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LA-UR- 03-2425

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Title: ESTIMATING THE ERROR IN SIMULATION PREDICTION OVER THE DESIGN SPACE (U)

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Submitted to: LANL Uncertainty Quantification Working Group (UQWG)
Los Alamos National Laboratory, Los Alamos, New Mexico
August 27, 2002

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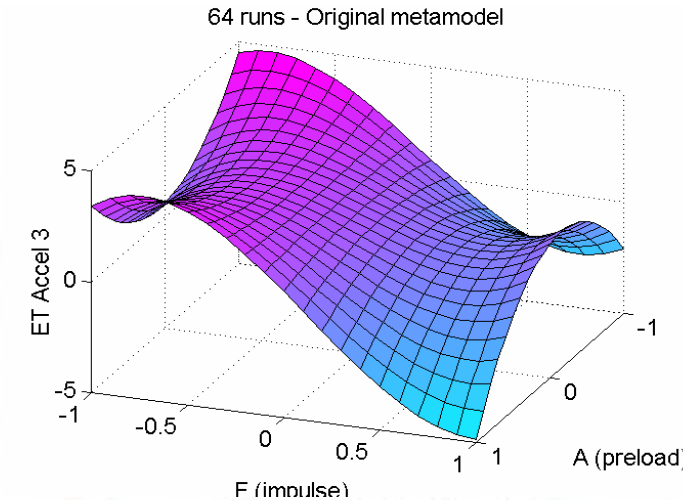
ESTIMATING THE ERROR IN SIMULATION PREDICTION OVER THE DESIGN SPACE (U)



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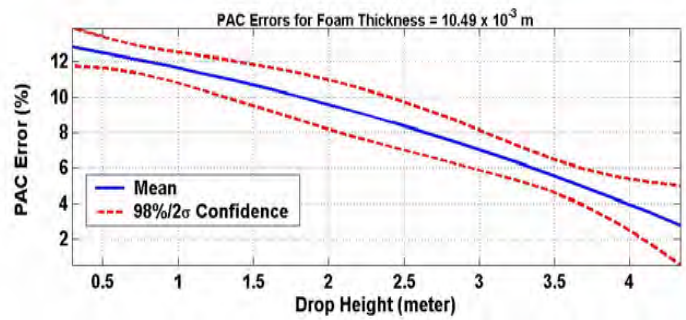

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Abstract

Estimating the Error in Simulation Prediction Over the Design Space (U)

This study addresses the assessment of accuracy of simulation predictions. A procedure is developed to validate a simple non-linear model defined to capture the hardening behavior of a foam material subjected to a short-duration transient impact. Validation means that the predictive accuracy of the model must be established, not just in the vicinity of a single testing condition, but for all settings or configurations of the system. The notion of validation domain is introduced to designate the design region where the model's predictive accuracy is appropriate for the application of interest. Techniques brought to bear to assess the model's predictive accuracy include test-analysis correlation, calibration, bootstrapping and sampling for uncertainty propagation and metamodeling. The model's predictive accuracy is established by training a metamodel of prediction error. The prediction error is not assumed to be systematic. Instead, it depends on which configuration of the system is analyzed. The study shows how predictive accuracy can be assessed even in the presence of a calibrated model by calibrating to one point in the design space, then assessing with respect to experimental data elsewhere in the design space. Finally, the prediction error's confidence bounds are estimated by propagating the uncertainty associated with specific modeling assumptions.

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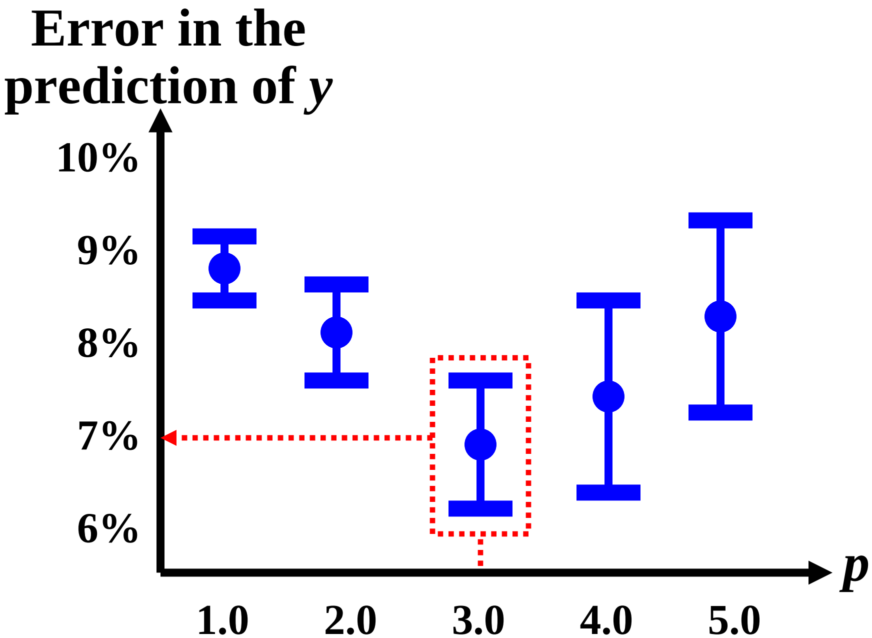
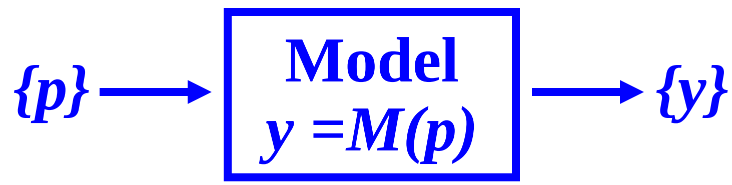
Motivation

- **The motivation of this work is the development of tools for Verification and Validation (V&V) because our objective is to make decisions based on *validated* simulations.**
- **A key component of V&V is the assessment of predictive accuracy.**
- **Example: Bill Press is asking us to demonstrate that our "science-based predictions" are *credible*.**
- **Example: What are the benefits in terms of improving the confidence in our simulations of performing another test?**

Illustration

- **What do we mean by “assessing the predictive accuracy” of a numerical simulation?**





“For the setting of p=3, we can predict y with an expected accuracy of 7% +/- 1%, at the significance level of 96%.”

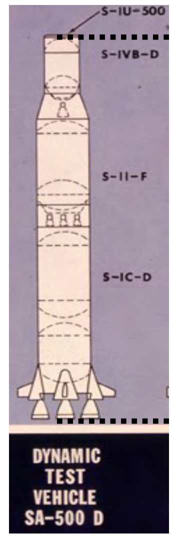
- **Prediction accuracy includes the assessment of the sources of uncertainty and *lack-of-knowledge*.**

Why Do We Make Assumptions?

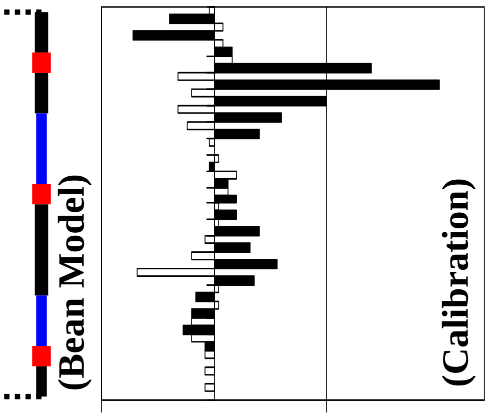
- Assumptions enable model-building.

