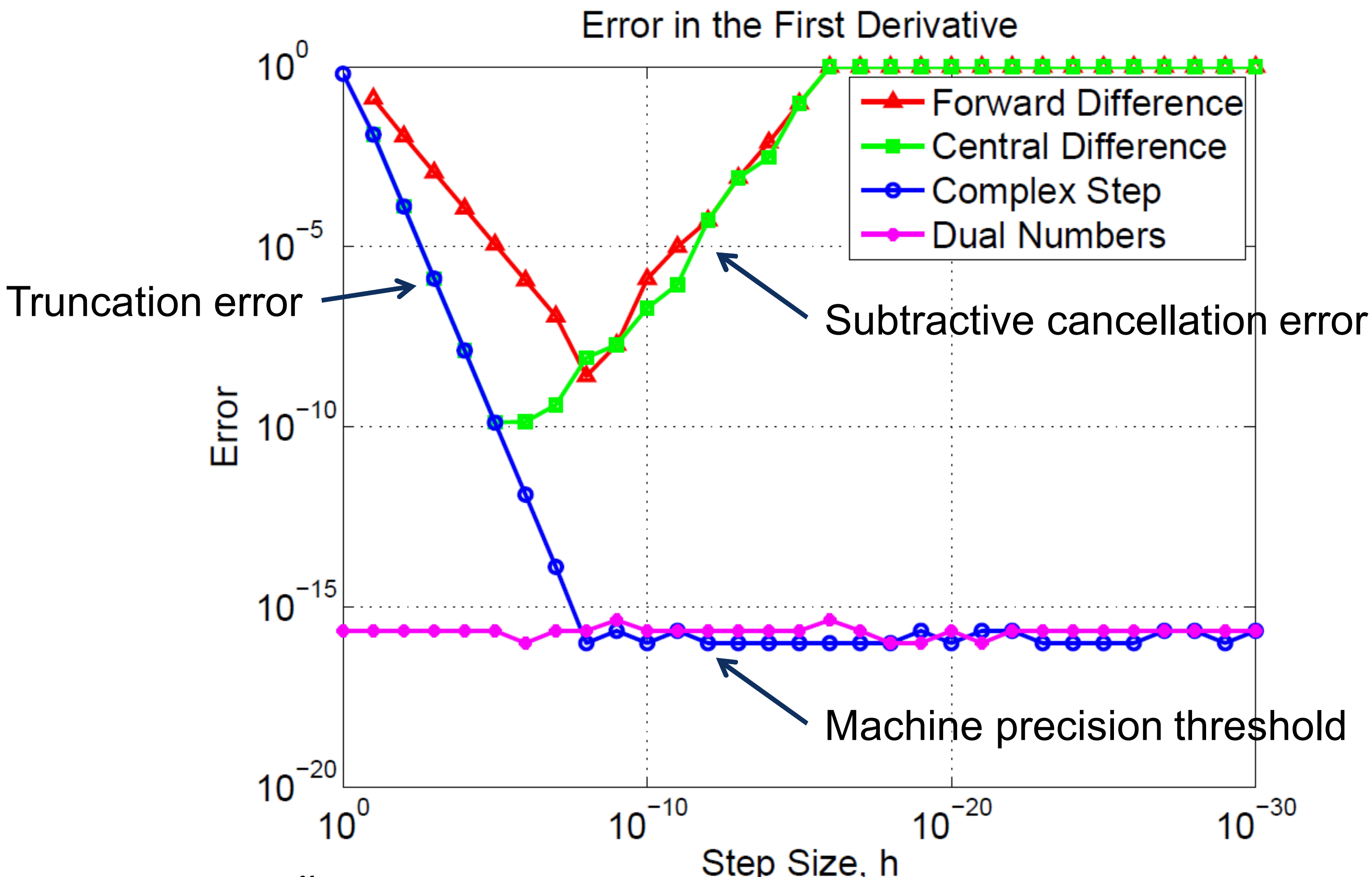
- Double numbers ($E^2 = e^2 = 1$)

$$f(x+he) = \underbrace{\left(f(x) + \frac{1}{2!}h^2 f''(x) + \cdots\right)}_{\text{Real}} + h\underbrace{\left(f'(x) + \frac{1}{3!}h^3 E^3 f'''(x) + \cdots\right)}_{\text{Non-Real}} e$$

