LA-UR- 04-4650

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Title:

THE MYTH OF SCIENCE-BASED PREDICTIVE MODELING (U)

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Submitted to:

View-graphs for presentation at the National Institute of Aerospace, NASA Langley Research Center, Hampton, Virginia, October 6, 2004.

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The Myth of Science-based Predictive Modeling (U)

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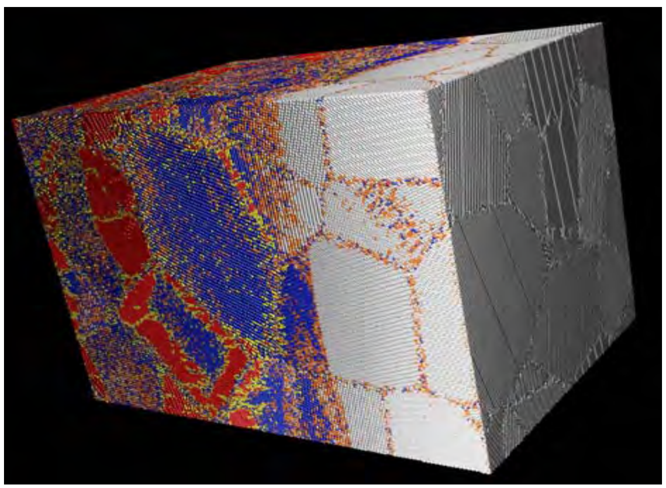
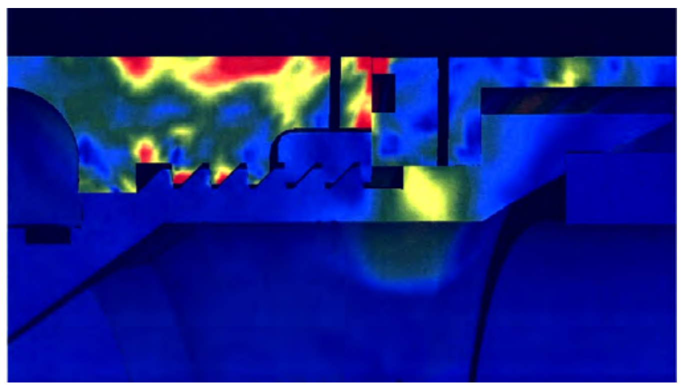




Abstract

The Myth of Science-based Predictive Modeling (U)

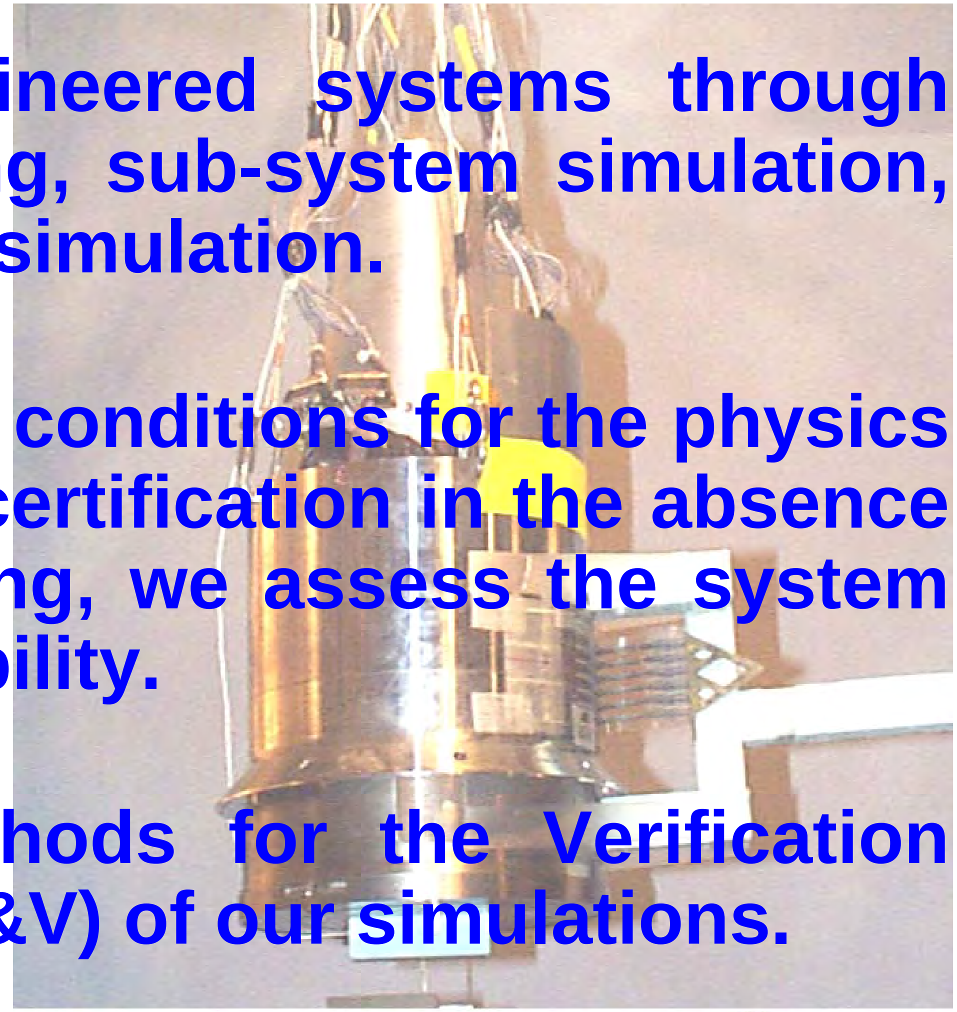
In computational physics and engineering, numerical models are developed to predict the behavior of a system whose response cannot be measured experimentally. A key aspect of science-based predictive modeling is the assessment of prediction credibility. Credibility, which is usually demonstrated through the activities of model Verification and Validation, quantifies the extent to which simulation results can be analyzed with confidence to represent the phenomenon of interest with an accuracy consistent with the intended use of the model.