Reality of Interest

Conceptual Model



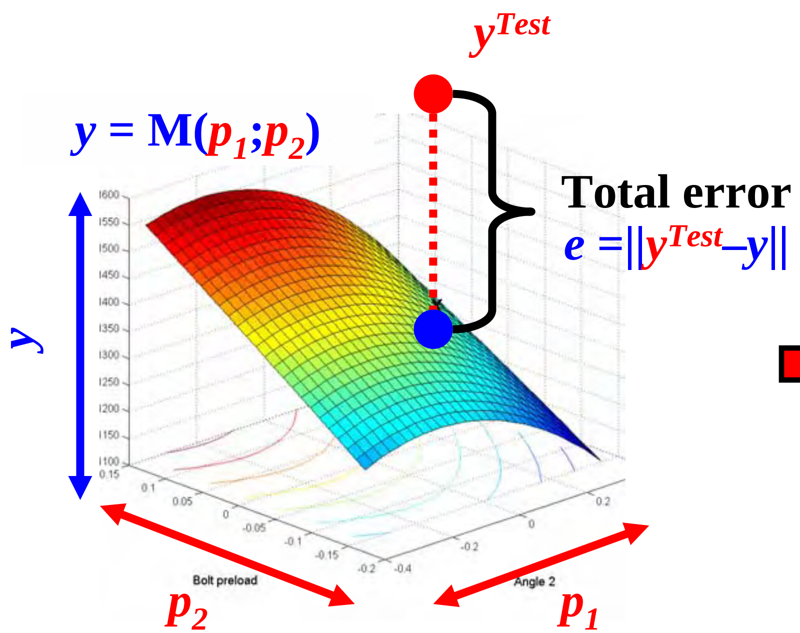
Computational Model

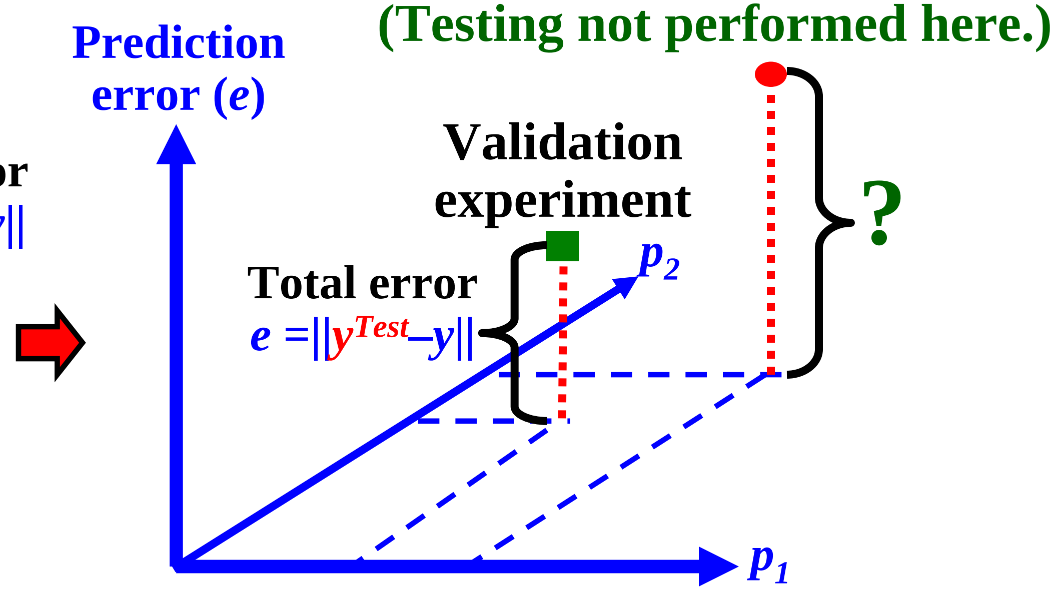


(From Collins, Hasselman & al., AIAA Journal, 1974.)

- Modeling assumptions ***reduce*** the uncertainty! It may result into a false sense of confidence in the predictions.
- The extent to which modeling assumptions influence the predictions and decisions must be quantified.

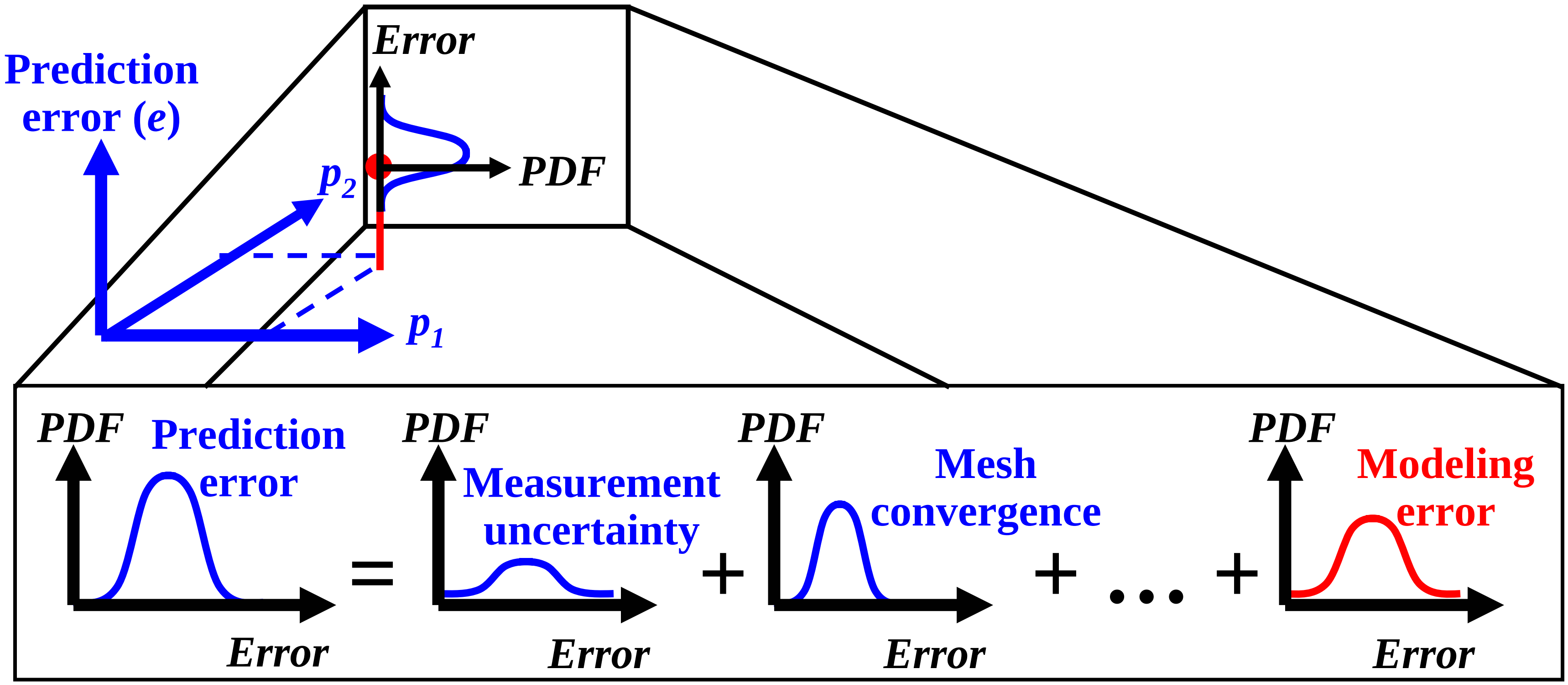
The First Step is the Definition of the Domain of Validation





