UNCERTAINTY QUANTIFICATION
WORKING GROUP

A Definition of Simulation Uncertainty & A View of Total Uncertainty

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PART 1—A DEF’N OF SIMULATION UNCERTAINTY

Overview

- Why do we care?
- What is it?
- How does it apply to our models?
- What technologies are available?
- What technologies are being developed?
- What is the path forward?

WHY DO WE CARE ABOUT UNCERTAINTY?

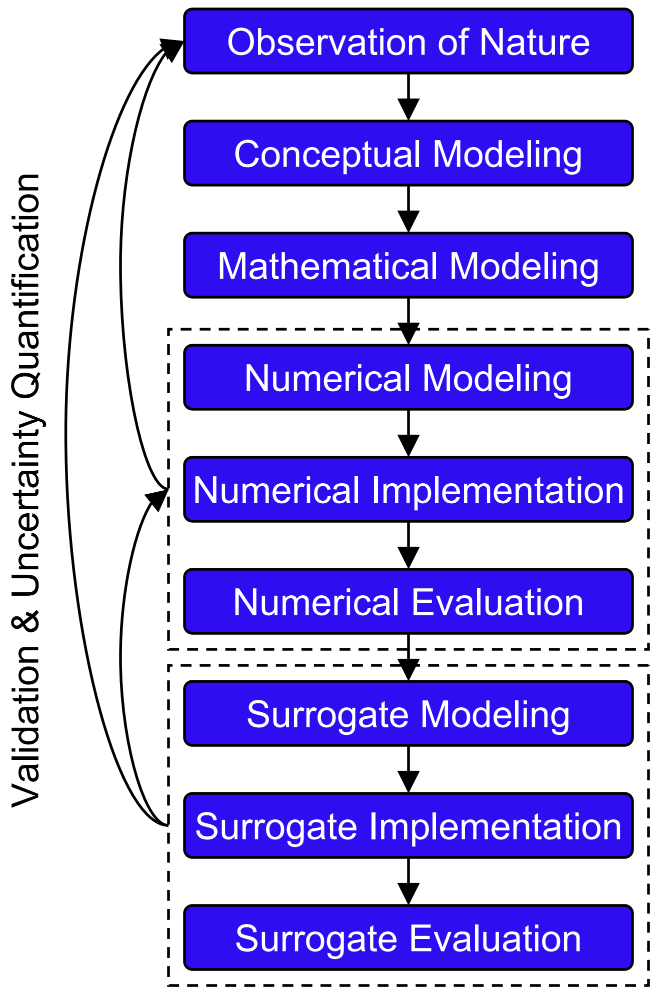
- Science-based stockpile stewardship requires data and models
  - Test measurements
  - High-fidelity physics-based models (FEM, etc.)
  - Low-fidelity physics-based models (SDOF, etc.)
  - Surrogate models
- Decisions will be based on our model predictions
  - Safety
  - Security
  - Economic
  - Military
- Accuracy and robustness is crucial to acceptance
- Accuracy/robustness $\Rightarrow$ quantified uncertainties

WHAT IS UNCERTAINTY?

- Aleatoric uncertainty (also called Variability)
  - Inherent variation
  - Irreducible
- Epistemic uncertainty (also called simply Uncertainty)
  - Potential deficiency
  - Lack of knowledge
  - Reducible?
- Prejudicial uncertainty (also called Error)
  - Recognizable deficiency
  - Bias
  - Reducible

HOW DOES IT APPLY TO OUR MODELS?

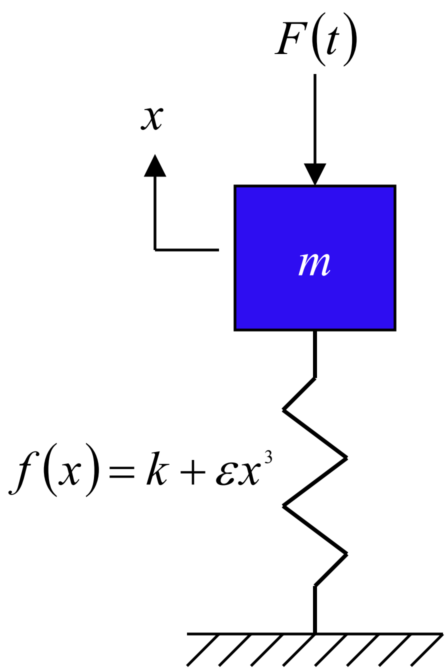
- Phases of the modeling process



- Sources of uncertainty
  - Measurements
    - Noise
    - Resolution,
    - Quantization
    - Processing
  - Mathematical models
    - Equations
    - Geometry
    - BCs/ICs
    - Inputs
    - Deterministic chaos
  - Numerical models
    - Weak formulations
    - Discretizations
    - Approximate solution algorithms
    - Truncation and roundoff
  - Surrogate models
    - Approximation error
    - Interpolation error
    - Extrapolation error
  - Model parameters

A SIMPLE EXAMPLE

"Truth" Model



$$m\ddot{x} + kx + \varepsilon x^3 = F(t)$$
$$x(0) = x_0,\ \dot{x}(0) = \dot{x}_0$$

- **Measurement uncertainty**
  - Forcing function & ICs
  - Response
- **Math model uncertainty**

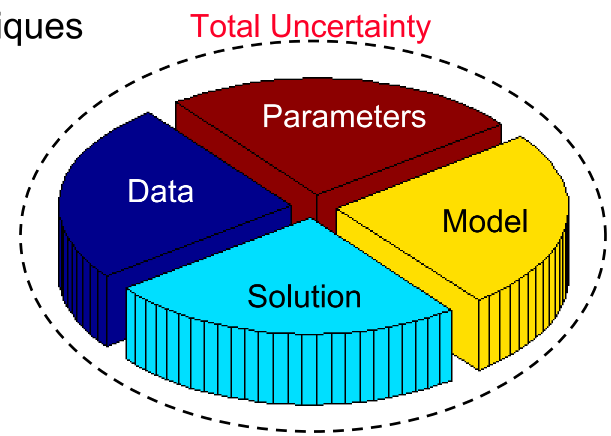
$$m\ddot{x} + kx = \hat{F}(t)$$
$$x(0) = \hat{x}_0,\ \dot{x}(0) = \hat{\dot{x}}_0$$

  - Equation form
  - Forcing function & Ics
  - Sensitive dependence on ICs
- **Numerical solution uncertainty**
  - Integration algorithm
  - Time step (discretization)
- **Parameters**

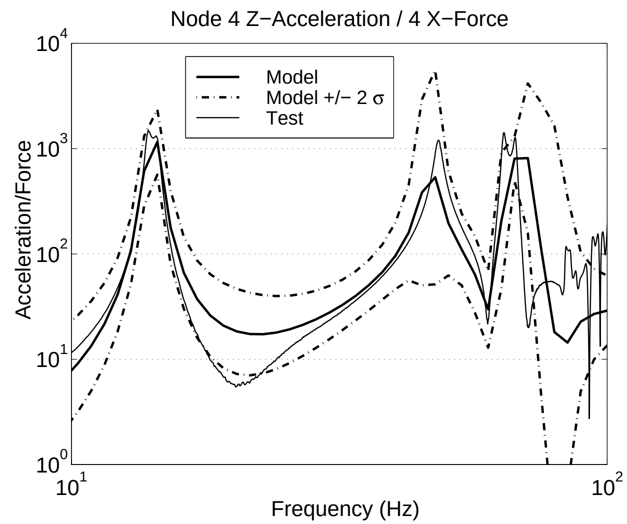
$$\hat{m},\ \hat{k}$$

WHAT TECHNOLOGIES ARE AVAILABLE?