The presentation develops the idea that assessing the credibility of a mathematical or numerical model must combine three components: 1) Improving the fidelity to test data; 2) Studying the robustness of prediction-based decisions to variability, uncertainty, and lack-of-knowledge; and 3) Establishing the expected prediction accuracy of the models in situations where test measurements are not available. A Theorem is established that demonstrates the irrevocable trade-off between fidelity to data, robustness to uncertainty, and confidence in prediction. Clearly, fidelity to data matters because no analyst will trust a simulation that does not reproduce the measurements of past experiments. Robustness to uncertainty is equally critical to minimize the vulnerability of decisions to uncertainty and lack-of-knowledge. It may be argued, however, that the most important aspect of credibility is the assessment of confidence in prediction, which is generally not addressed in the literature. The antagonism between three objectives (fidelity to data, robustness to uncertainty, and confidence in prediction) suggests a decision-making strategy in situations where knowledge is severely lacking. These concepts are illustrated with an engineering application for which simplistic numerical simulations are implemented, yet, severe sources of lack-of-knowledge are considered.

This presentation has been approved for unlimited, public release on July 8th, 2004. LA-UR-04-4650.

What We Do at LANL

- We analyze engineered systems through component testing, sub-system simulation, and system-level simulation.
- We provide initial conditions for the physics simulations and certification in the absence of full-scale testing, we assess the system engineering reliability.
- We develop methods for the Verification and Validation (V&V) of our simulations.



Main Messages of This Talk

- **Decisions based on predictive modeling are not *credible* until the simulations have been rigorously verified and validated.**

  … which includes a thorough quantification of all sources of uncertainty and lack-of-knowledge, and their effects on predictions.

- **Prediction credibility cannot be achieved without first understanding the trade-offs between robustness-to-uncertainty, fidelity-to-data, and confidence-in-prediction.**

Disclaimer

- **The opinions expressed in this presentation are mine only.**
- **The theoretical results and computational tools suggested in this material are not official policy of the Department of Energy, LANL, or the ASC Program.**
- **This lecture is not a criticism of ASC. I am a firm believer in physics-based Modeling and Simulation (M&S) as a major driving force behind the advancement of sciences.**

Outline

- Modeling and Simulation (M&S)
- Robustness, fidelity, and confidence
- Illustration with an engineering example

The Relationship Between Experiments and Simulations is Changing …

- ***Old paradigm:***

  Experiments are qualification tests, proof that something does or does not "break". Simulations are used to understand what happened, generally, after the fact.