- **Prediction errors must be estimated through the design space, including in regions where physical experiments are *not* available.**

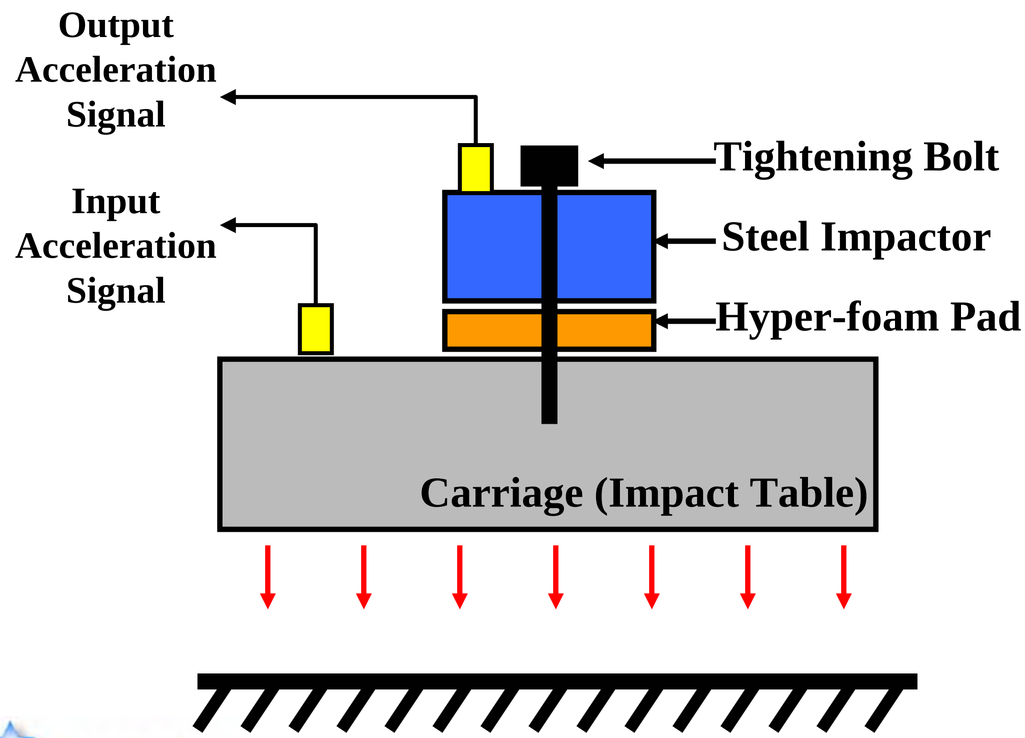
The Second Step is the Assessment of Uncertainty From Modeling Assumptions

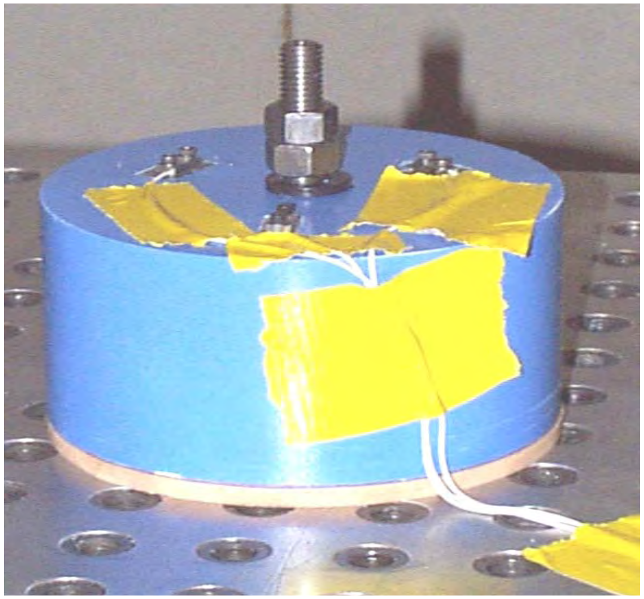


- The uncertainty introduced by the modeling assumptions (or *modeling error*) must be assessed and quantified.

Hyper-foam Impact Experiments

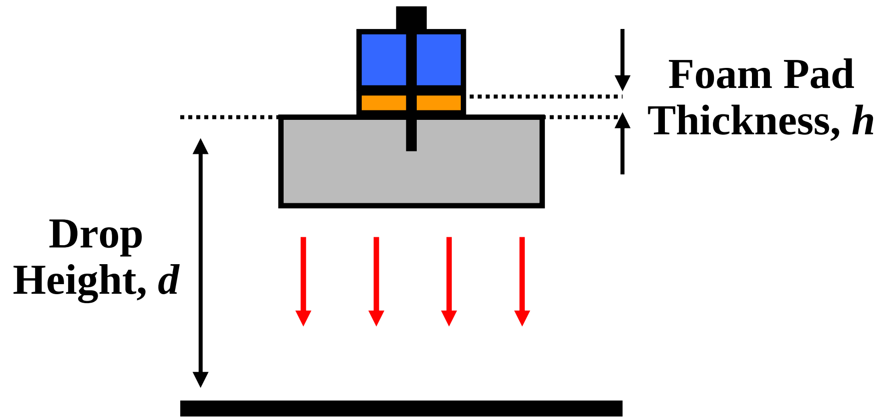
- **Physical experiments are performed to study the propagation of an impact through an assembly of metallic and crushable (foam pad) components.**

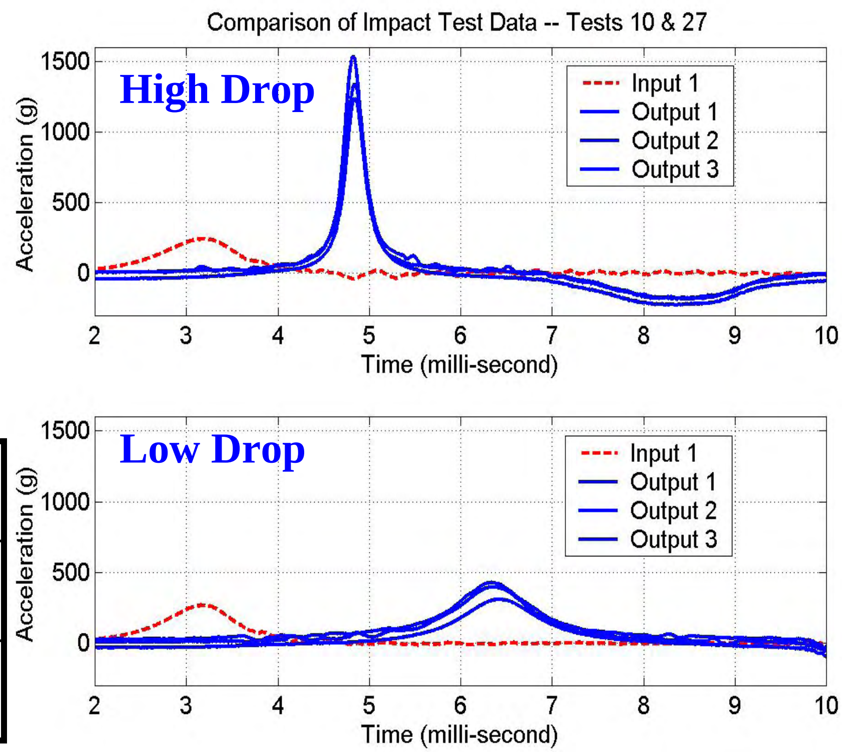




Configurations Tested

- **Several configurations of the system are tested by varying the foam pad thickness (*h*) and drop height (*d*).**