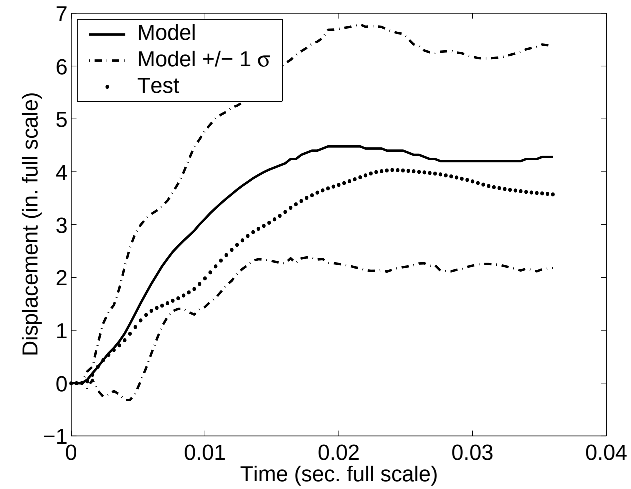
- Data
  - Calibration w.r.t. conventional standards
  - Noise characterization
  - “Similar” or “inverse” signal processing
- Mathematical models (Not much!)
- Numerical models
  - Bounds for discretization errors
  - Bounds for approximate solution techniques
  - Bounds for truncation/roundoff errors
- Surrogate models
  - DOE
  - Residual analysis
  - ANOVA
- Parameters
  - Sensitivity analysis
  - Monte Carlo
  - Reliability methods (FORM, SORM, AMV, AMV+, FPI)
  - Fuzzy set & interval propagation methods
  - Stochastic FEM
- Total uncertainty



GENERIC VIEW OF TOTAL UNCERTAINTY

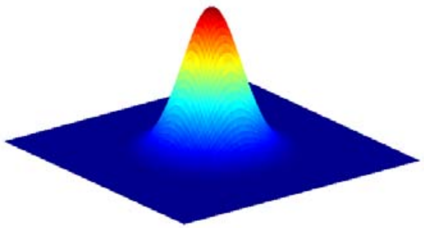


- Generic class of model-test pairs
- Normalized comparisons
- Uncertainty propagation

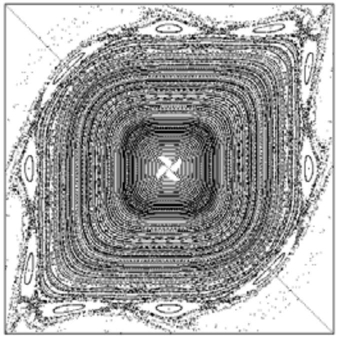


WHAT TECHNOLOGIES ARE BEING DEVELOPED?

- **Measure theoretic methods**
  - Probability theories—frequentist, Bayesian, Koopman-Carnap
  - Dempster-Schafer theory
  - Possibility theory



- **Set theoretic methods**
  - Fuzzy set theories—classical, grey, intuitionistic, rough
  - Interval arithmetic
  - Convex sets & convex modeling



- **Dynamical systems methods**
  - Strange attractor theory
  - Liapunov exponents
  - Complexity theory

PROBABILITY THEORY V. DST

- Probability theory—
  Based on classical measure theory (additivity)

$$\Pr : 2^X \to [0,1]$$
$$\Pr(\varnothing) = 0$$
$$\Pr(X) = 1$$

$$\Pr\left(\bigcup_i A_i\right) = \sum_i \Pr(A_i) - \sum_{j<k} \Pr(A_j \cap A_k) + \cdots + (-1)^{n+1} \Pr\left(\bigcap_i A_i\right)$$

$$\Pr\left(\bigcap_i A_i\right) = \sum_i \Pr(A_i) - \sum_{j<k} \Pr(A_j \cup A_k) + \cdots + (-1)^{n+1} \Pr\left(\bigcup_i A_i\right)$$

- Dempster-Schafer theory—
  Based on fuzzy measure theory (monotonicity & semicontinuity)

$$\mathrm{Bel} : 2^X \to [0,1] \qquad \mathrm{Pl} : 2^X \to [0,1]$$
$$\mathrm{Bel}(\varnothing) = 0 \qquad \mathrm{Pl}(\varnothing) = 0$$
$$\mathrm{Bel}(X) = 1 \qquad \mathrm{Pl}(X) = 1$$

$$\mathrm{Bel}\left(\bigcup_i A_i\right) \geq \sum_i \mathrm{Bel}(A_i) - \sum_{j<k} \mathrm{Bel}(A_j \cap A_k) + \cdots + (-1)^{n+1} \mathrm{Bel}\left(\bigcap_i A_i\right)$$

$$\mathrm{Pl}\left(\bigcap_i A_i\right) \leq \sum_i \mathrm{Pl}(A_i) - \sum_{j<k} \mathrm{Pl}(A_j \cup A_k) + \cdots + (-1)^{n+1} \mathrm{Pl}\left(\bigcup_i A_i\right)$$

PROBABILITY THEORY V. POSSIBILITY THEORY

- Probability theory—
  Based on classical measure theory (additivity)

$$\Pr : 2^X \to [0,1]$$
$$\Pr(\varnothing) = 0$$
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$$\Pr\left(\bigcap_i A_i\right) = \sum_i \Pr(A_i) - \sum_{j<k} \Pr(A_j \cup A_k) + \cdots + (-1)^{n+1} \Pr\left(\bigcup_i A_i\right)$$

- Possibility theory—
  Based on fuzzy measure theory (semicontinuity)

$$\mathrm{Pos} : 2^X \to [0,1] \qquad \mathrm{Nec} : 2^X \to [0,1]$$
$$\mathrm{Pos}(\varnothing) = 0 \qquad \mathrm{Nec}(\varnothing) = 0$$
$$\mathrm{Pos}(X) = 1 \qquad \mathrm{Nec}(X) = 1$$

$$\mathrm{Pos}\left(\bigcup_i A_i\right) = \sup_i \mathrm{Pos}(\mathrm{A}_\mathrm{i})$$

$$\mathrm{Nec}\left(\bigcap_i A_i\right) = \inf_i \mathrm{Nec}(A_i)$$

POTENTIAL UNCERTAINTY METRICS

- Hartley measure for nonspecificity

$$H(A) = \log_2 |A|, |A| \text{ is cardinality of } A$$

- Generalized Hartley measure for nonspecificity in DST

$$N(m) = \sum_{A \in 2^X} m(A) \log_2 |A|, m : 2^X \to [0,1], m(\varnothing) = 0, \sum_{A \in 2^X} m(A) = 1$$