- ***New paradigm:***

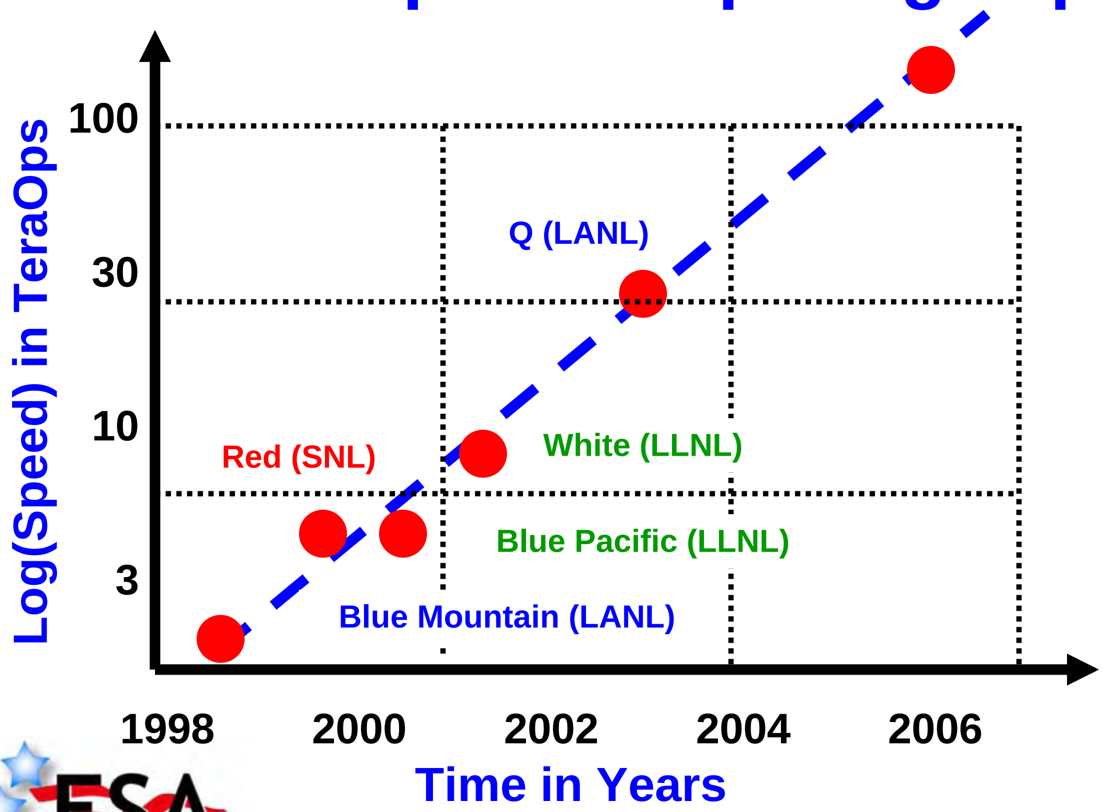
  Experiments explore the mechanics and validate predictions. Simulations are used to predict, with *quantifiable confidence* , across the *operational space*.

➡ ***Key:*** **Demonstrate the *credibility* of predictions.**

Platform Resources

- ASC platforms at Los Alamos, Livermore, and Sandia National Laboratories deliver TeraOps(*) computing capabilities.

(*) 1 TeraOps = 10^{+12} FLOPS.

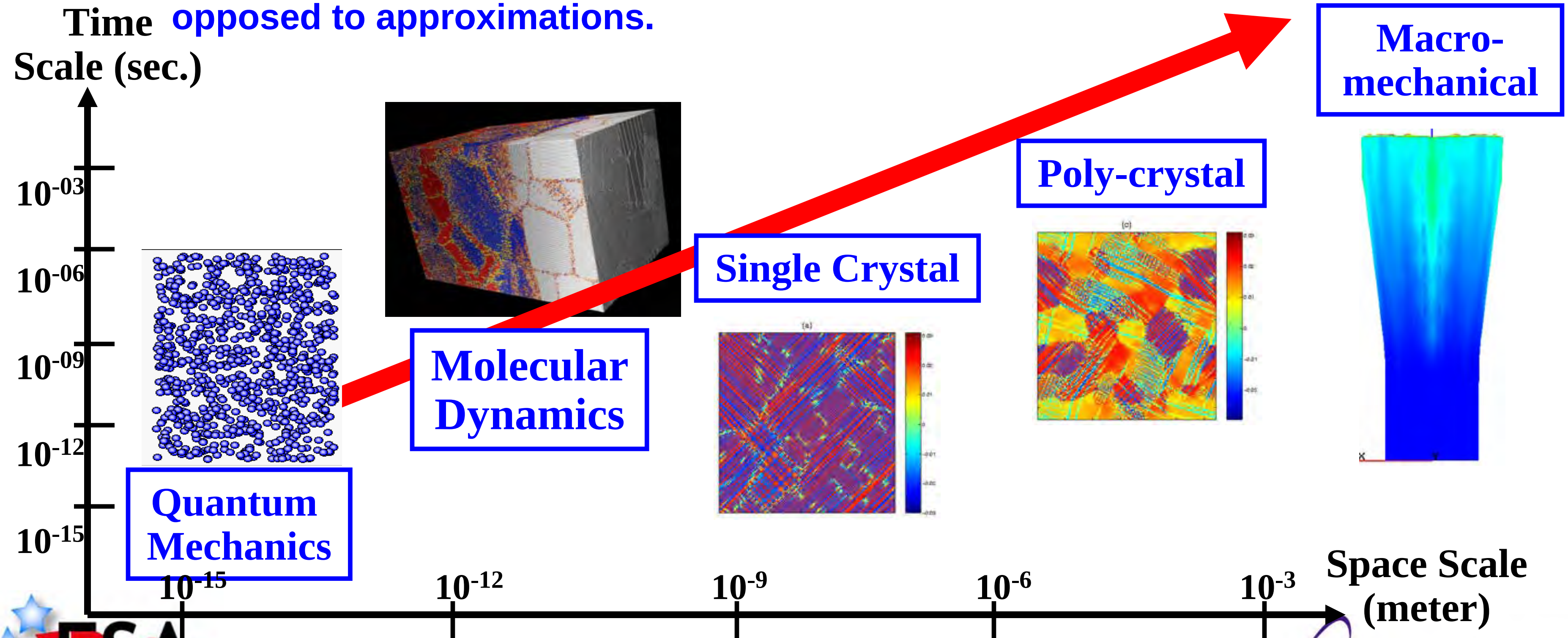


ASCI Q at Los Alamos (Nov. 2002)

Code Resources

- **High-fidelity predictive codes are developed through "first principle" physics.(*)**

(*) Examples are the full, three-dimensional representation of the geometry; better coupling algorithms; and increased reliance on physics principles as opposed to approximations.



