Error Budget for the Validation of Physics-Based Predictive Models

Roger Ghanem
Alireza Doostan
University of Southern California
Los Angeles, California

John Red-Horse
Sandia National Laboratories
Albuquerque, NM

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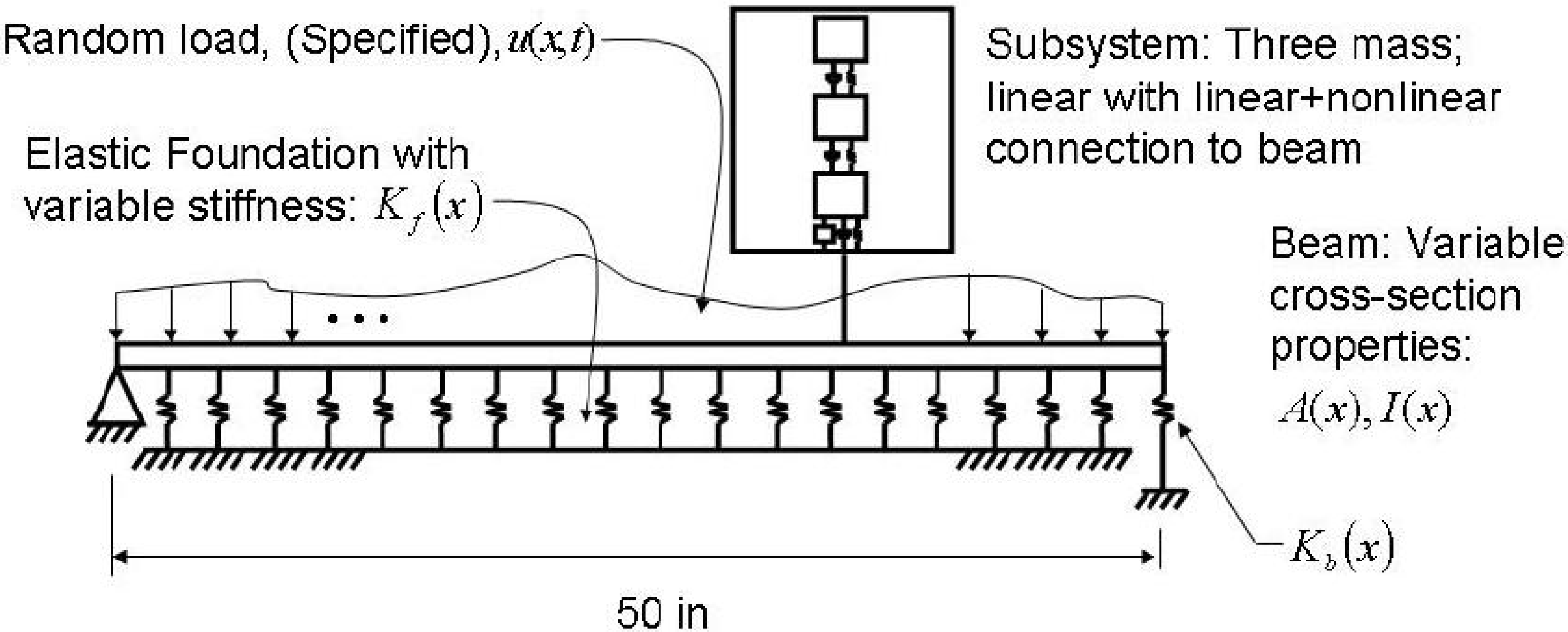
Outline

- Validation philosophy
- Uncertainty representation and estimation
  - Develop intuition on simple problems
- Challenge problem

The Physical Problem

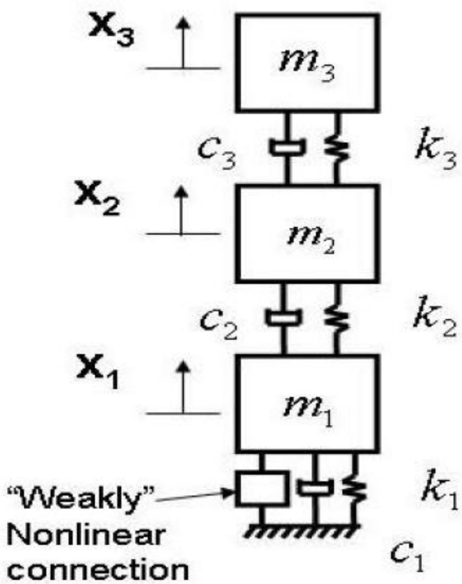
Problem Description:

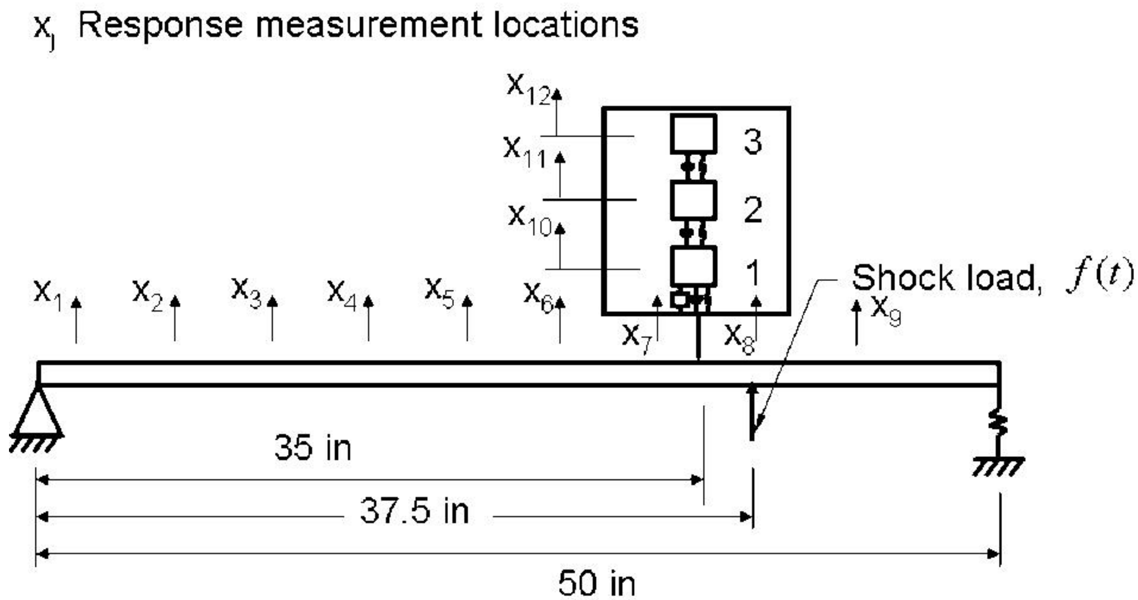


Objective:

Is a linear model valid for representing the weak nonlinearity of the subsystem-to-beam connection?

Validation Procedure





- Subsystem calibration (20 physical specimens, each subjected to three different input excitation)
- Subsystem validation (20 new specimens, each subjected to three new input excitation)
- System Validation (3 physical specimens, each subjected to one input excitation)
- System Accreditation (based on prediction - no data)

Validation philosophy

Given a (physics model, data, and computational resources):

- compute limits on predictability

  i.e. which statements about system performance can be certified

- compute resource allocation (data/computing) along validation path

Given a (physics model - with infinite data/computing resources):

- compute limits on predictability

  i.e. which statements about system performance can be certified

Error budget

$$\mathrm{U} = \hat{\mathrm{U}}|_{h,d,p,m} + \epsilon_h|_{p,d,m} + \epsilon_p|_{d,m} + \epsilon_d|_m + \epsilon_m$$

limit on predictability, given a model

MUST BE QUANTIFIED !!!!

$\epsilon_h|_{d,m}$: can be reduced through better numerics.

$\epsilon_p|_{d,m}$: can be reduced through better statistics.

$\epsilon_d|_m$: can be reduced through better data.

ϵ_m: can be reduced through better models.

Motivation of approach

Package information efficiently for intended purpose:

- propagate information through large scale computational models.
- decide on a path for validation:
  - sensitivity to additional information
  - sensitivity to uncertainty in model components
  - sensitivity to numerical approximations

Representing uncertainty

The random quantities are resolved as surfaces in a normalized space:

$$\alpha(\mathbf{x},\theta) = \sum_{i=1}^{\infty} \alpha_i(\mathbf{x}) \Psi_i(\{\boldsymbol{\xi}(\theta)\})$$

$$\begin{aligned}
\psi_0 &= 1 \\
\psi_1 &= \xi_1 \\
\psi_2 &= \xi_2 \\
\psi_3 &= \xi_1^2 - 1 \\
\psi_4 &= \xi_1 \xi_2 \\
\psi_5 &= \xi_2^2 - 1 \\
\ldots
\end{aligned}$$

Independent random variables

Multidimensional Orthogonal Polynomials

Dimension of vector ξ reflects complexity of α

These could be, for example:

- Parameters in a PDE
- Boundaries in a PDE (e.g. Geometry)
- Field Variable in a PDE

Error budget

$$\mathrm{U} = \hat{\mathrm{U}}|_{h,d,p,m} + \epsilon_h|_{p,d,m} + \epsilon_p|_{d,m} + \epsilon_d|_m + \epsilon_m$$

IF PREDICTION IS OBTAINED USING A WEAK FORM OF SOME GOVERNING EQUATION:

- Joint error estimation is possible, for special cases:
  - infinite-dimesional gaussian measure: Benth et.al, 1998
  - tensorized iid measure: Babuska et.al, 2004
- Joint error estimation is possible, for general measures, using nested approximating spaces (Doostan, Ghanem, Rozovsky, 2006)

Characterization of Uncertainty

$$\alpha(\mathbf{x},\theta) = \sum_{i=1}^{\infty} \alpha_i(\mathbf{x})\Psi_i(\{\xi(\theta)\})$$

- Galerkin Projections
  - Efficient - unsuitable for dependent scales
- Maximum Likelihood
- Maximum Entropy
  - Suitable for data-driven constraints
- Bayes Theorem