- U-uncertainty measure for nonspecificity in possibility theory

$$U(r) = \sum_{i=2}^{n} (r_i - r_{i+1}) \log_2 i, r(x) = \mathrm{Pos}(\{x\}), r_i \geq r_{i+1} \forall i$$

- Shannon entropy for total uncertainty in probability theory

$$S(p) = -\sum_{x \in X} p(x) \log_2 p(x)$$

- Generalized Shannon entropy for total uncertainty in DST

$$AU(\mathrm{Bel}) = \max_{p_x} \left(-\sum_{x \in X} p_x \log_2 p_x \right), Bel(A) \leq \sum_{x \in A} p_x \forall A \in 2^X$$

- Hamming distance for fuzzy sets

$$f(A) = \sum_{x \in X} \left[1 - |2A(x) - 1| \right], A(x) \text{ is membership function}$$

WHAT IS THE PATH FORWARD?

- Some type of uncertainty quantification is required
- Salient points
  - Measure predictive capability $\Rightarrow$ Compare data & predictions
  - Experiments should be designed to facilitate comparisons
  - “Adequate” quantification of predictive capability $\Rightarrow$ lots of data
  - Interpolation/extrapolation beyond observations $\Rightarrow$ inference
- No comprehensive framework/toolbox exists
  - Application dependent
  - Different types of uncertainty require different tools
- Hypothetical approach
  - Characterize measurement uncertainty
  - Characterize/propagate parametric uncertainty
  - Bound/propagate solution uncertainty
  - Estimate (generically) total uncertainty
  - “Subtract” to estimate model uncertainty

PART 2—A VIEW OF TOTAL UNCERTAINTY

Overview

- What is total uncertainty?
- Prototypical application: linear structural dynamics
  - Methodology
  - Example: Space truss structure
- Generalization to arbitrary applications
  - Methodology
  - Example: Nose cone crushing
  - Example: Blast response of R/C wall
- Conclusions

WHAT IS TOTAL UNCERTAINTY?

- *Total uncertainty* is simply a measure of the difference between experimental data and model predictions

- Practical considerations
  - There rarely exists enough samples for a given simulation scenario
  - Simple differencing leads to “small differences of large numbers”

- A candidate approach
  - Consider “generic classes” of test-analysis comparisons
  - Normalize information so that differences are “perturbations”

PROTOTYPICAL APPLICATION: LINEAR DYNAMICS

- Classical normal modes

$$\left({}^{0}K - {}^{0}\lambda^{0}M^{0}\right)\phi = 0 \quad \ldots\text{analysis}$$
$$\left(K - \lambda M\right)\phi = 0 \quad \ldots\text{test}$$

- Modal mass and stiffness matrices

$${}^{0}m = {}^{0}\phi^{T\,0}M\,{}^{0}\phi = I$$
$${}^{0}k = {}^{0}\phi^{T\,0}K\,{}^{0}\phi = {}^{0}\lambda$$

- Assumed "true" modal mass and stiffness matrices

$$m = {}^{0}m + \Delta m = I + \Delta m$$
$$k = {}^{0}k + \Delta k = {}^{0}\lambda + \Delta k$$

- Normalization of test modes

$$\phi^{T\,0}M\phi = I$$

- Cross-orthogonality of analysis and test modes

$$\phi = {}^{0}\phi\psi \ldots\text{assumed}$$
$${}^{0}\phi^{T\,0}M\phi = {}^{0}\phi^{T\,0}M\,{}^{0}\phi\psi = \psi$$

- Differences between analysis and test modes

$$\Delta\lambda = \lambda - {}^{0}\lambda$$
$$\Delta\phi = \phi - {}^{0}\phi = {}^{0}\phi\left(\psi - I\right) = {}^{0}\phi\Delta\psi$$

PROTOTYPICAL APPLICATION (CONT'D)

- Normalized modal metrics for total uncertainty quantification

$$\Delta m = -\left(\Delta\psi + \Delta\psi^{T}\right)$$
$$\Delta\tilde{k} = {}^{0}\lambda^{-1/2}\left(\Delta\lambda - {}^{0}\lambda\Delta\psi - \Delta\psi^{T\,0}\lambda\right)^{0}\lambda^{-1/2}$$
$$\Delta\zeta = \zeta - {}^{0}\zeta$$

- Vectorization of normalized differences

$$\Delta\tilde{r} = \begin{Bmatrix} \mathrm{vec}(\Delta m) \\ \mathrm{vec}(\Delta\tilde{k}) \\ \mathrm{vec}(\Delta\zeta) \end{Bmatrix}$$

- Structure-specific covariance matrix of uncertainty (biased)

$$\mu_{\Delta\tilde{r}} = E[\Delta\tilde{r}]$$
$$S_{\tilde{r}\tilde{r}} = E\left[\left(\Delta\tilde{r} - \mu_{\Delta\tilde{r}}\right)\left(\Delta\tilde{r} - \mu_{\Delta\tilde{r}}\right)^{T}\right]$$

- Generic covariance matrix of total uncertainty (unbiased)

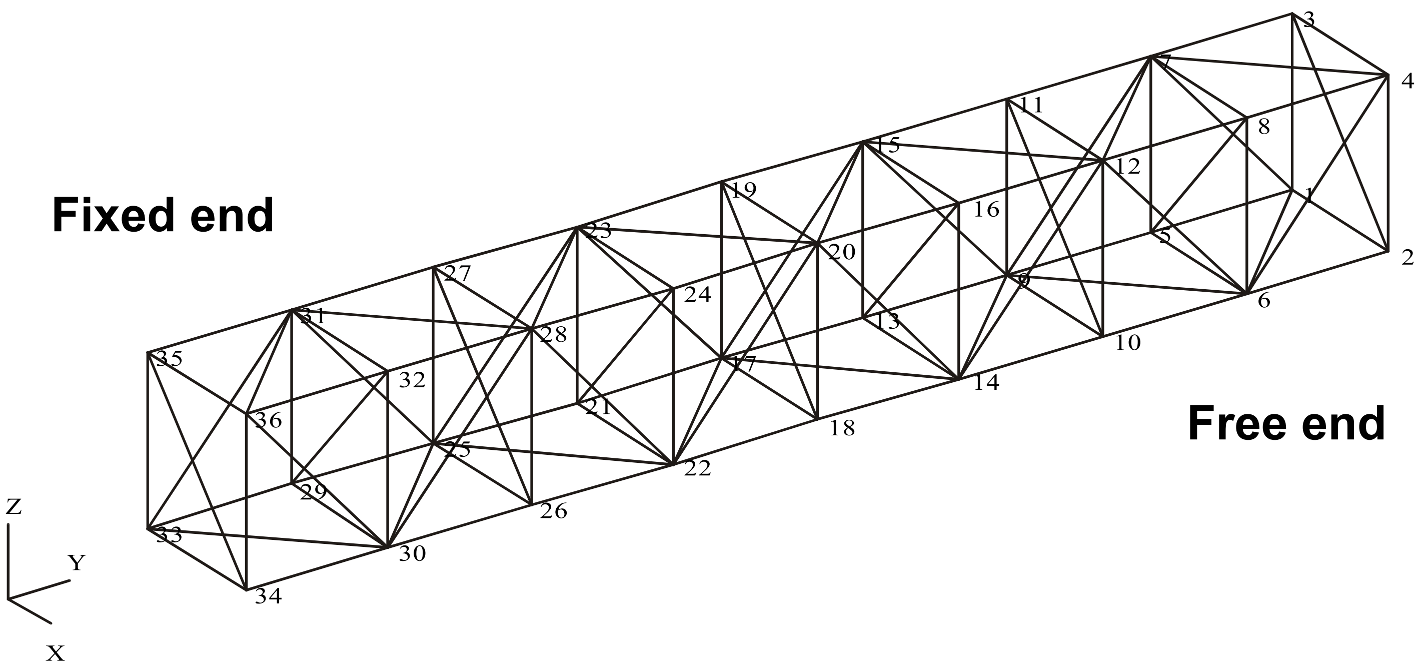
$$\mu_{\Delta\tilde{r}} = 0\ldots\text{assumed}$$
$$S_{\tilde{r}\tilde{r}} = E\left[\Delta\tilde{r}\Delta\tilde{r}^{T}\right]$$