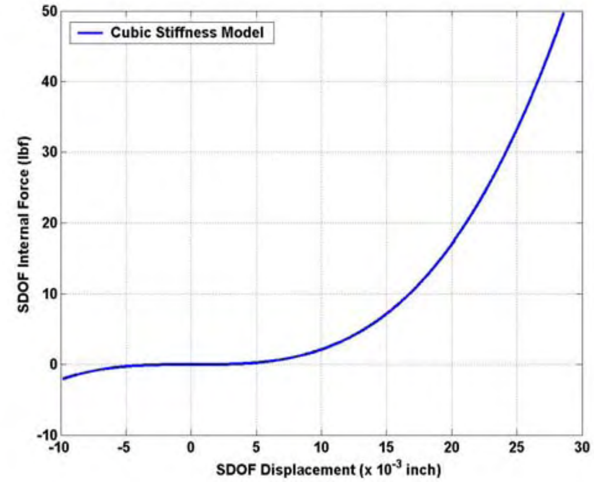


	Low Drop (*d*=13", 0.3 m)	High Drop (*d*=155", 4.0 m)
Thin Layer (*h*=0.25", 6.3 mm)	10 Replicates	5 Replicates
Thick Layer (*h*=0.50", 12.6 mm)	10 Replicates	5 Replicates

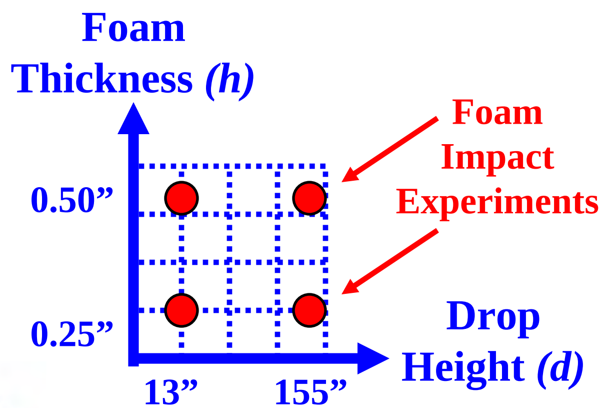
The Domain of Validation

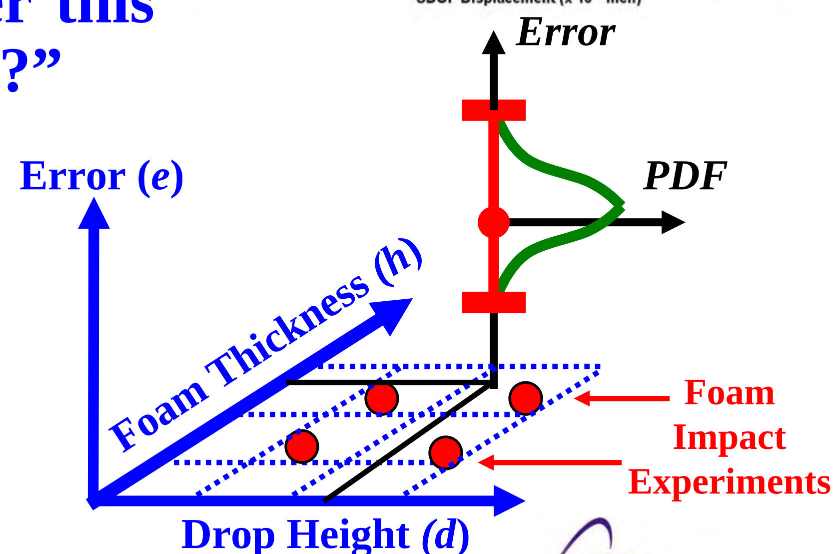
- **The crushing behavior of the foam material is represented by a 1D strain-stress constitutive equation.**

$$F(x(t)) = k_{nl}(x(t))^q$$



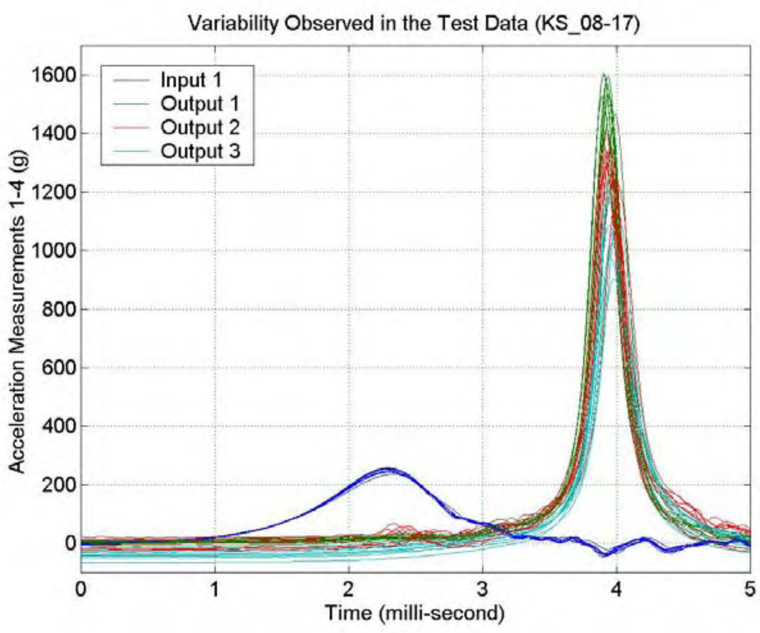
- **"How good is this model over this range of operating conditions?"**