Characterize $\alpha_i(x)$ as random variables

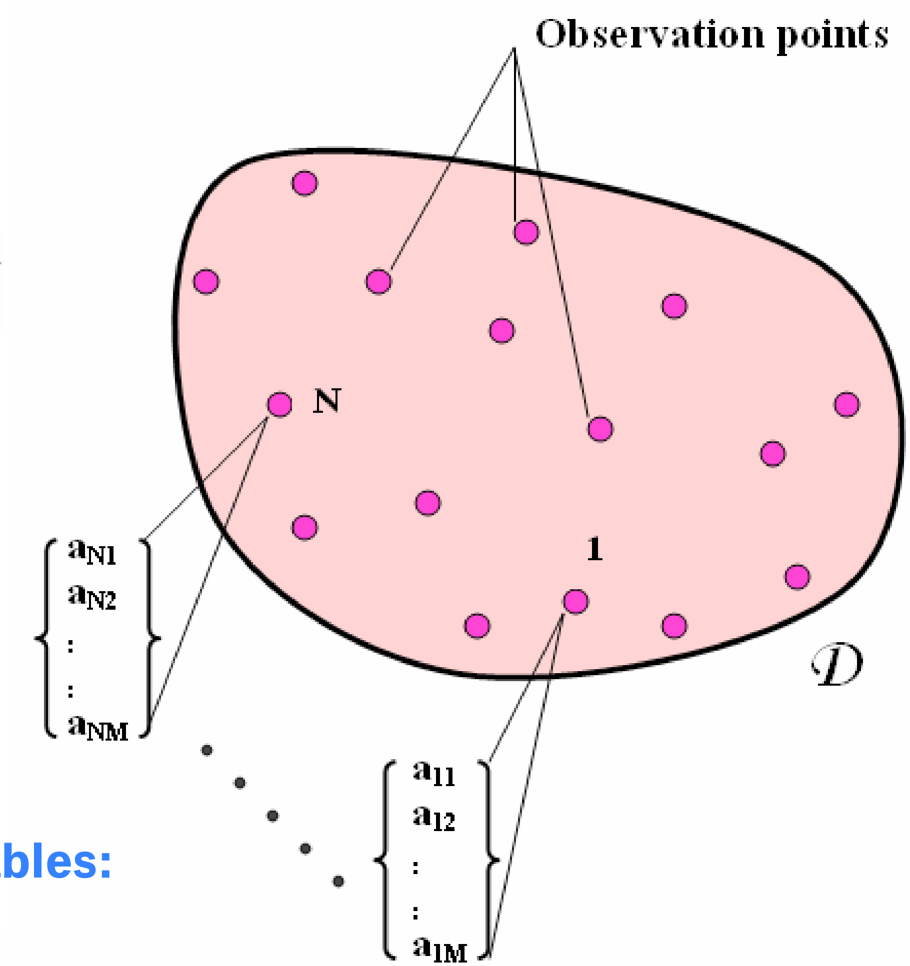
Representing uncertainty

Starting with observations of process over a limited points on the domain:

Reduced order representation:

$$a(\theta) \approx \bar{a} + \sum_{i=1}^{\mu} \sqrt{\lambda_i}\eta_i(\theta)\phi_i$$

$$\begin{cases} \eta_i^{(j)} = \dfrac{1}{\sqrt{\lambda_i}}\langle a^{(j)} - \bar{a}, \phi_i\rangle_{l_2}, & j = 1, \cdots, M \\ E[\eta_i] = 0 & \\ E[\eta_i\eta_j] = \delta_{ij} & i, j = 1, \cdots, \mu \end{cases}$$



Polynomial representation of KL variables:

$$\eta_i(\theta) = \sum_{j=1}^{p} \gamma_j^{(i)}\psi_j(\xi_i), \quad i = 1, \cdots, \mu \qquad \xi_i \sim N(0,1) \quad i.i.d$$

Characterizing Uncertainty
Maximum Likelihood Estimation

Physical object: Linear Elasticity

Convergence as function of "dimensionality"

Stochastic parameters

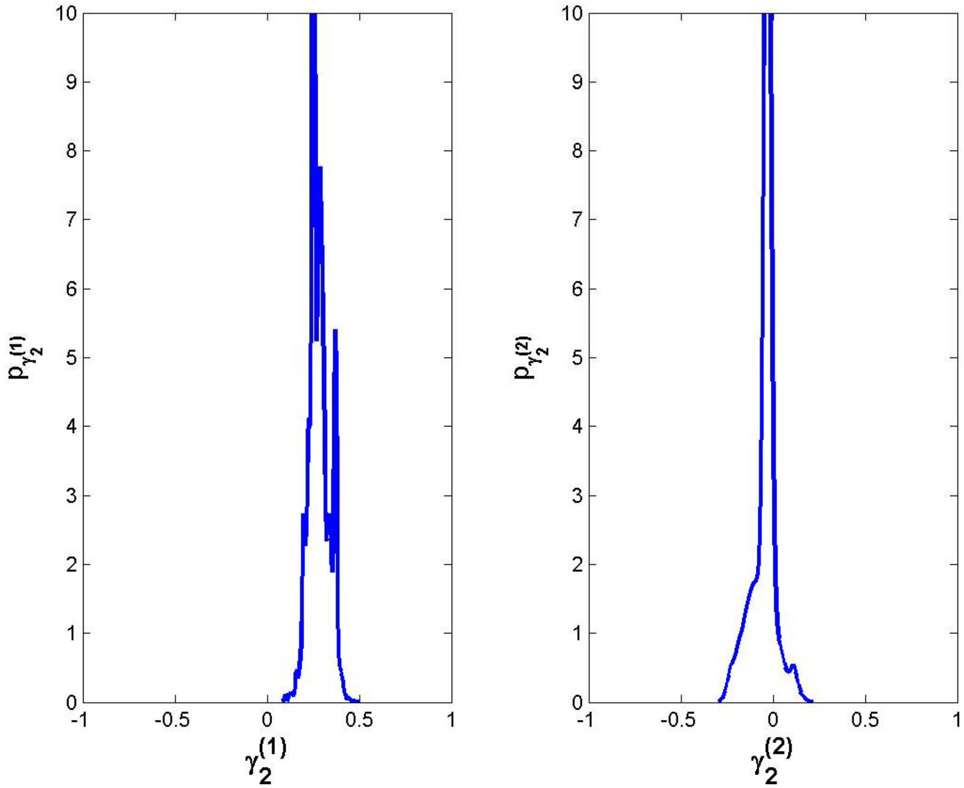
Beam with random heterogeneous material properties.