Our Core Mission

- **From publications of the ASC Program:(*)**

"The development of high-fidelity applications for execution on massively parallel computers is required to properly steward the enduring stockpile and maintain a credible deterrent."

"Advanced physics and material models, and the coupling of such models to these applications, are required to create a predictive capability for the modeling of nuclear weapons as our stockpile continues to age."

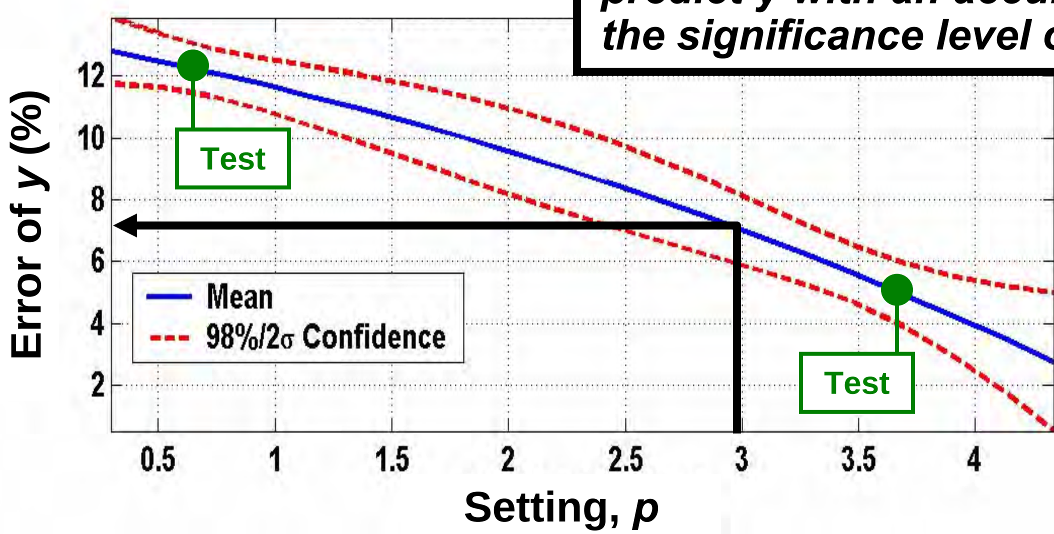
"An essential task of the weapons program has always been to determine, with confidence, the performance of stockpile weapons."

(*) One reference is: Kusnezov, D., Soudha, J., ASC Program Plan FY05, *Publication NA-ASC-101R-04-Vol. 1-Rev. 0 of the Office of Advanced Simulation & Computing*, NNSA Defense Programs, Department of Energy, Washington, D.C., September 2004.

What Does it Mean to Establish a "Predictive Capability"?

- **Prediction accuracy must be assessed throughout the operating regime, especially away from settings that have been tested experimentally.**

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



What Types of Uncertainty Are We Dealing With?

- **Beyond randomness & parametric variability, we also deal with ambiguity, conflict, and unknown physics in our applications.**