- Dual numbers ($E^2 = \varepsilon^2 = 0$)

$$f(x+h\varepsilon) = \underbrace{f(x)}_{\text{Real}} + \underbrace{hf'(x)\varepsilon}_{\text{Non-Real}}$$

Accuracy of First Derivative Calculations



$$f(x) = \frac{e^{x}}{\sqrt{(\sin x)^3 + (\cos x)^3}}$$

What About Higher Derivatives?

- Complex step method requires a differencing operation, which leads to subtractive cancellation error…
- Hyper dual numbers are dual numbers defined in multiple dimensions (Fike, 2011 & 2012)

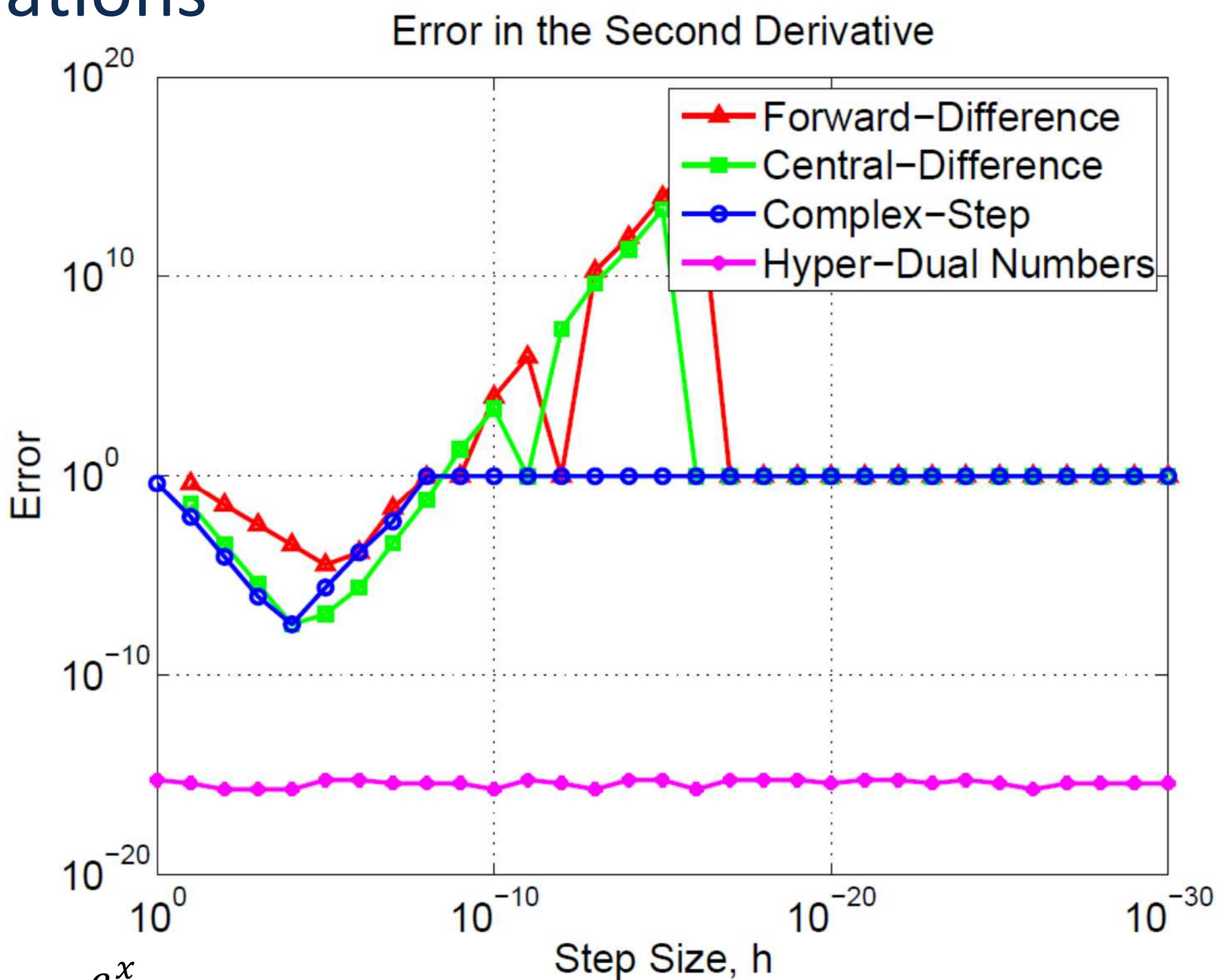
$$x = x_0 + x_1\varepsilon_1 + x_2\varepsilon_2 + x_3\varepsilon_1\varepsilon_2$$
$$\varepsilon_1^2 = \varepsilon_2^2 = 0$$
$$\varepsilon_1 \neq \varepsilon_2 \neq 0$$
$$\varepsilon_1\varepsilon_2 = \varepsilon_2\varepsilon_1 \neq 0$$