Observe realizations of system response

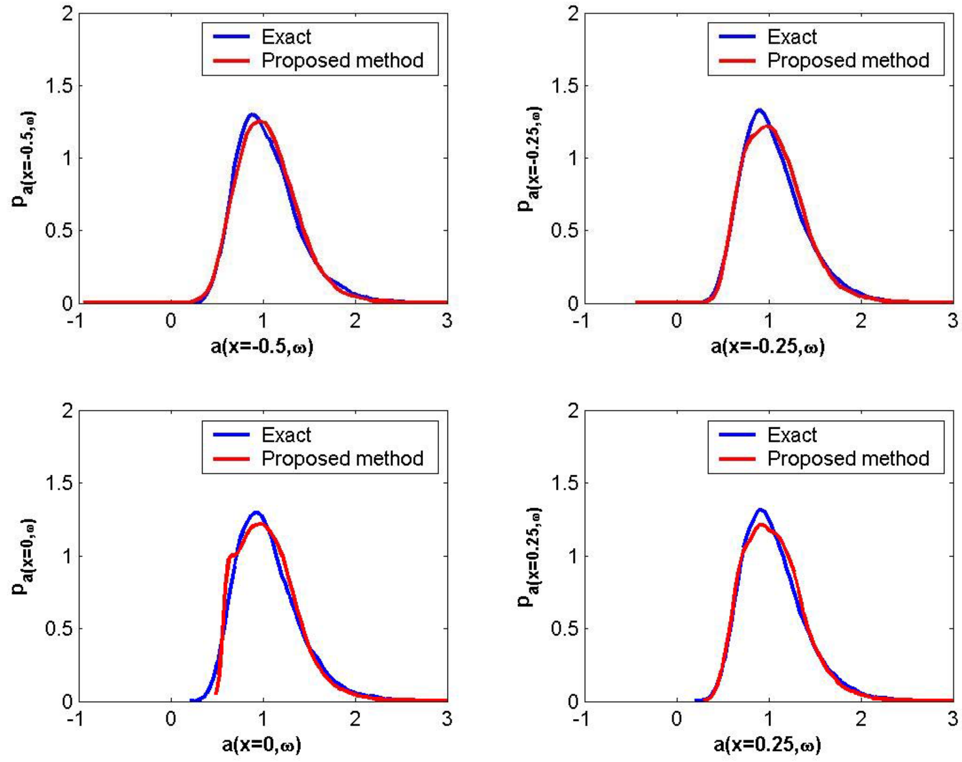
$$\alpha(\mathbf{x},\theta) = \sum_{i=1}^{\infty} \alpha_i(\mathbf{x})\Psi_i(\{\xi(\theta)\})$$

Reference: Desceliers, Ghanem amd Soize, , IJNME, 2006.

Characterization of Uncertainty:
Bayesian Inference



Posterior distributions of coefficients in polynomial Expansion η_i of

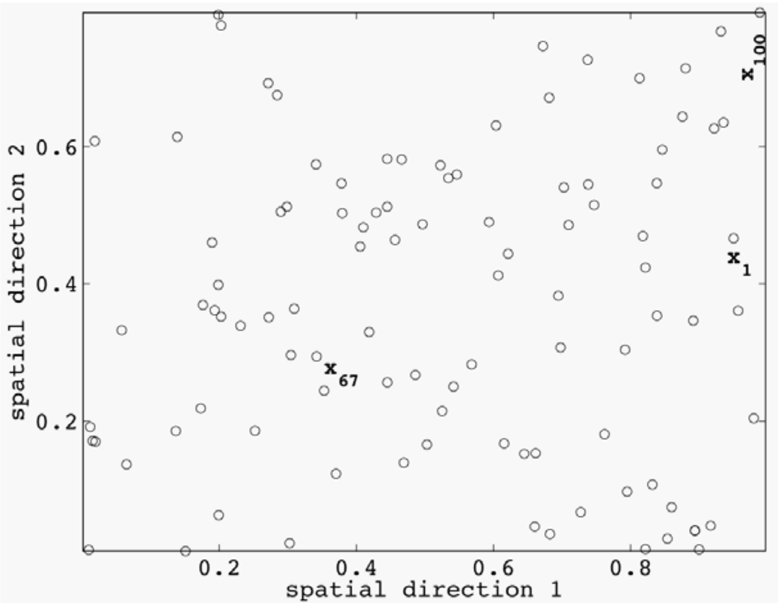


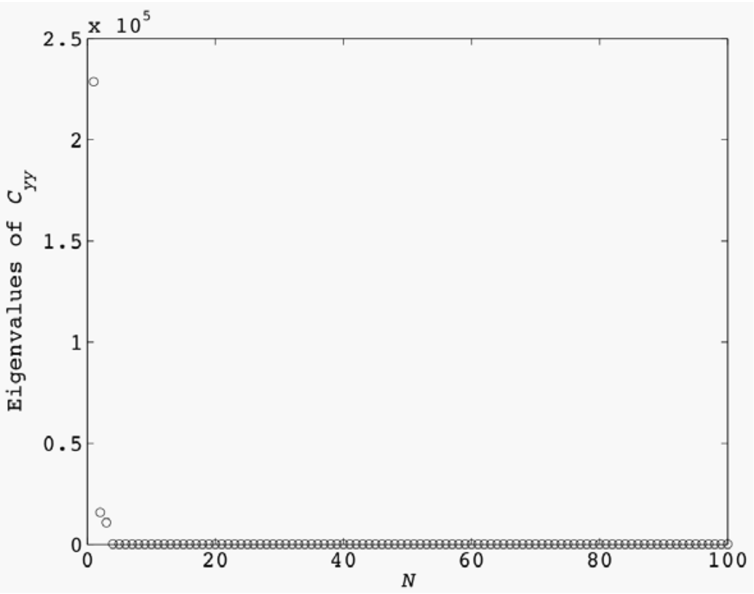
Distribution of the recovered process:

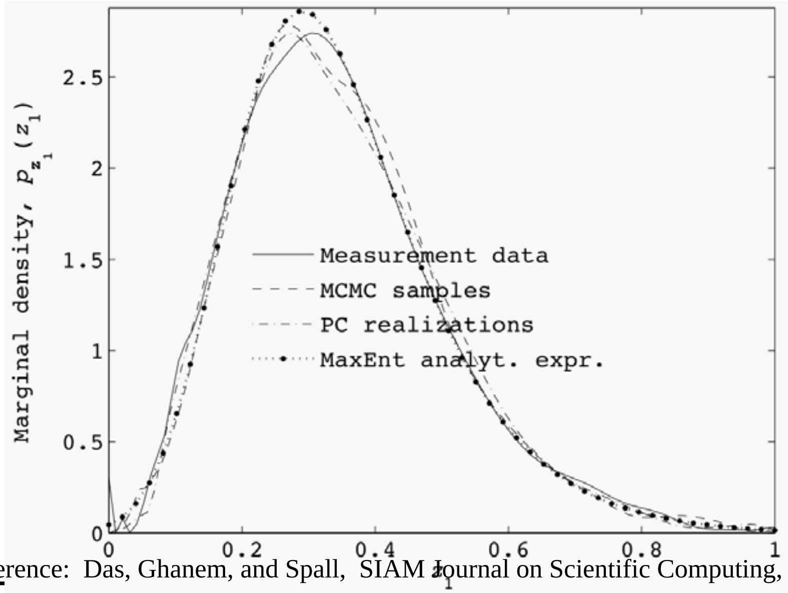
$$\approx \bar{a} + \sum_{i=1}^{\mu} \sqrt{\lambda_i}\,\eta_i(\omega)\phi_i$$

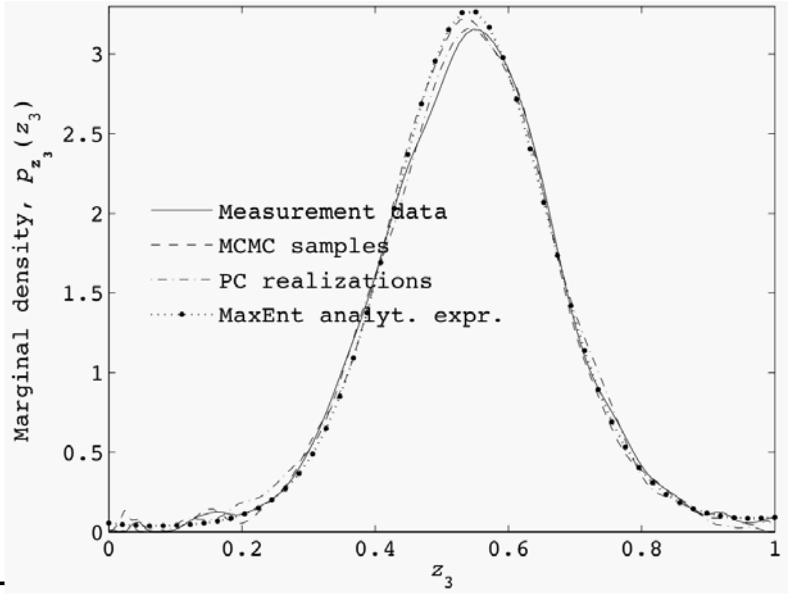
Reference: Doostan and Ghanem, , Journal of Computational Physics, 2006.

Characterization of Uncertainty:
Maximum Entropy Estimation with Moment Constraints









Reference: Das, Ghanem, and Spall, SIAM Journal on Scientific Computing, 2006.

Characterization of Uncertainty

Maximum Entropy Estimation / Spatio-Temporal Processes

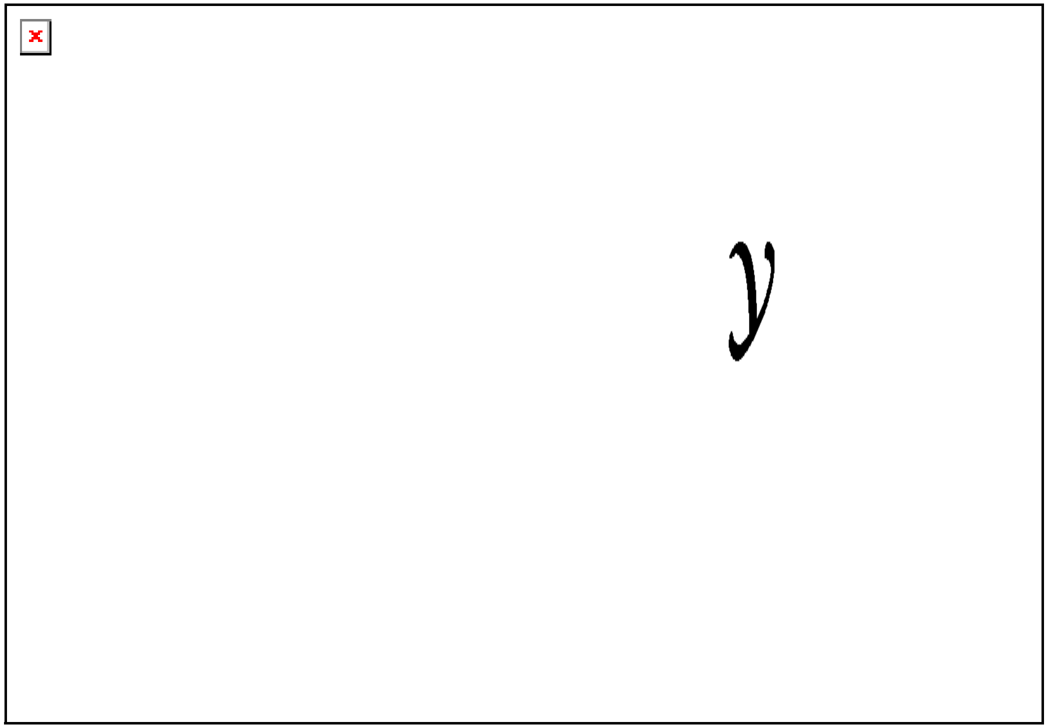
Temperature time histories, $\mathbf{T}(z, t)$, at various depths.