- Propagate thru model
  - Linear covariance propagation
  - Interval propagation
  - Monte Carlo simulation

EXAMPLE: SPACE TRUSS STRUCTURE

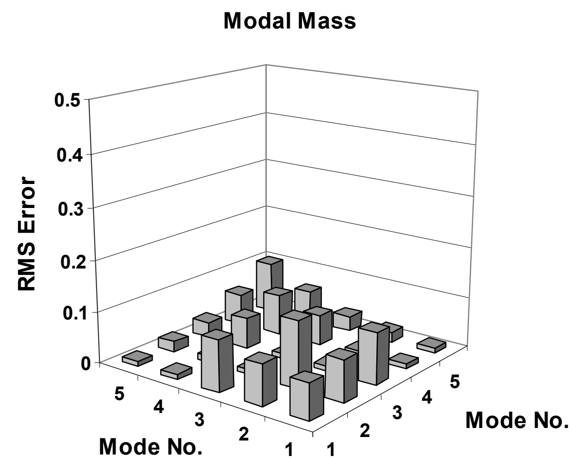
NASA/LaRC 8-bay truss structure

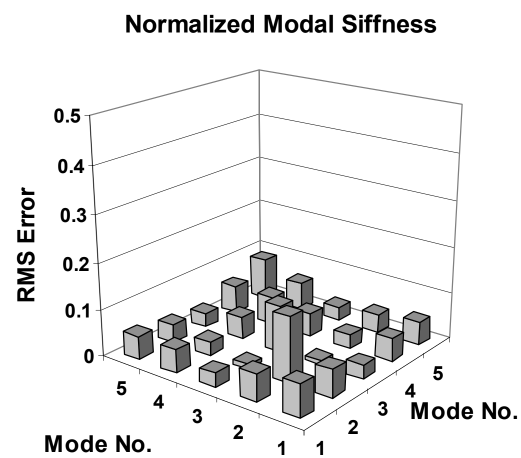
- Force input at Nodes 4 and 7
- Acceleration response measured at Nodes 1 through 32