- This leads to the expansion

$$f(x + h_1\varepsilon_1 + h_2\varepsilon_2 + 0\varepsilon_1\varepsilon_2) = f(x) + h_1 f'(x)\varepsilon_1 + h_2 f'(x)\varepsilon_2 + h_1 h_2 f''(x)\varepsilon_1\varepsilon_2$$

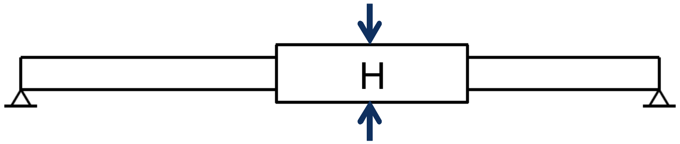
which has exact first and second derivatives

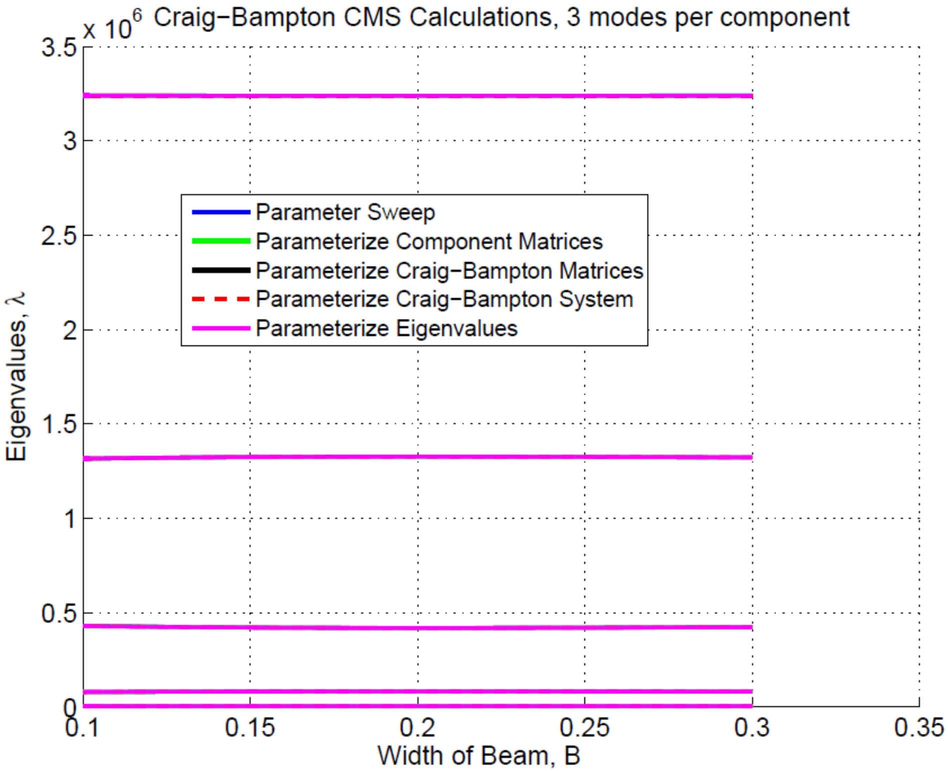
Accuracy of Second Derivative Calculations