Characterization of Uncertainty

Maximum Entropy Estimation with Histogram Constraints

- Reduced order model of → $\eta, \quad \dim(\eta) = M = 23$

KL expansion



A typical plot of marginal pdf for a Karhunen-Loeve variable.

Spearman Rank Correlation Coefficient is also matched:

$$100 \frac{\left(\| [\rho_s^{(PC)}] - [\hat{\rho}] \| \right)}{\| [\hat{\rho}] \|}$$

$$= 0.5743\%$$

Reference: Das, Ghanem, Finette, , Journal of Geophysical Research, 2006.

Uncertainty modeling for system parameters

Approximate asymptotic representation:

$$\sqrt{M}(\tilde{\gamma} - \hat{\gamma}) \xrightarrow{\text{dist}} N(0, \hat{J}(\hat{\gamma})^{-1})$$

Representation on the set of observation:

$$\hat{\boldsymbol{a}} = \bar{\boldsymbol{a}} + \sum_{i=1}^{\mu} \sqrt{\lambda_i} \left(\sum_{j=1}^{p} \tilde{\gamma}_j{}^{(i)} \bar{\psi}_j(\xi_i) \right) \boldsymbol{\phi}_i$$

Remark: Both intrinsic uncertainty and uncertainty due to lack of data are represented.

Representation smoothed on the whole domain:

$$\hat{a}(x, \omega) = \tilde{\bar{a}}(x) + \sum_{i=1}^{\mu} \sqrt{\lambda_i} \left(\sum_{j=1}^{p} \tilde{\gamma}_j{}^{(i)} \bar{\psi}_j(\xi_i) \right) \tilde{\phi}_i(x)$$

Remark: $\tilde{\gamma}$ is formulated by spectral decomposition of $\hat{J}(\hat{\gamma})^{-1}$.

Additional information and sensitivity analysis

Important remarks:

- Asymptotically, the total uncertainty reduces to intrinsic uncertainty.
- Contribution of uncertainty due to limited information could be separated from that of the intrinsic uncertainty both at parameter level and response level.
- Sensitivity of the statistics of SRQ to parameters of $\tilde{\gamma}$ can be quantified.

CDF of system parameters: m_1, c_1, k_1

Estimate

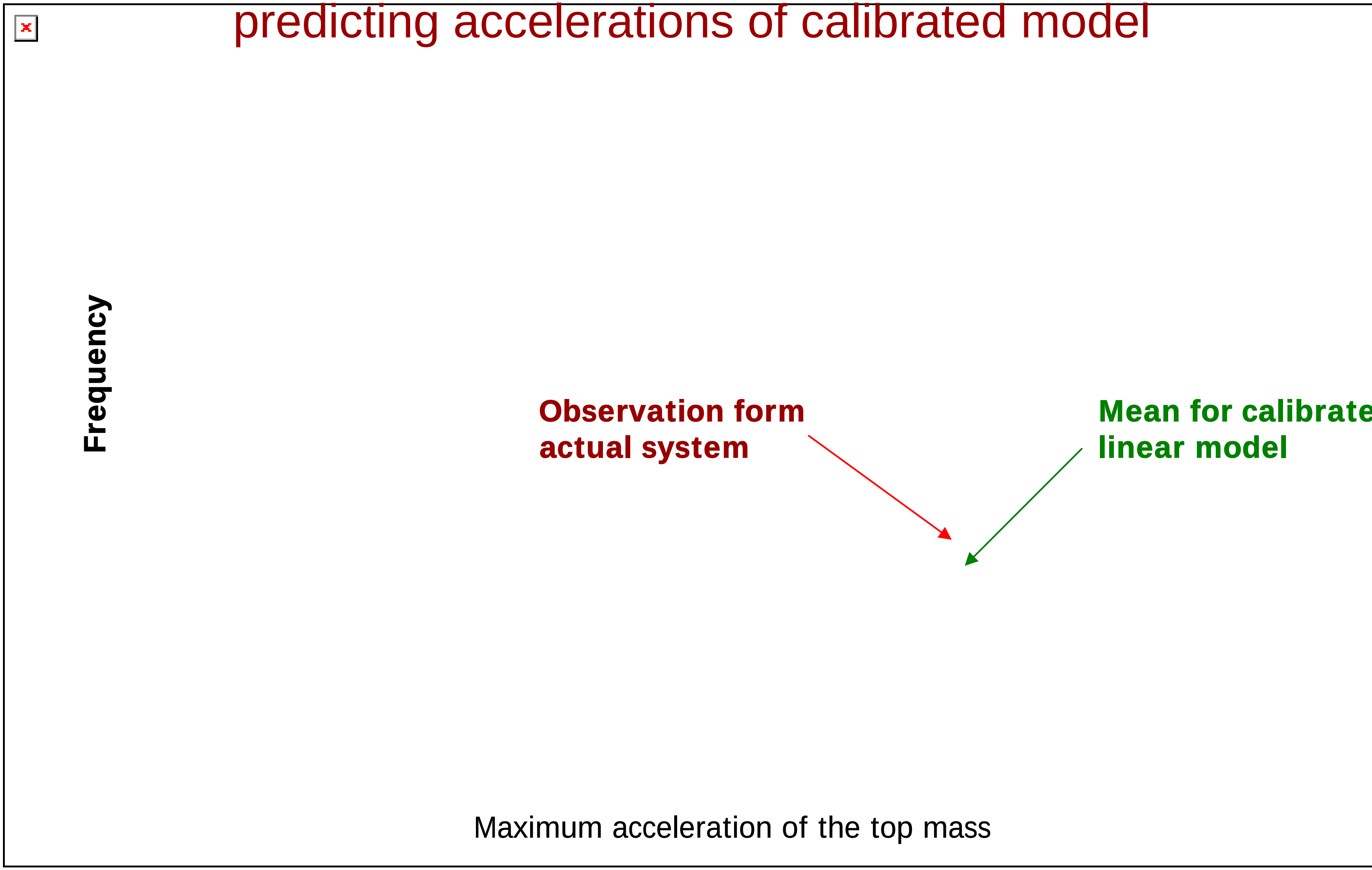
%95 probability box

Remarks:

- Confidence intervals are due to finite sample size.