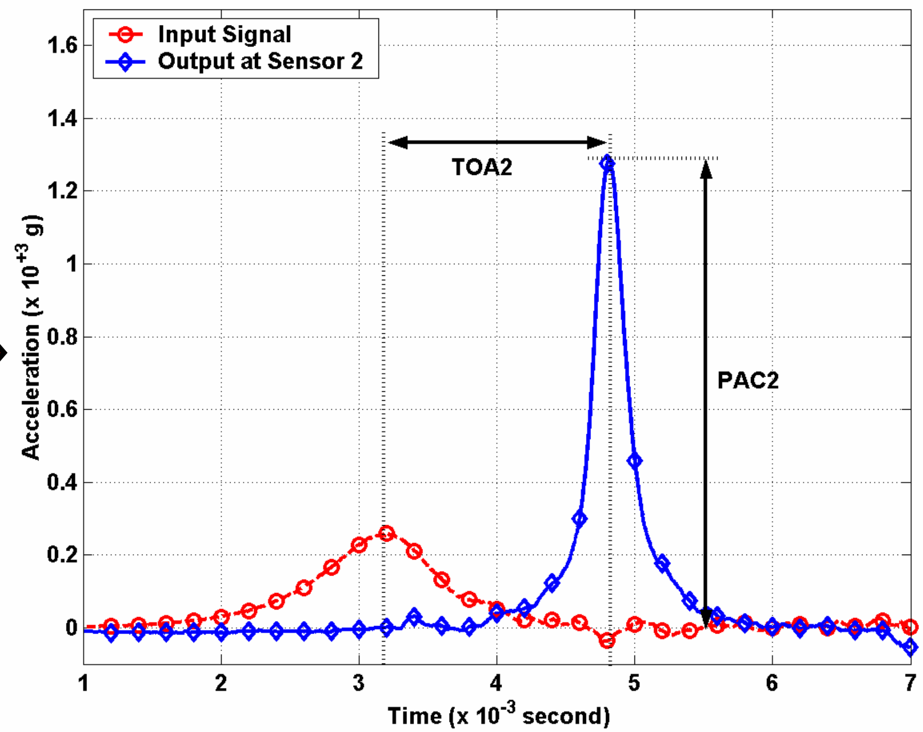




Response Features

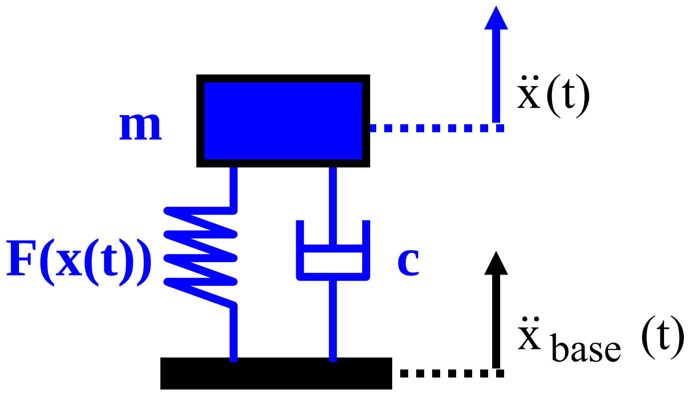
- The response features of interest are the peak acceleration (*PAC*) and the time-of-arrival (*TOA*) at output sensor 2.





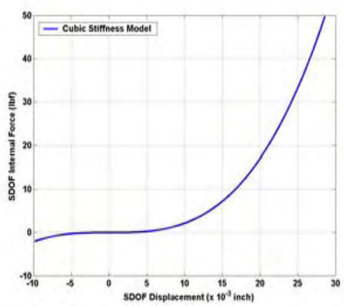
Single Degree of Freedom Modeling

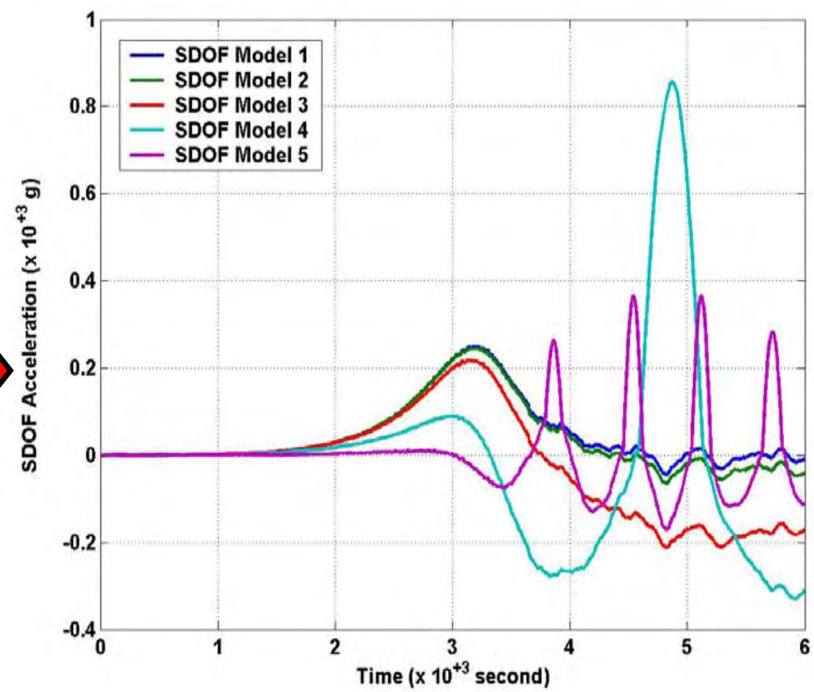
- **A single degree-of-freedom (SDOF) oscillator is developed to predict the features *PAC* and *TOA* without describing the crushable foam and dynamics with high-fidelity.**



$$m\ddot{x}(t)+c\dot{x}(t)+F(t)=m\ddot{x}_{base}(t)$$

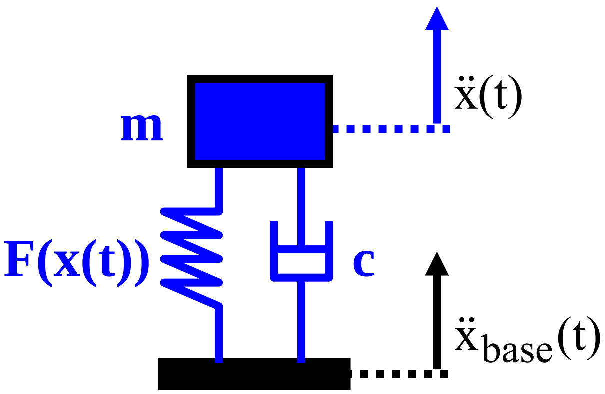
$$F(x(t))=k_{nl}(x(t))^q$$



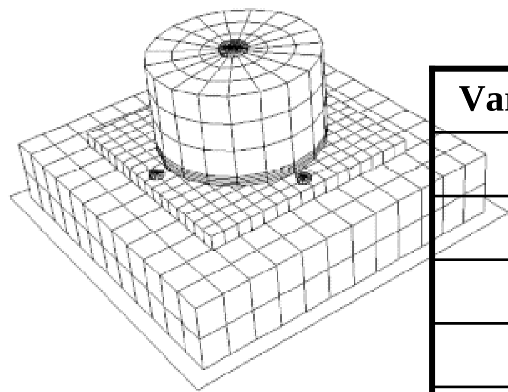


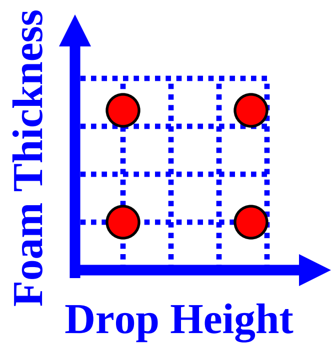
Dimensionality

- **The dimensionality of the problem remains 2D, no matter which numerical simulation is implemented.**



Variable	Description
1	Foam Thickness (inch)
2	Drop Height (inch)
3	Damping (lbf sec/inch)
4	Stiffness (lbf/inch^q)
5	Exponent (unitless)