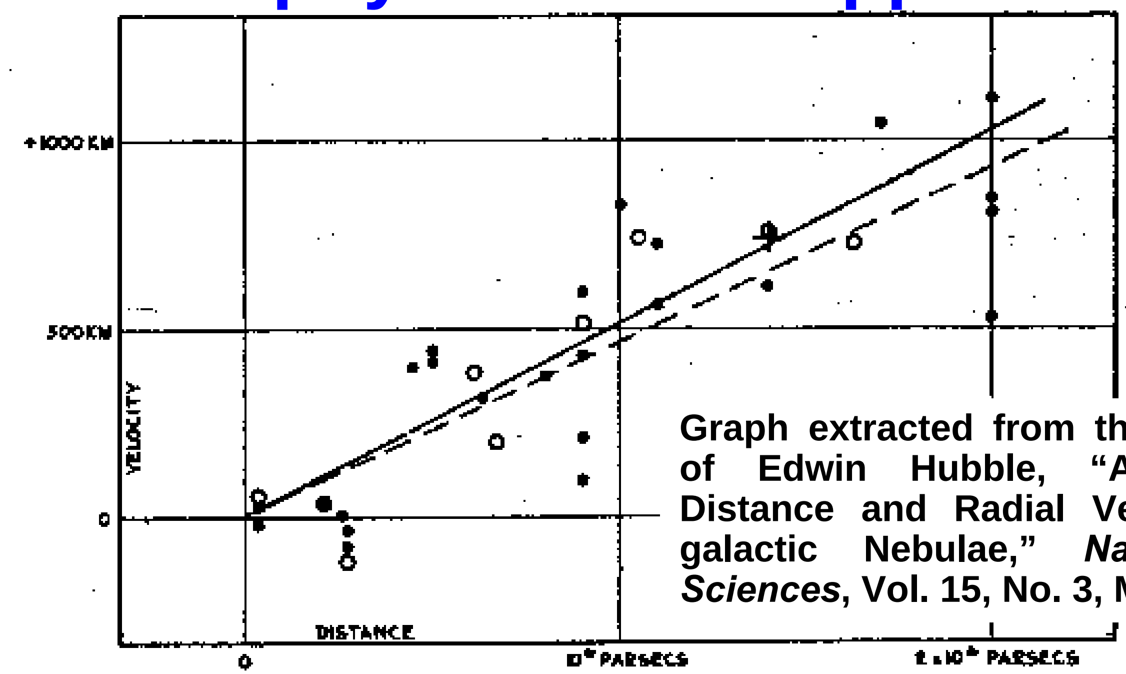


FIGURE 1

Graph extracted from the original publication of Edwin Hubble, "A Relation Between Distance and Radial Velocity Among Extra-galactic Nebulae," *National Academy of Sciences*, Vol. 15, No. 3, March 1929.

Modeling & Uncertainty

- "Models" and "families of models" are defined in a broad sense to include physics-based models, phenomenological models, test data, historical databases, regression models, expert opinion, etc.
- Uncertainty is defined in a broad sense; it includes variability and randomness and also ambiguity, conflict, lack-of-knowledge.
- Our focus is on decision-making, and not so much on the representation of uncertainty.

Path Forward

- Decisions should be robust with respect to the assumptions upon which the models are built. (This is important because ignorance manifests itself through the modeling assumptions we make.)
- To demonstrate credibility and provide confidence, the uncertainty and its effect on simulation-based decisions must be assessed.
  - ➡ *Are decisions robust to the uncertainty?*
  - ➡ *Is confidence vulnerable to what we do not know?*
- Each source of uncertainty should be represented using the most appropriate theory. The difficulty then becomes information integration.
  - ➡ *What is the total uncertainty?*

Outline

- Modeling and Simulation (M&S)
- Robustness, fidelity, and confidence
- Illustration with an engineering example

Common Objectives for Modeling and Simulation

- **Predictions must agree with the available test data.**

  ➡ ***High fidelity-to-data.***

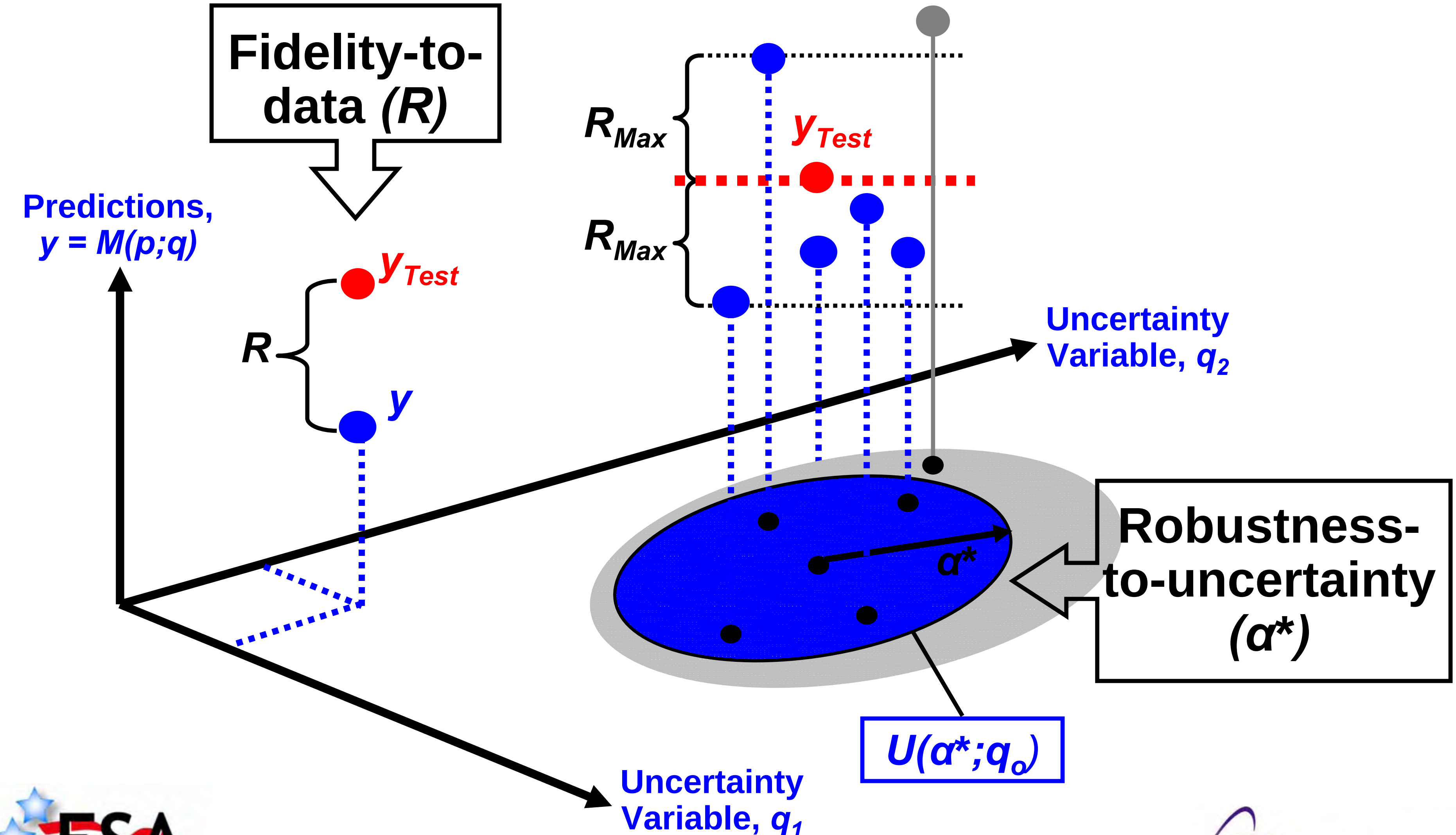
- **Decisions must be robust with respect to the sources of modeling uncertainty.**