Model accuracy

predicting accelerations of calibrated model



Calibration Excitation = Low

Validation path: hypothesis test

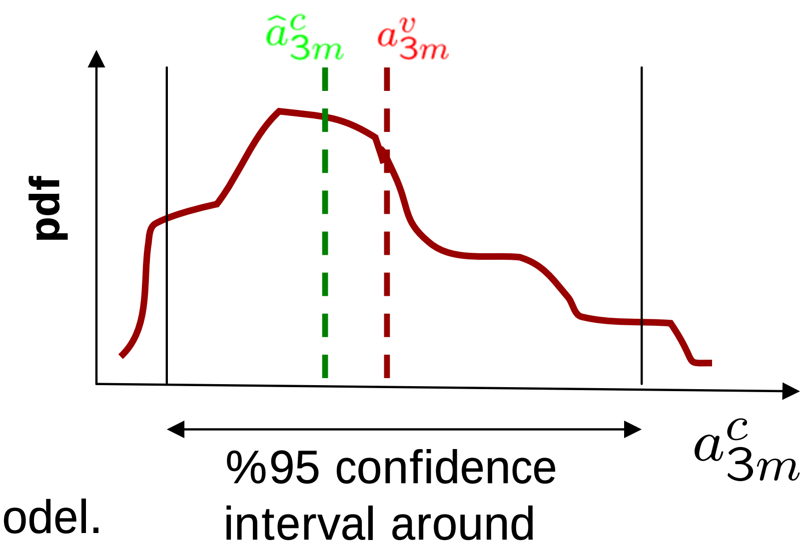
System Response Quantity (SRQ):

Maximum acceleration of the top mass = $\mathbf{a_{3m}}$

Propagation using calibrated stochastic linear model:

Equivalent hypothesis test:

$$H_0 : \hat{a}_{3m}^c = a_{3m}^v$$



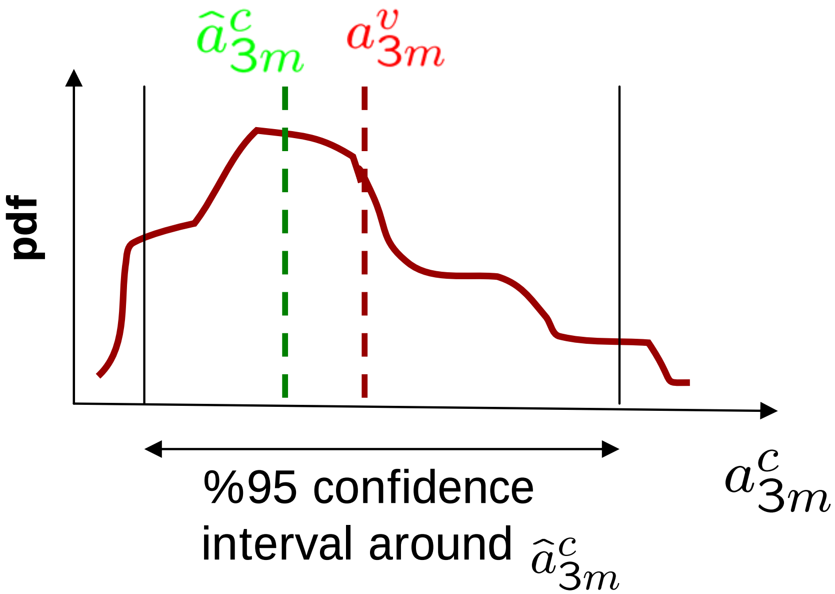
Remark:

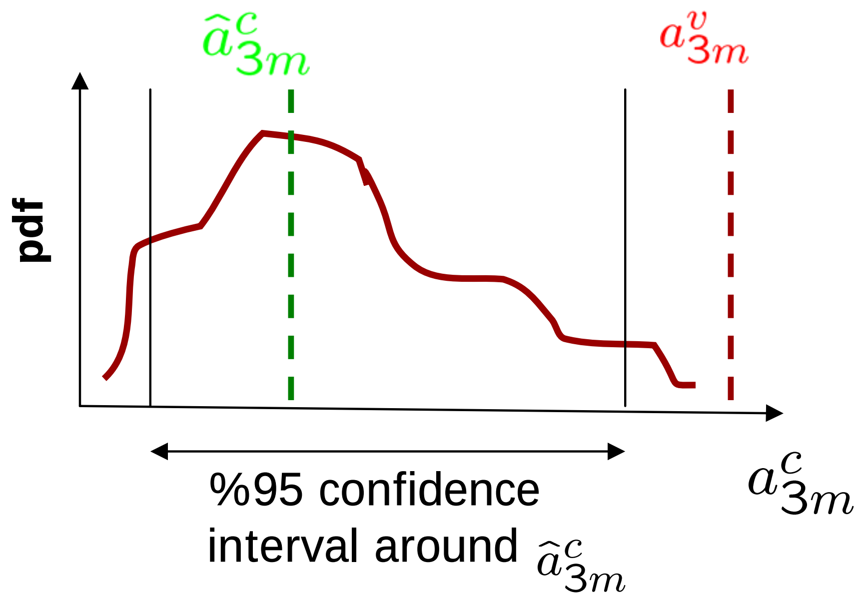
Parameters are calibrated under H_0 .

$\hat{a}_{3m}^c$ = mean of predicted a_{3m}^c from linear model.