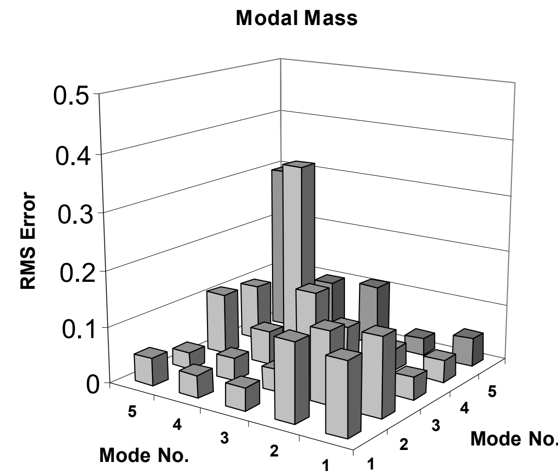
STRUCTURE-SPECIFIC VS. GENERIC VARIATION

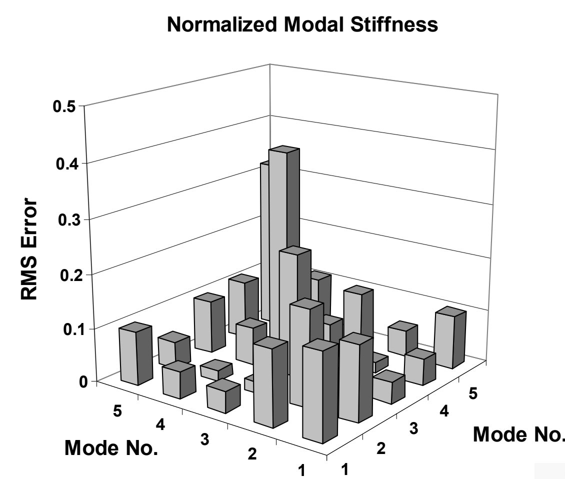
Structure-specific variability



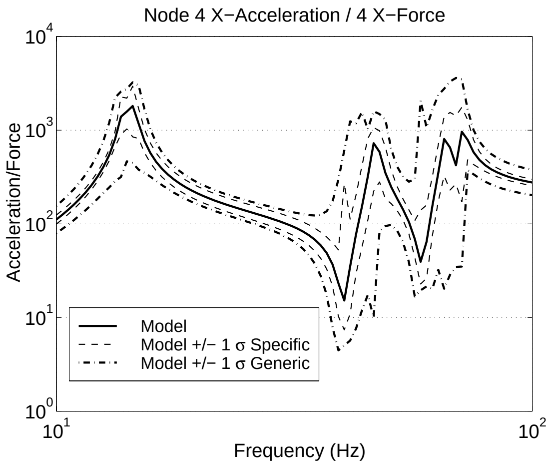


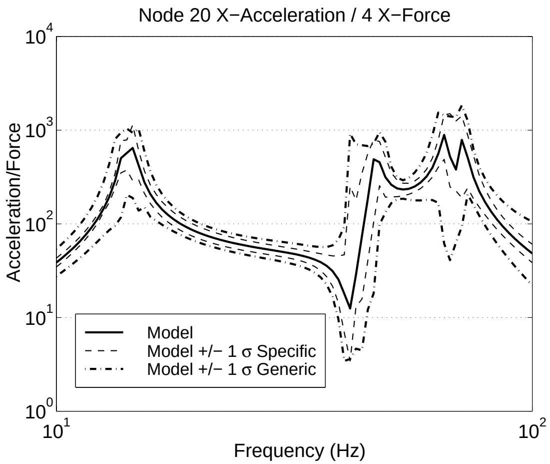
Generic class variability

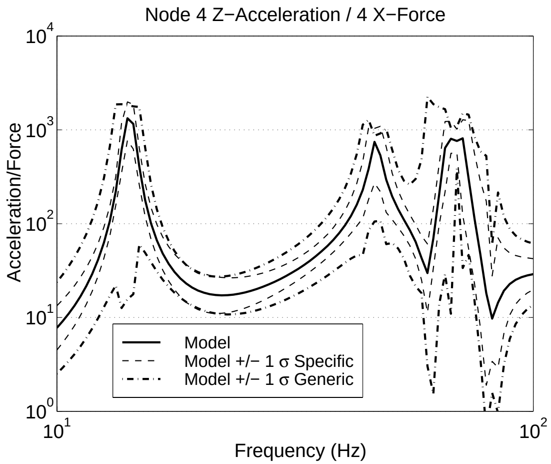


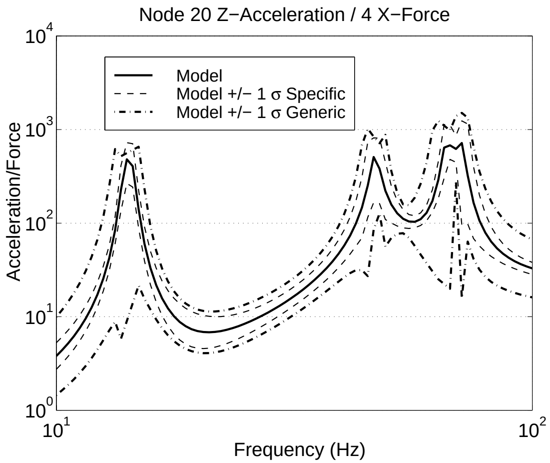


PREDICTIVE ACCURACY FOR SPACE TRUSS









GENERALIZATION TO ARBITRARY APPLICATIONS

- Response matrix

$$X = \begin{bmatrix} x(t_1;\theta_1) & x(t_1;\theta_2) & \cdots & x(t_1;\theta_n) \\ x(t_2;\theta_1) & x(t_2;\theta_2) & \cdots & x(t_2;\theta_n) \\ \vdots & \vdots & \ddots & \vdots \\ x(t_m;\theta_1) & x(t_m;\theta_2) & \cdots & x(t_m;\theta_n) \end{bmatrix}$$

- Singular value decomposition

$$X = U\Sigma V^T$$

$$= \underbrace{\left[\begin{array}{c:c} \overbrace{\eta^T}^{m\times p} & \overbrace{\eta_\perp^T}^{m\times(m-p)} \end{array}\right]}_{m\times m} \underbrace{\left[\begin{array}{c:c} \overbrace{D}^{p\times p} & \overbrace{0}^{p\times(n-p)} \\ \hdashline \overbrace{0}^{(m-p)\times p} & \overbrace{0}^{(m-p)\times(n-p)} \end{array}\right]}_{m\times n} \underbrace{\left[\begin{array}{c} \overbrace{\phi^T}^{p\times n} \\ \hdashline \overbrace{\phi_\perp^T}^{(n-p)\times n} \end{array}\right]}_{n\times n}$$

$$= \eta^T D\phi^T, \quad \eta\eta^T = \phi^T\phi = I_p$$

[Note: Papers use "X" $= X^T = \phi D\eta$]

GENERALIZATION (CONT'D)

- Differences between analysis and test

$$\Delta\phi = \phi - {}^{0}\phi$$
$$\Delta D = D - {}^{0}D$$
$$\Delta\eta = \eta - {}^{0}\eta$$

- Cross-orthogonality matrices

$$\psi = {}^{0}\phi^{T}\phi$$
$$\nu = {}^{0}\eta\eta^{T}$$

- Normalized differences

$$\Delta\psi = \psi - I_p$$
$$\Delta\nu = \nu - I_p$$
$$\Delta\tilde{D} = \frac{1}{\mathrm{Trace}\left({}^{0}D\right)}\left(D - {}^{0}D\right)$$

- Vectorization of differences

$$\Delta\tilde{r} = \begin{Bmatrix} \mathrm{vec}(\Delta m) \\ \mathrm{vec}(\Delta\tilde{k}) \\ \mathrm{vec}(\Delta\zeta) \end{Bmatrix}$$

- Structure-specific covariance matrix of uncertainty (biased)

$$\mu_{\Delta\tilde{r}} = E[\Delta\tilde{r}]$$
$$S_{\tilde{R}\tilde{R}} = E\left[(\Delta\tilde{r} - \mu_{\Delta\tilde{r}})(\Delta\tilde{r} - \mu_{\Delta\tilde{r}})^{T}\right]$$

- Generic covariance matrix of total uncertainty (unbiased)

$$\mu_{\Delta\tilde{r}} = 0 \ldots \text{assumed}$$
$$S_{\tilde{R}\tilde{R}} = E\left[\Delta\tilde{r}\Delta\tilde{r}^{T}\right]$$

GENERALIZATION (CONT'D)

- Consider data as function of normalized parameters

$$u(\tilde{r}) = \text{vec}\left[X(\tilde{r})\right]$$

- First order Taylor series approximation of data

$$\Delta u \approx T_{u\tilde{r}} \Delta\tilde{r}, \quad \Delta u = u(\tilde{r}) - u\left({}^{0}\tilde{r}\right), \quad \left(T_{u\tilde{r}}\right)_{ij} = \left.\frac{\partial u_i}{\partial \tilde{r}_j}\right|_{\tilde{r} = {}^{0}\tilde{r}}$$

- "Propagate" uncertainty

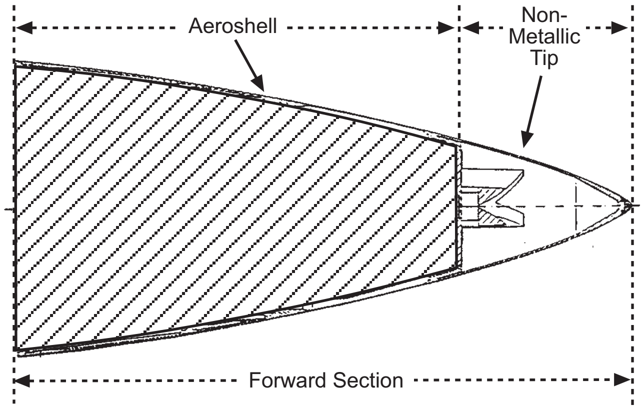
$$\begin{aligned} S_{UU} &= E\left(\Delta u \Delta u^T\right) \\ &\approx E\left(T_{u\tilde{r}} \Delta\tilde{r} \Delta\tilde{r}^T T_{u\tilde{r}}^T\right) \\ &\approx T_{u\tilde{r}} S_{\tilde{R}\tilde{R}} T_{u\tilde{r}}^T \end{aligned}$$