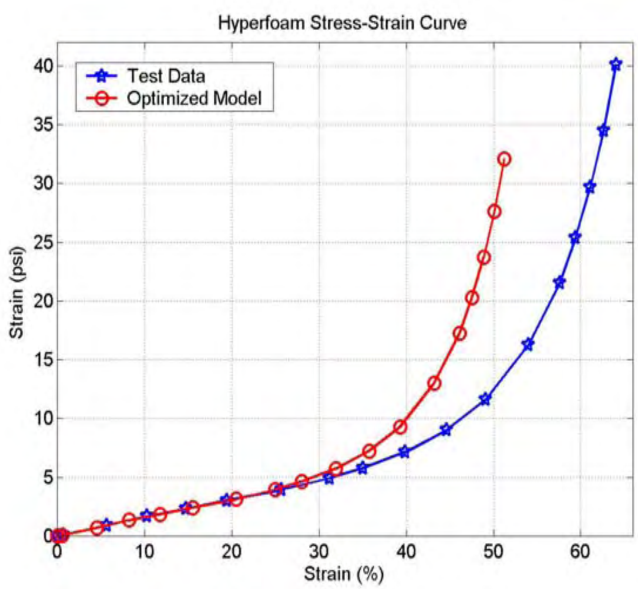




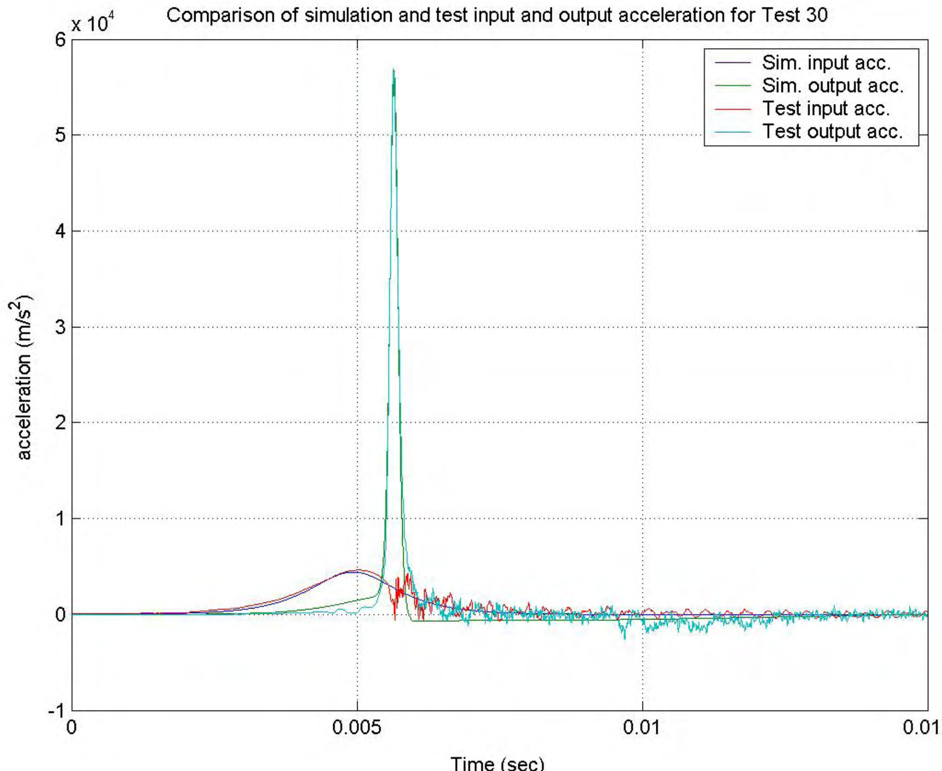
Variable	Description
1	Foam Thickness (inch)
2	Drop Height (inch)
3	Tilt Angle 1 (degree)
4	Tilt Angle 2 (degree)
5	Bolt Preload (psi)
6	Stress Scaling (unitless)
7	Strain Scaling (unitless)
8	Input Scaling (unitless)
9	Friction (unitless)
10	Bulk Viscosity (unitless)

Calibration

- **Material model parameters are calibrated by optimizing a multivariate T-test statistics of test-analysis correlation.**



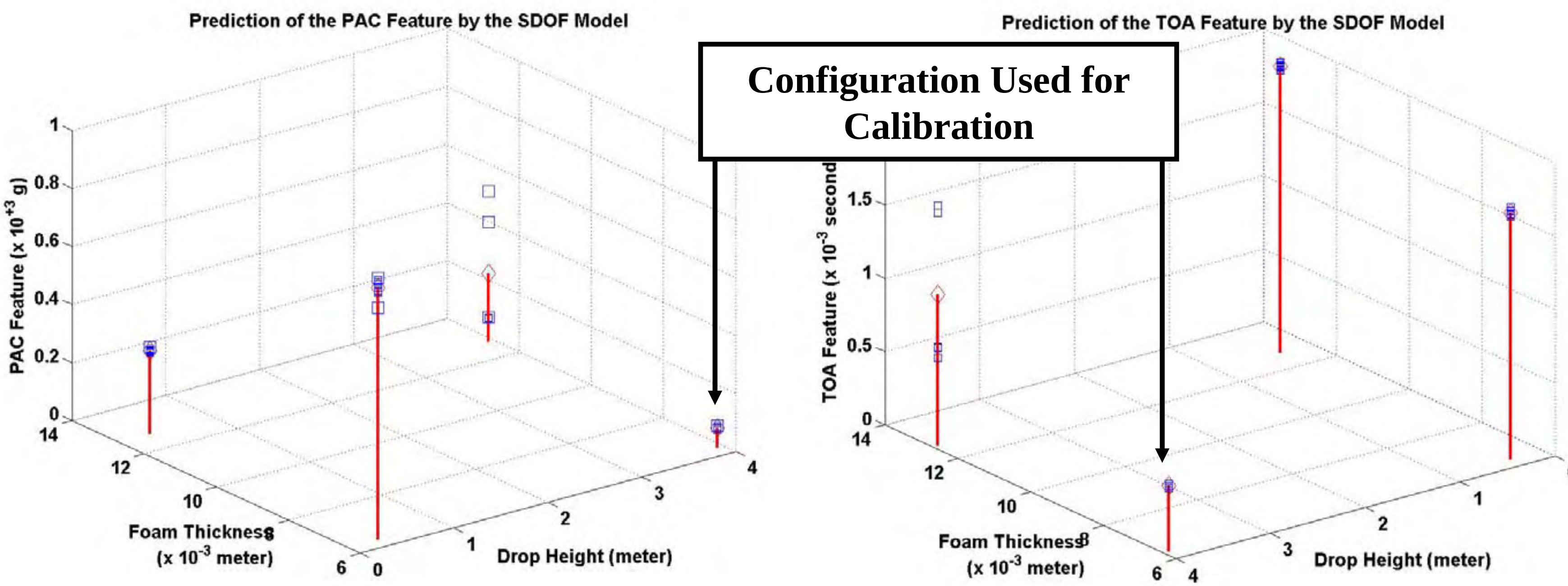
Calibrated Strain-stress Curve



Post-calibration Correlation

Prediction Errors Are Estimated at Discrete Locations in the Design Space

- **The material model $F = k_{nl}\, x^q$ is calibrated w.r.t. settings *(h=¼”; d=13”)*, then used to predict other configurations.**



Prediction of *PAC* Features **Prediction of *TOA* Features**

Prediction Errors Are Extrapolated Throughout the Design Space

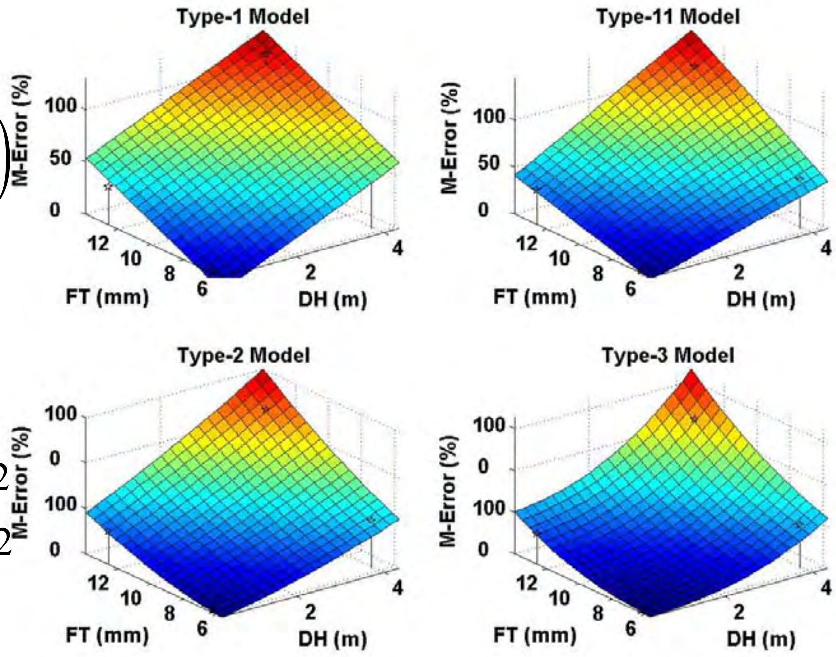
- **The prediction errors are extrapolated over the design space using a family of polynomial metamodels.**