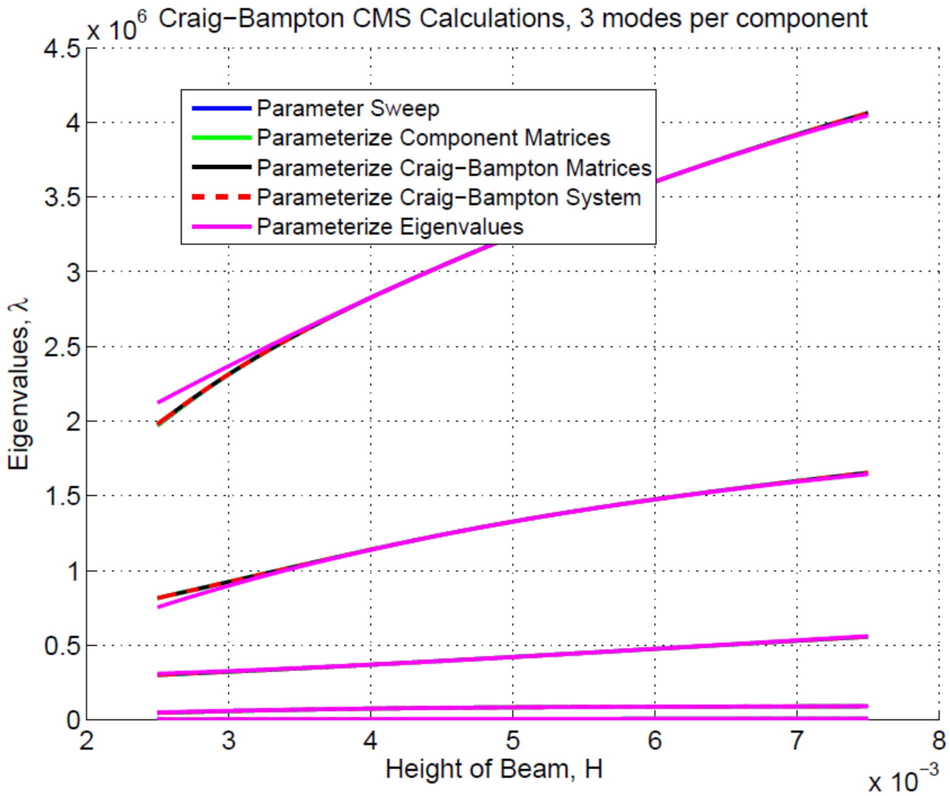


$$f(x) = \frac{e^x}{\sqrt{(\sin x)^3 + (\cos x)^3}}$$

Results of PROMs Constructed With Hyper Dual Numbers







- Cubic expansion, based off of a single mesh of the beam