  ➡ ***High robustness-to-uncertainty.***

- **Predictions from a family of models must establish a consistent body of evidence.**

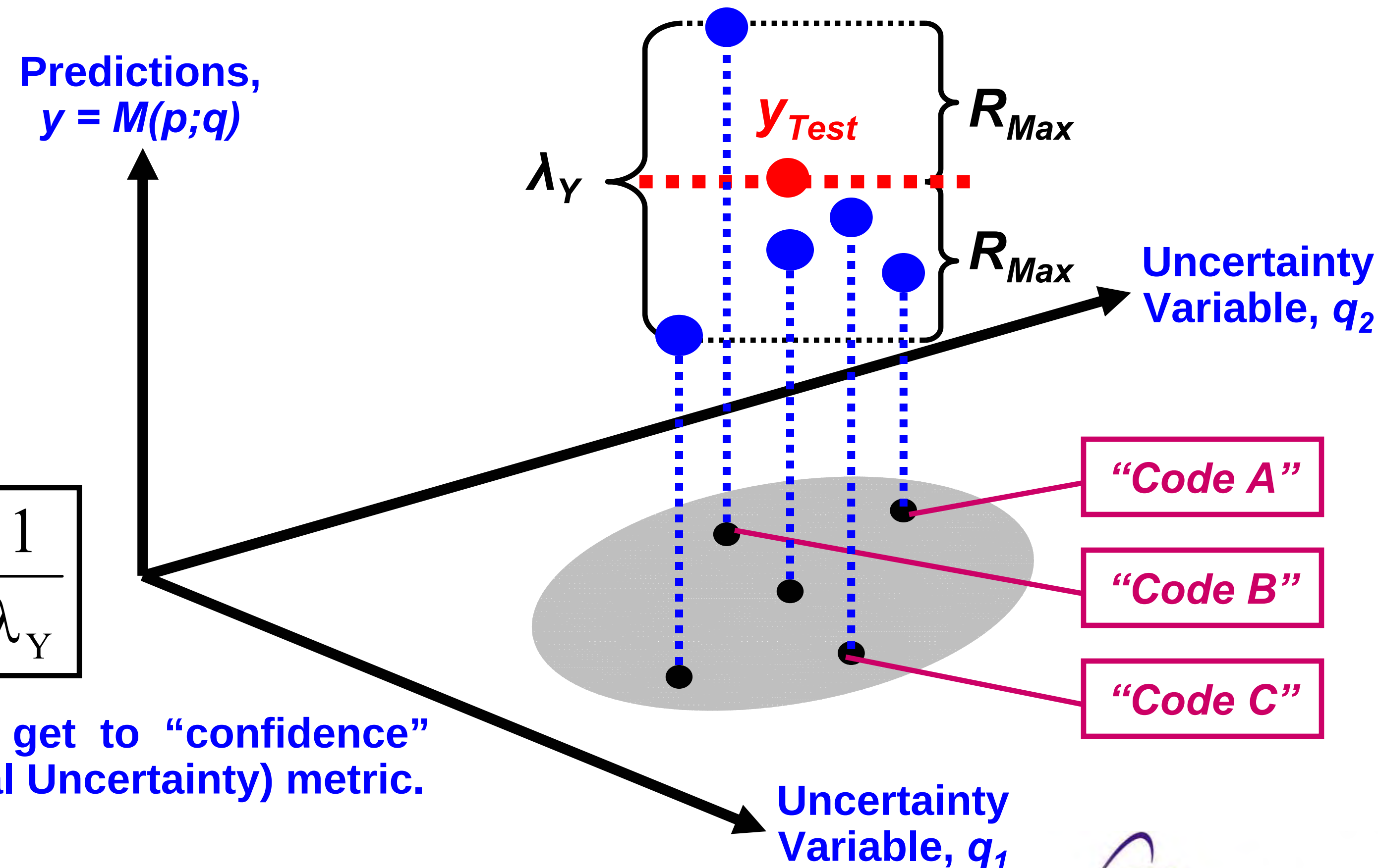
  ➡ ***High confidence-in-prediction.***