- Generate uncertainty bands

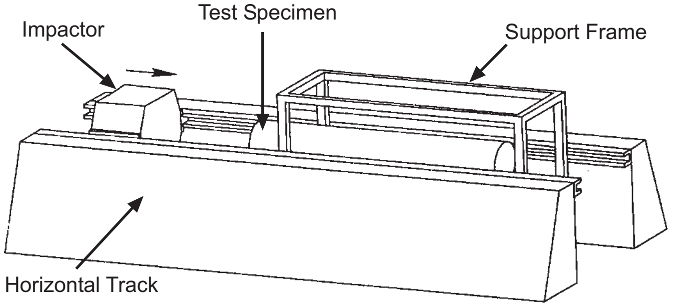
$$\sigma_U = \text{diag}\begin{bmatrix} \sqrt{\left(S_{UU}\right)_{11}} & & 0 \\ & \ddots & \\ 0 & & \sqrt{\left(S_{UU}\right)_{n_u n_u}} \end{bmatrix}$$

EXAMPLE: NOSE CONE CRUSHING

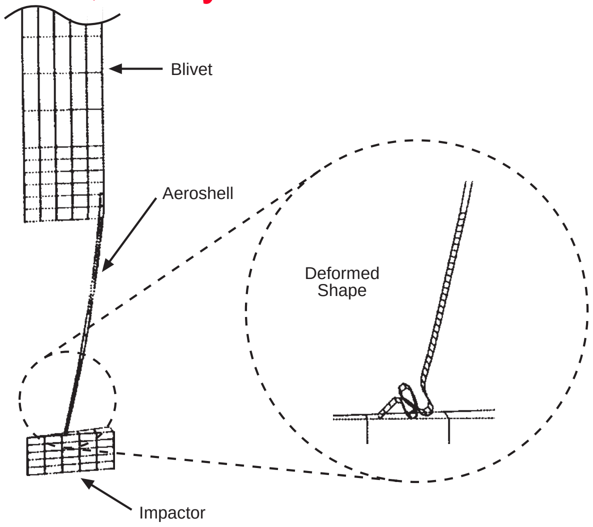
Nosecone aeroshell



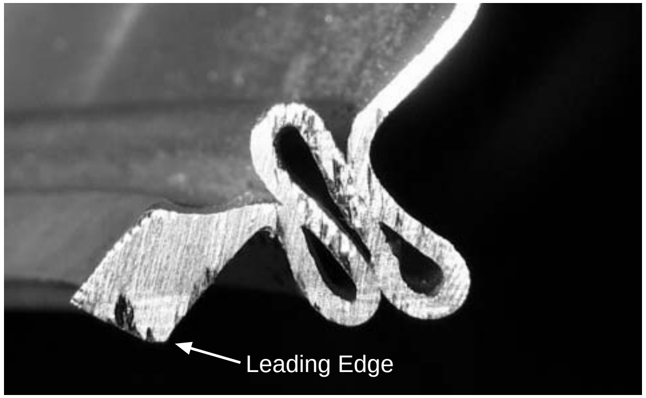
Test setup



Simplified, axisymmetric DYNA3D model

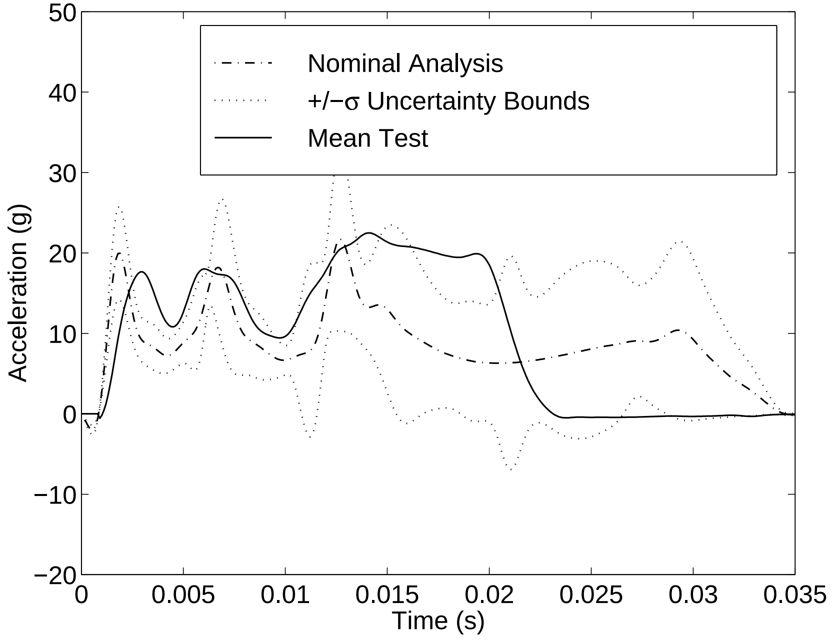


Actual buckling pattern

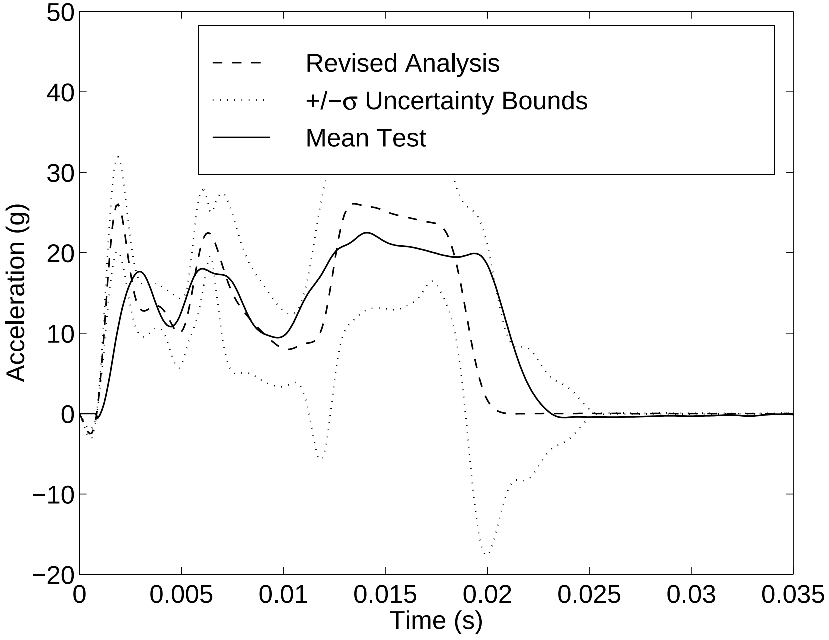


PREDICTIVE ACCURACY FOR NOSE CONE

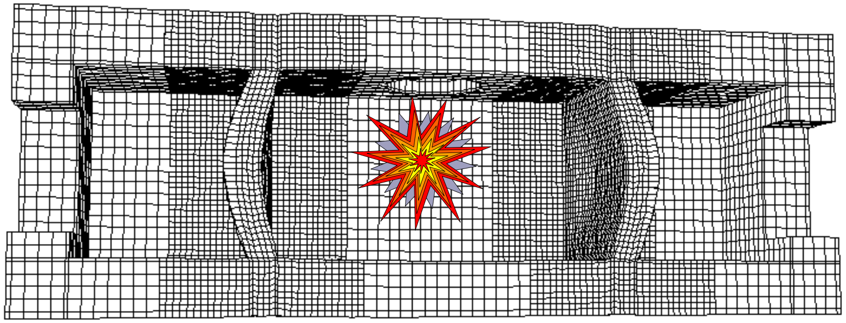
Pre-update predictive accuracy



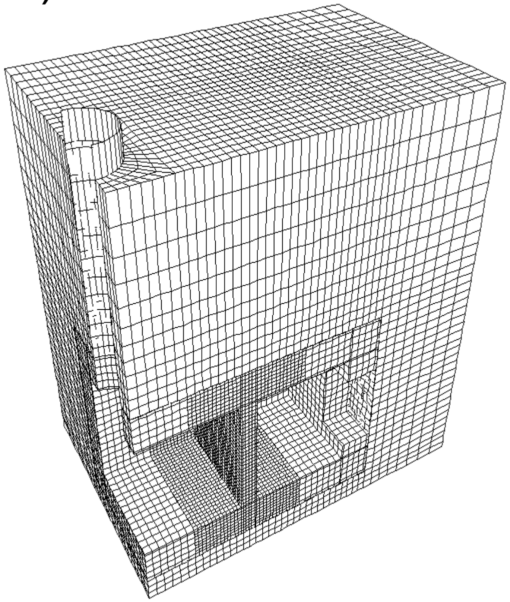
Post-update predictive accuracy



EXAMPLE: BLAST RESPONSE OF R/C WALL

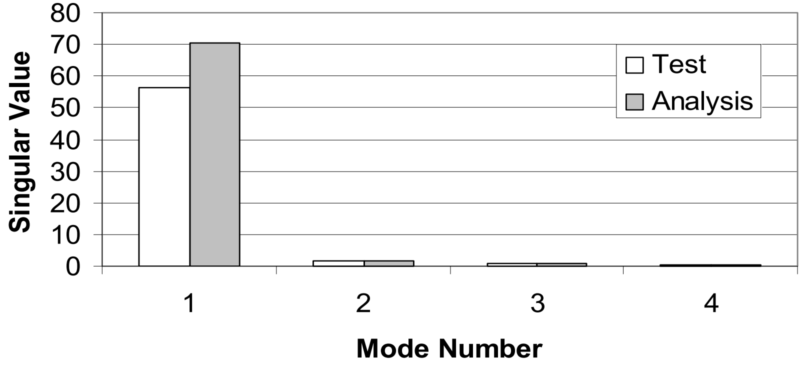


- Scenario
  - 3-room buried bunker
  - Explosion in center room
- Measurements
  - Displacements (12 sensors, 4 locations)
  - Pressures (10 sensors, 9 distinct locations)
- Structure model
  - DYNA3D (customized LLNL version)
  - ~80,000 continuum elements
  - ~20,000 beam elements
- Load model
  - CFD code (SHARC?)
  - Uncoupled from structure
  - Validated w.r.t. pressure measurements