Validation path: hypothesis test

Possible scenarios: Repeat for all validation data





No sufficient evidence to reject H_0

H_0 is rejected

Therefore:

Validation metric: $d = |\hat{a}^c_{3m} - a^v_{3m}|$

Typical subsystem validation result

a^v_{3m} $\hat{a}^c_{3m}$

Calibration Excitation = Medium

Validation Excitation = High

Frequency

a^c_{3m}

Typical subsystem validation result

neglecting effect of finite sample

a^{v}_{3m} $\hat{a}^{c}_{3m}$

Calibration Excitation = Medium

Validation Excitation = High

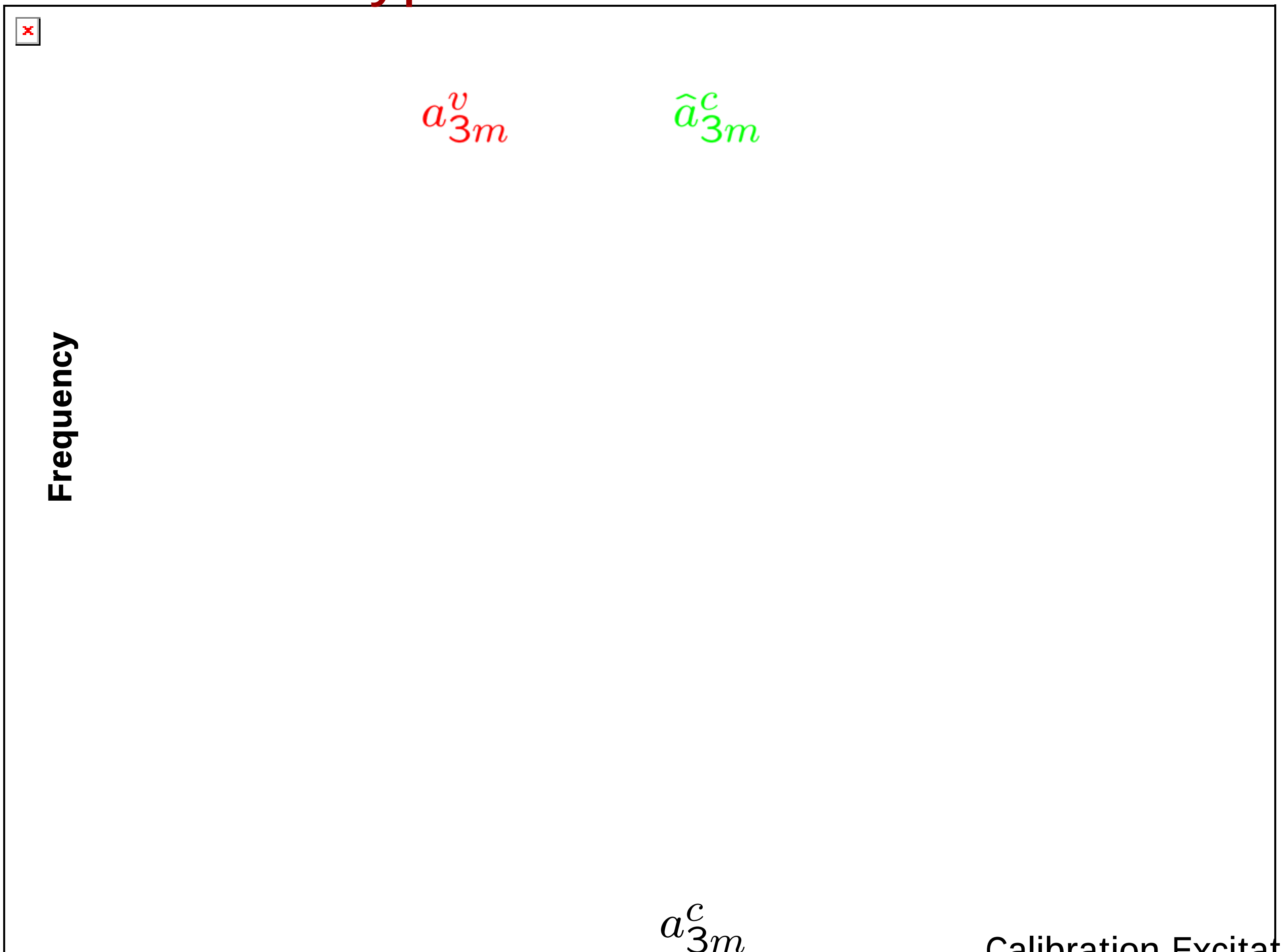
Frequency

a^{c}_{3m}

Subsystem validation outcome

Calibration Based On Excitation Level	Validation Excitation Level	Hypothesis
Low	Low	Accepted
	Medium	Accepted
	High	Accepted
Medium	Low	Accepted
	Medium	Accepted
	High	Accepted
High	Low	Accepted
	Medium	Accepted
	High	Accepted

Typical accreditation result



Calibration Excitation = Medium

Accreditation Excitation = 2

System accreditation outcome

Calibration Based On Excitation Level	Accreditation Excitation Number	Hypothesis
Low	1	Accepted
	2	Accepted
	3	Accepted
Medium	1	Accepted
	2	Accepted
	3	Accepted
High	1	Accepted
	2	Accepted
	3	Accepted

Prediction on target application

$$P_{am} := \text{Prob}\left\{\max_{t>0} |a(t)| > 1.8(10^4) in/sec^2\right\} < 10^{-2}$$

Calibration Based On Excitation Level	Sample Mean of P_{am}	Sample Variance of P_{am}
Low	0.0835	0.000830
Medium	0.0662	0.001500
High	0.1269	0.004300

Remark: Based on only 25 samples.

Conclusion

- Suitable Uncertainty Quantification can provide an integrated path for model validation.