Results of PROMs Constructed With Hyper Dual Numbers

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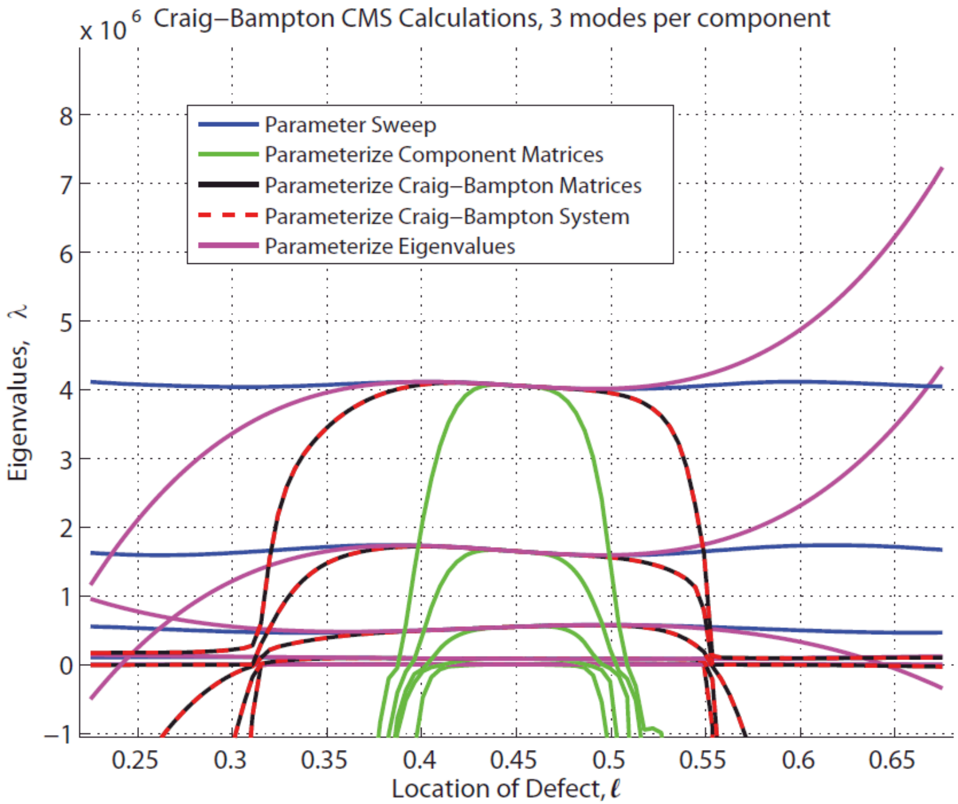
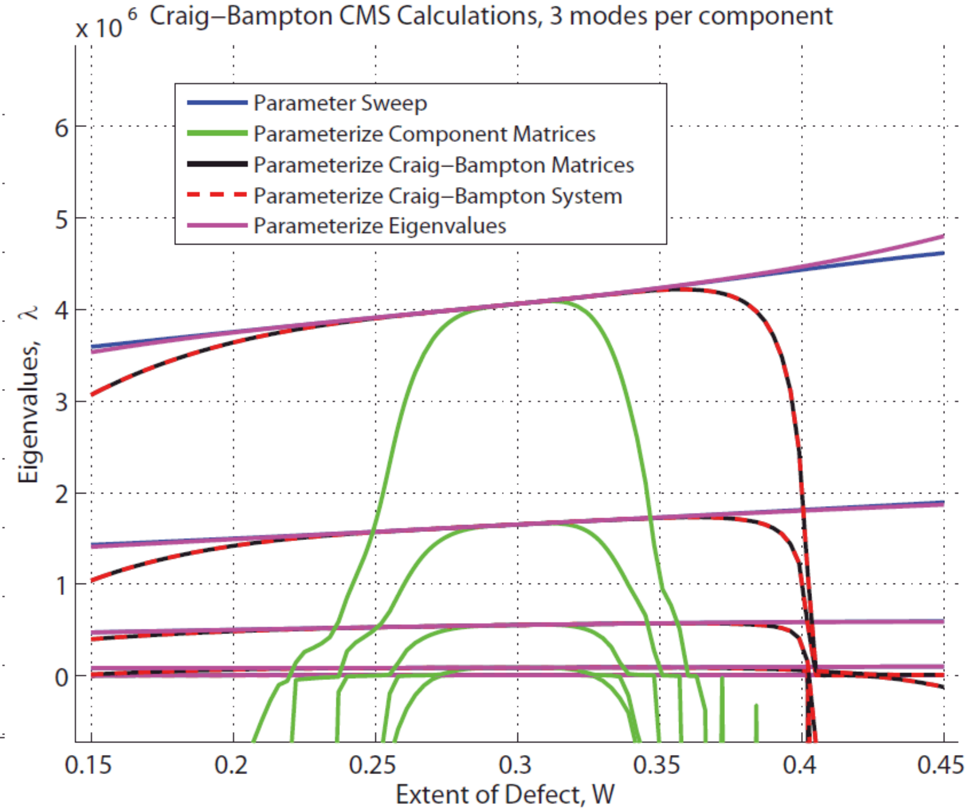
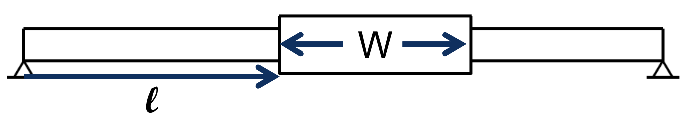