Fidelity *(R)*, Robustness *(α*)*



"Looseness" (λ_Y)

- **There is no formal definition of *confidence* within ASC. Looseness is a way to get to it.(*)**



$$\text{Confidence} \propto \frac{1}{\lambda_Y}$$

(*) **In this work, we get to "confidence" through our *TU* (Total Uncertainty) metric.**

Definitions

- ***Fidelity-to-data (R)***: **Degree of correlation between test data and simulation predictions.**

$$R^2 = \sum_{k=1 \ldots N_{Test}} \left(y_{Test}^{(k)} - M(p^{(k)};q) \right)^2$$

- ***Prediction looseness (λ_Y)***: **Range of predictions expected from a family of equally-robust models.**

$$\lambda_Y = \max_{M \in U(\alpha^*;q_o)} M(p;q) - \min_{M \in U(\alpha^*;q_o)} M(p;q)$$

- ***Robustness-to-uncertainty (α*)***: **Maximum value of the horizon-of-uncertainty for which all models of the corresponding family *$U(\alpha;q_o)$* meet a given fidelity requirement *R_{Max}*.**

$$\alpha^* = \max_{\alpha \geq 0} \left\{ R \leq R_{Max} \text{, for all } M \in U(\alpha;q_o) \right\}$$

First Theorem

- ***Theorem 1:*** **Let $\{U(\alpha;q_o)\}$ denote an info-gap family of models that obeys the axiom of nesting.[1] Let $R_{A,Max}$ and $R_{B,Max}$ denote two requirements of fidelity. If $R_{A,Max} \geq R_{B,Max}$, then $\alpha^*(q_o;R_{A,Max}) \geq \alpha^*(q_o;R_{B,Max})$.[2]**

[1] Both Theorems rely on the theory of information gap to represent uncertainty. Info-gap formulates convex models of ignorance, which introduces no serious practical limitation.

[2] Credit for establishing both Theorems goes to Professor Yakov Ben-Haim, Yitzhak Moda'i Chair in Technology and Economics, The Israel Institute of Technology, Haifa, Israel.

Second Theorem

- ***Theorem 2:*** **Let $U(\alpha;q_o)$ be an info-gap family of models that obeys the axioms of nesting and translation.[1] Let q_o and q_o' denote two families of models. If $\alpha^*(q_o;R_{Max}) \geq \alpha^*(q_o';R_{Max})$, then $\lambda_Y(q_o) \geq \lambda_Y(q_o')$.[2]**

$$\text{Simply put} \quad \ldots \quad \frac{\partial \text{ Prediction Looseness}}{\partial \text{ Robustness} - \text{to} - \text{uncertainty}} \geq 0$$

[1,2] Credit for establishing both Theorems goes to Professor Yakov Ben-Haim. Proofs rely on the theory of information gap to represent uncertainty, which introduces no serious practical limitation.

What the Theorems Imply …

- Robustness-to-uncertainty and fidelity-to-data are *antagonistic* attributes of any family of models.

$$\text{Theorem 1} \;\Rightarrow\; \frac{\partial\,\text{Robustness} - \text{to} - \text{uncertainty}}{\partial\,\text{Fidelity} - \text{to} - \text{data}} \leq 0$$

- Confidence-in-prediction and robustness-to-uncertainty are *antagonistic* attributes of any family of models.

$$\text{Theorem 2} + \text{"Confidence} \propto \frac{1}{\lambda_Y}\text{"} \;\Rightarrow\; \frac{\partial\,\text{Confidence} - \text{in} - \text{prediction}}{\partial\,\text{Robustness} - \text{to} - \text{uncertainty}} \leq 0$$

Trade-offs Established

- ***Robustness decreases as fidelity improves.***

  "Models" calibrated to better reproduce the available test data become more vulnerable to errors in modeling assumptions, errors in the functional form of the model, and uncertainty and variability in the model parameters.

- ***Confidence decreases as robustness improves.***

  "Models" made more immune to uncertainty and modeling errors provide a wider range of predictions, hence less consistency in their predictions (less predictive power).

- ***Confidence increases as fidelity improves.***

  "Models" calibrated to better reproduce the available test data provide more consistent forecasts, leading to a false sense of confidence ("over-calibration" or "over-fitting").