– **Definition of prediction errors:**

$$e(h;d) = \left(y^{Test} - y(h;d)\right)^T S_{yy}^{-1} \left(y^{Test} - y(h;d)\right)$$

– **Family of metamodels:**

$$\begin{cases} e(h;d) = c_1 + c_2 h + c_3 d \\ e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd \\ e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd + c_5 h^2 + c_6 d^2 \\ e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd + c_5 h^2 + c_6 d^2 \\ \qquad + c_7 dh^2 + c_8 hd^2 + c_9 h^3 + c_{10} d^3 \end{cases}$$

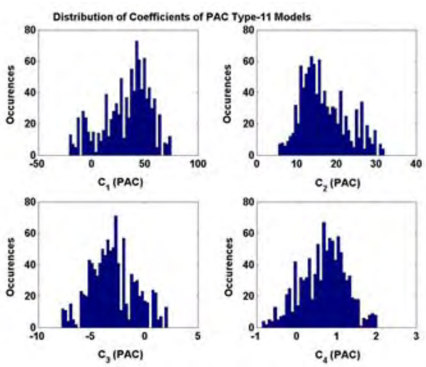


Criticism

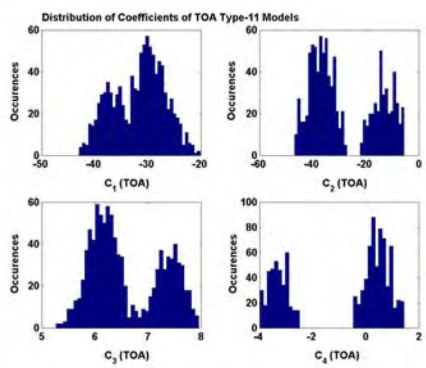
- Calibration can be useful, but it generally does not assess whether a numerical model can be used with *confidence*.
- Experimental variability has not been accounted for.
- The functional form of the prediction error metamodels has been assumed …
- … So are the material model, initial condition, physical modeling, parameter calibration values, and loading.
- The effect of these assumptions must be quantified.

Effect of Experimental Variability

- **The data features y^{Test} are bootstrapped from the available replicate impact tests for each configuration *(h;d)*.**



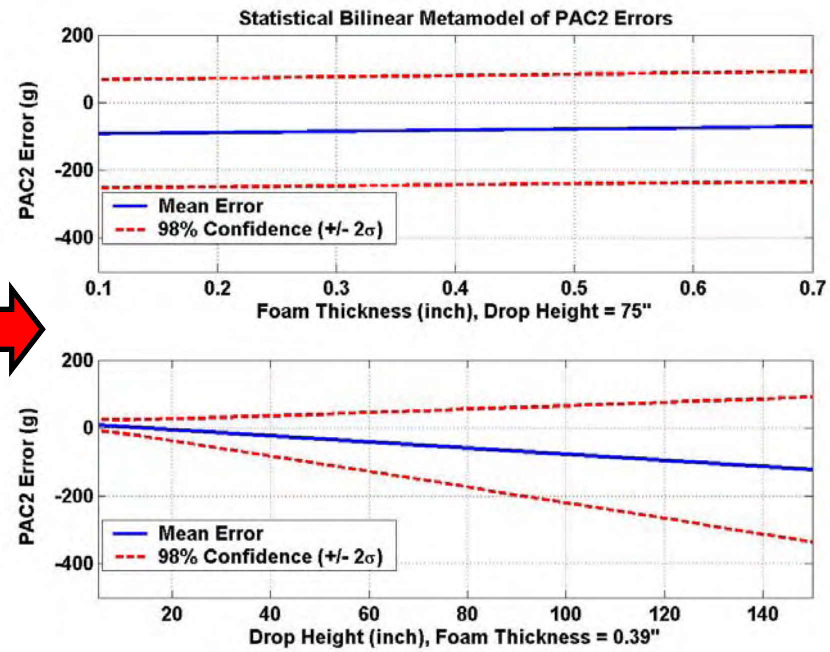
***PAC* Error Metamodel**



***TOA* Error Metamodel**

$$e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd$$

Bilinear Error Metamodel



Varying the Modeling Assumptions

- **Instead of neglecting a potential *lack-of-knowledge* about the form of the error metamodel, such uncertainty is represented, using probabilities here.**

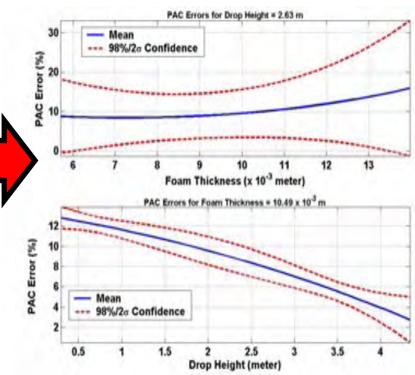
Define Possible Alternatives

"The model is linear." $e(h;d) = c_1 + c_2 h + c_3 d$
"The model is bilinear." $e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd$
"The model is quadratic." $e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd + c_5 h^2 + c_6 d^2$
"The model is cubic." $e(h;d) = c_1 + c_2 h + c_3 d + c_4 hd + c_5 h^2 + c_6 d^2 + c_7 dh^2 + c_8 hd^2 + c_9 h^3 + c_{10} d^3$

Assign a Probability

Assumption	Probability
Linear	1.5%
Bilinear	42.2%
Quadratic	42.2%
Cubic	14.1%

Sample a Probability Law to Propagate the Uncertainty



Prior and Posterior Probabilities

- **The Bayes Theorem is used to assign probabilities, based on *prior* information and *likelihood* of each assumption.**

Posteriors →

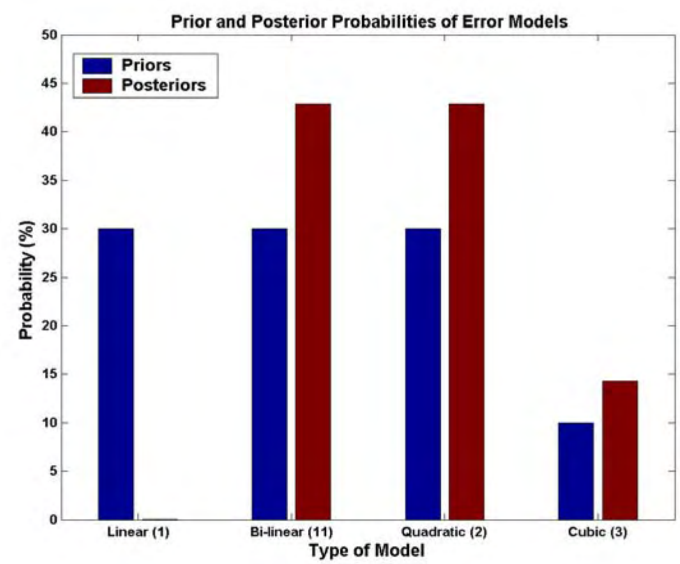
$$\Pr(p\mid y^{Test}) = \frac{L(y^{Test}\mid p)\Pr(p)}{\int_{p\in\Omega} L(y^{Test}\mid p)\Pr(p)}$$

← **Priors (May come from past experience, legacy data, expert judgment).**

Likelihood function ("goodness-of-fit" of each model).