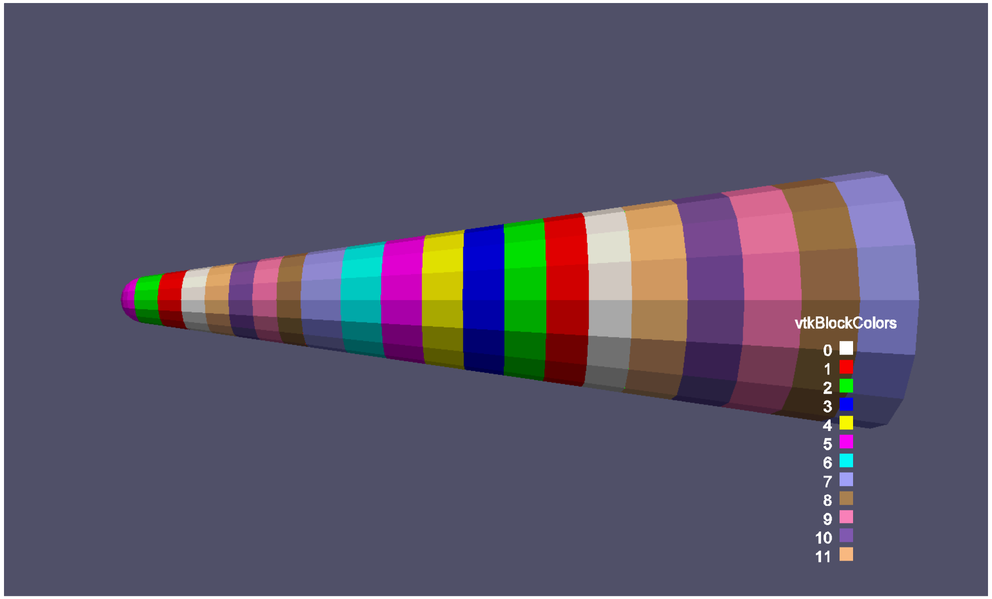




- Accuracy can be further improved with a meta-modeling approach, but that necessitates more meshes…