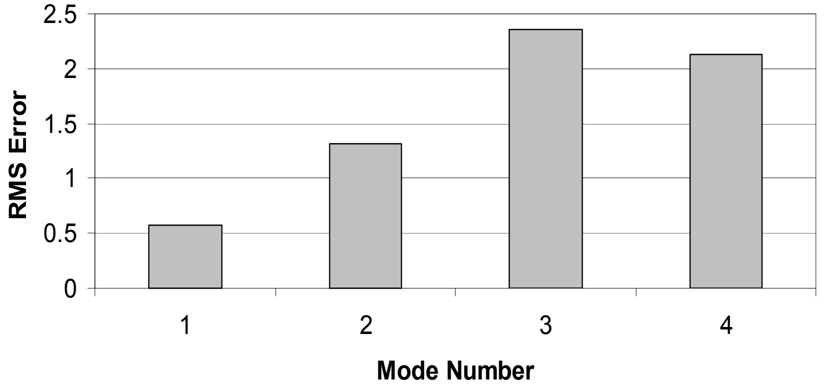


GENERIC CLASS VARIATION

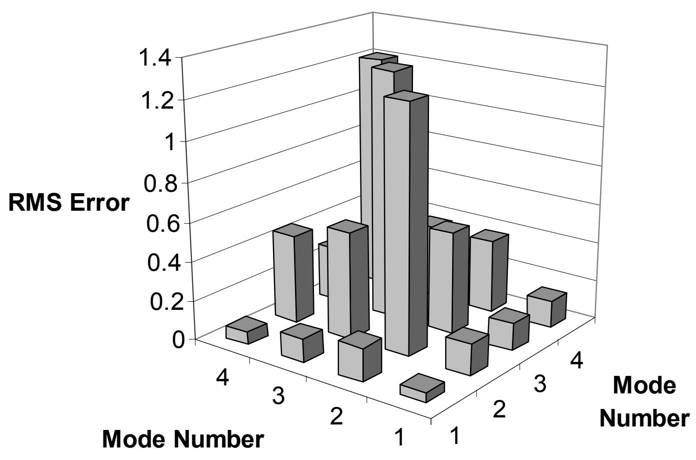
Typical Singular Values



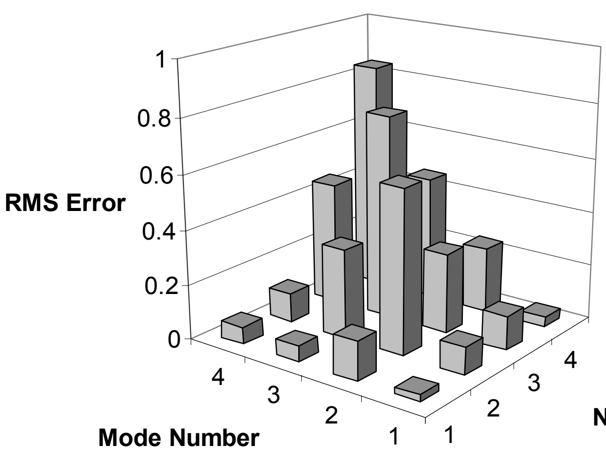
Normalized Singular Values



Left Eigenvector Cross-Orthogonality

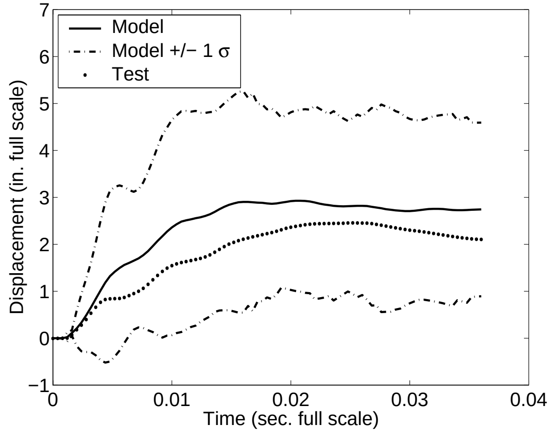


Right Eigenvector Cross-Orthogonality

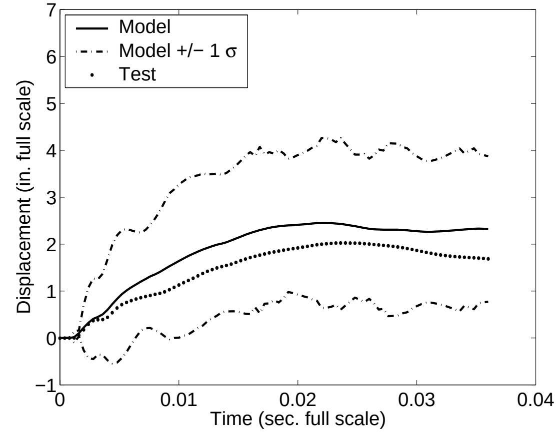


PRE-UPDATE PREDICTIVE ACCURACY FOR R/C WALL

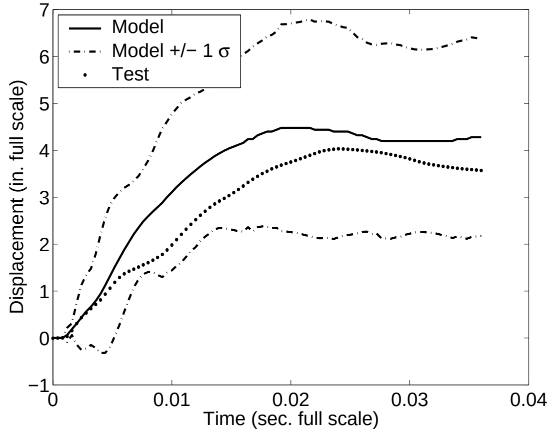
Left Horizontal Quarter Point



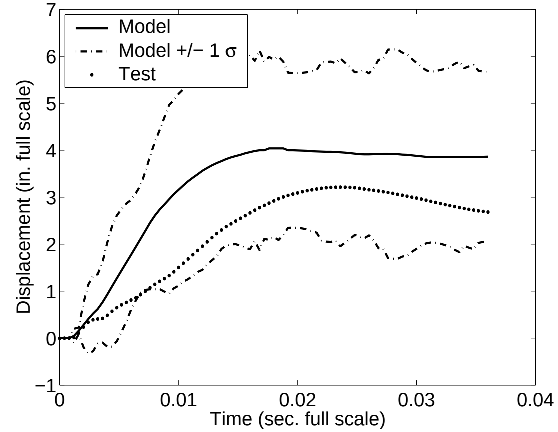
Upper Vertical Quarter Point



Center Point

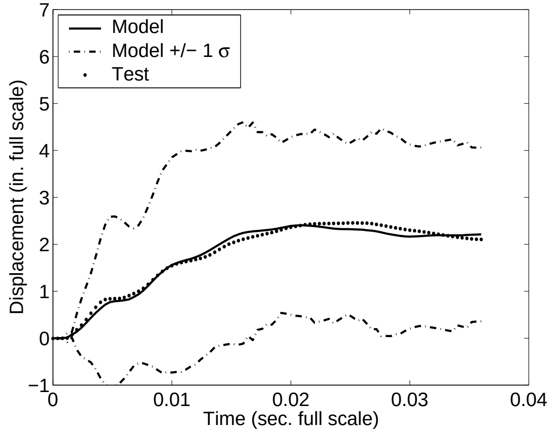


Lower Vertical Quarter Point

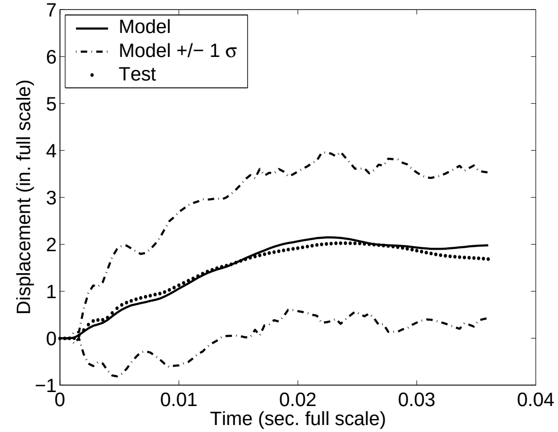


POST-UPDATE PREDICTIVE ACCURACY FOR R/C WALL