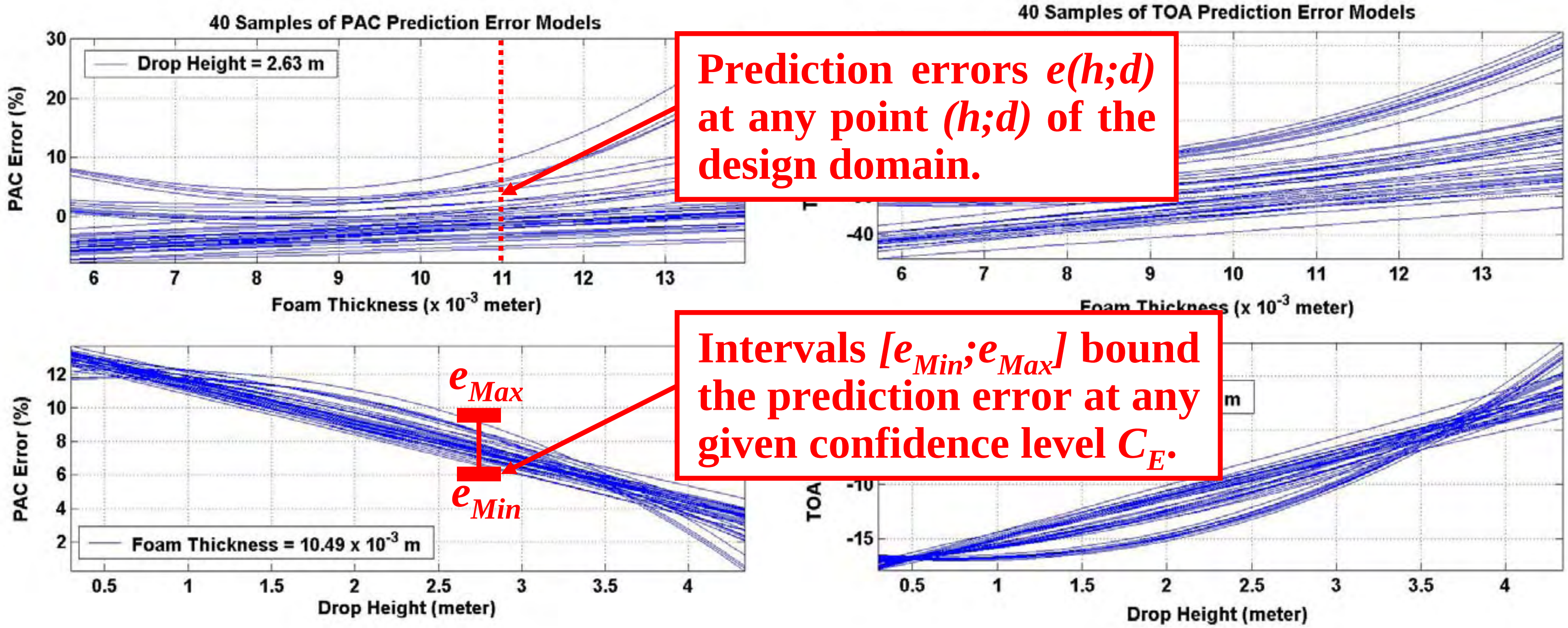
$$L(y^{Test}\mid p) = k e^{-(y^{Test}-y(p))^T S_{yy}^{-1}(y^{Test}-y(p))}$$

Assumption	Priors	Likelihood	Posteriors
Linear	30%	$4.59\ 10^{-5}$	1.5%
Bilinear	30%	$1.28\ 10^{-3}$	42.2%
Quadratic	30%	$1.28\ 10^{-3}$	42.2%
Cubic	10%	$1.28\ 10^{-3}$	14.1%



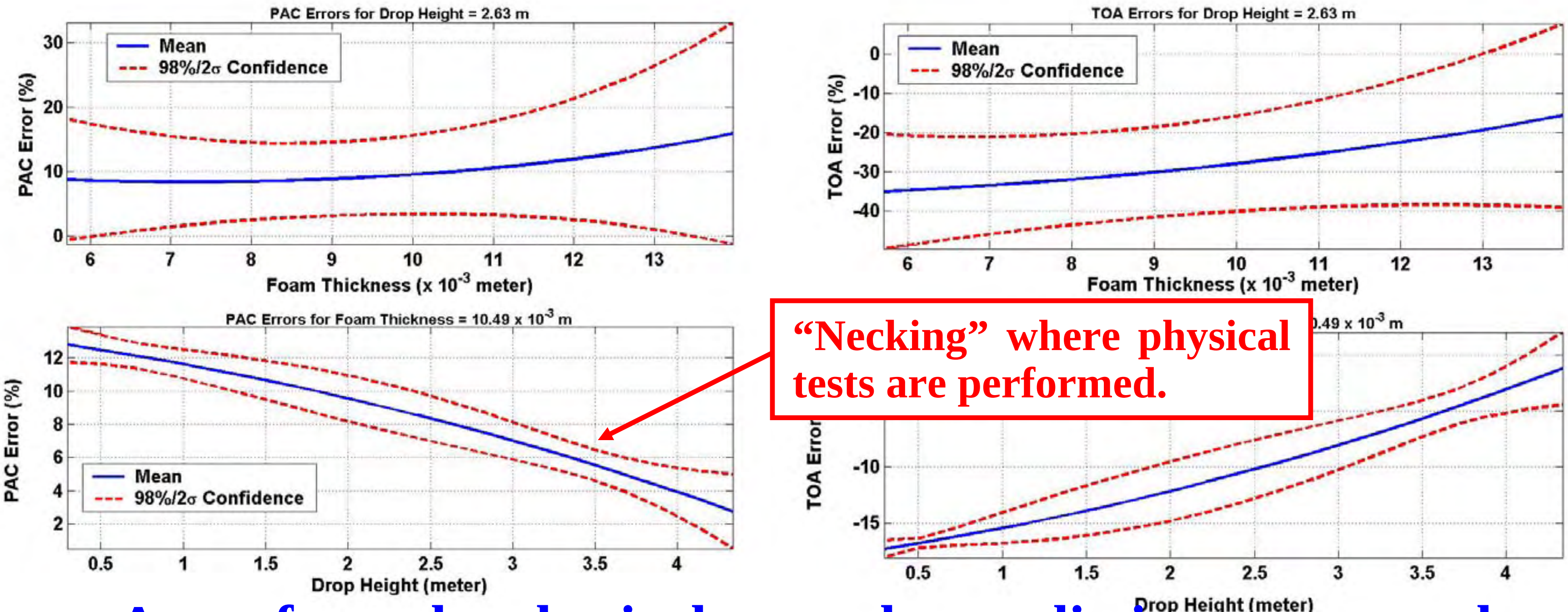
Propagation of Modeling Uncertainty

- **Sampling the posterior probability law provides a family of error metamodels (1,000 Monte Carlo simulation).**



Confidence Intervals of Accuracy

- **The confidence intervals express the effect that modeling uncertainty has on the expected prediction accuracy.**



- **Away from the physical tests, the prediction accuracy does not necessarily deteriorate … but the uncertainty of the predictive assessment tends to grow.**

Conclusion

- The concept of prediction accuracy is demonstrated with a simple model, a single source of experimental variability, and a single source of modeling uncertainty.
- The assessment of prediction accuracy is a pre-requisite to questions such as …
  - What is the benefit of another physical experiment?
  - Which model is the best one for a particular application?
- A calibrated model can still be used for making predictions elsewhere in the design space … as long as the prediction accuracy can be quantified.
- Extension to non-probabilistic approaches is considered.