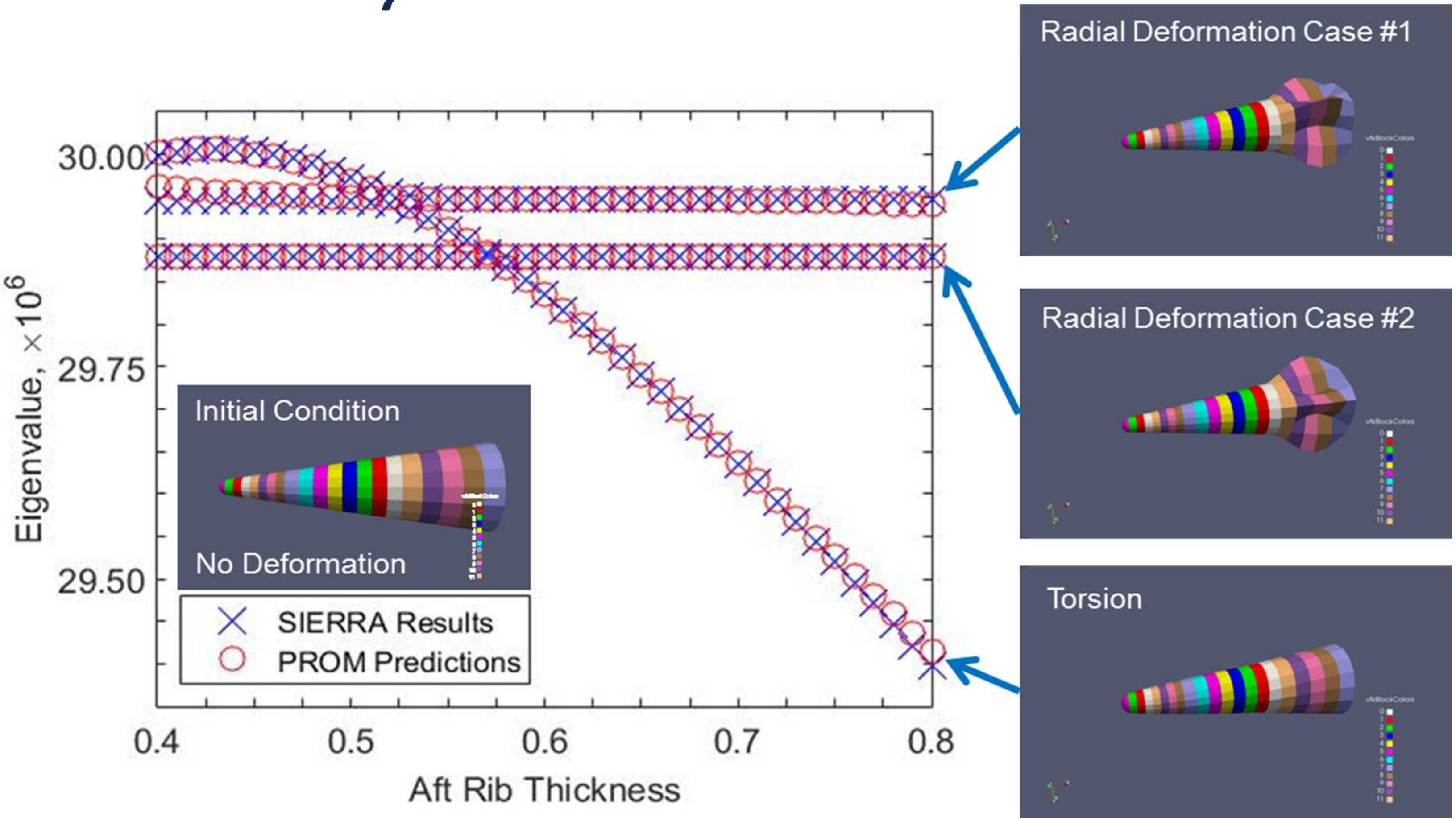
Application to Large Systems

- Mathematics the exact same as for previous system
- The challenge is in prescribing geometric dimensions for variation…



- Several internal components; design challenge: ribs connecting exterior to interior

Preliminary Results



- Computational time for the PROM approximately 1/40th that of the high fidelity model, and no additional costs to consider geometry changes.

Summary & Conclusions

- Hyper dual numbers are a branch of generalized complex numbers with the property $\varepsilon^2 = 0$, $\varepsilon \neq 0$
- Building hyper dual numbers into our FEA code allows us to develop parameterized reduced order models (PROMs) with a single mesh
- Multiple levels of parameterization are investigated, and the results indicate that this parameterization technique is an effective and efficient approach to modeling
- Generally, the closer a parameterization is to the high fidelity FEA model, the worse that the PROM constructed from it will perform
- Results match analytical solutions very well for PROMs constructed from Craig-Bampton models or Eigen representations

Acknowledgements

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