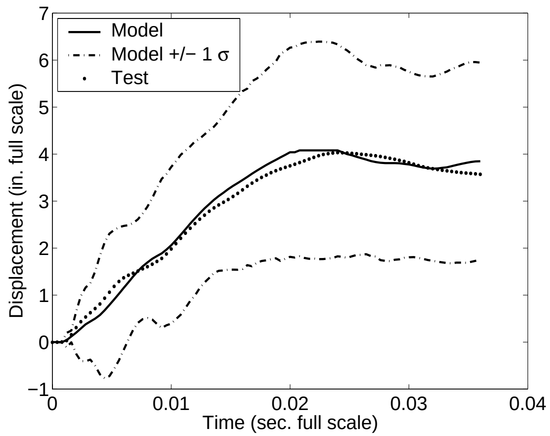
Left Horizontal Quarter Point



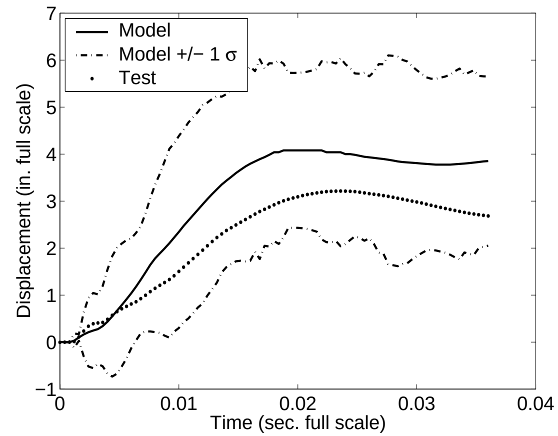
Upper Vertical Quarter Point



Center Point



Lower Vertical Quarter Point



CONCLUSIONS

- Total uncertainty quantification requires
  - A generic class of test-analysis pairs
  - A means of normalizing the differences
  - A method for propagating uncertainty thru the model
- Total uncertainty is more realistic than parametric uncertainty
- Some unresolved questions
  - How are generic classes defined/interpreted?
  - What are the statistical issues involved?
  - Can this approach be made rigorous?
  - Can total uncertainty be used in conjunction with other types of uncertainty quantification to deal with the issue of model uncertainty?