The "Sin" of Calibration

"Thou shalt not calibrate!"

Why?

- **Calibration reduces robustness.**
- **Provides a false sense of confidence.**

So what is the path forward?

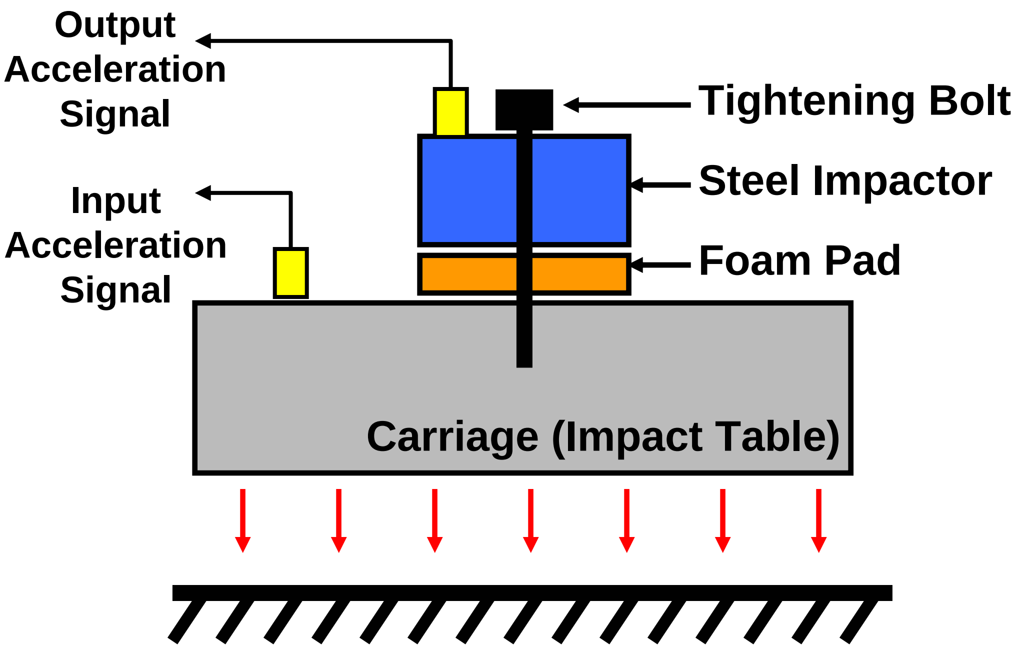
- **Fuse all sources of evidence.**
- **Assess the total uncertainty.**

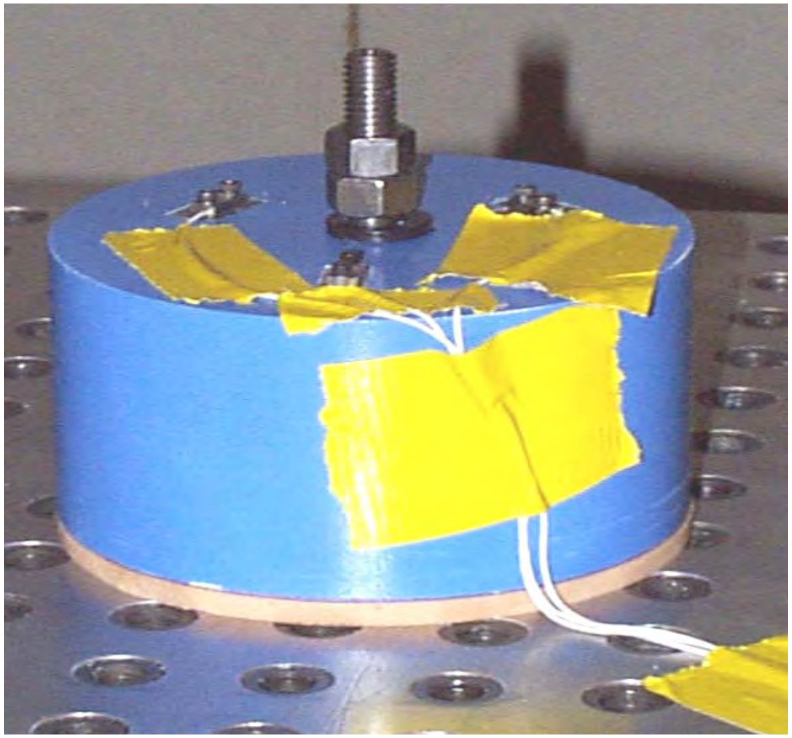
Outline

- Modeling and Simulation (M&S)
- Robustness, fidelity, and confidence
- Illustration with an engineering example

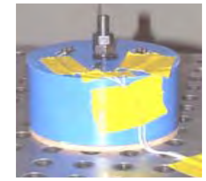
Engineering Application

- The application is the propagation of an impact through an assembly of metallic and crushable (foam pad) components.

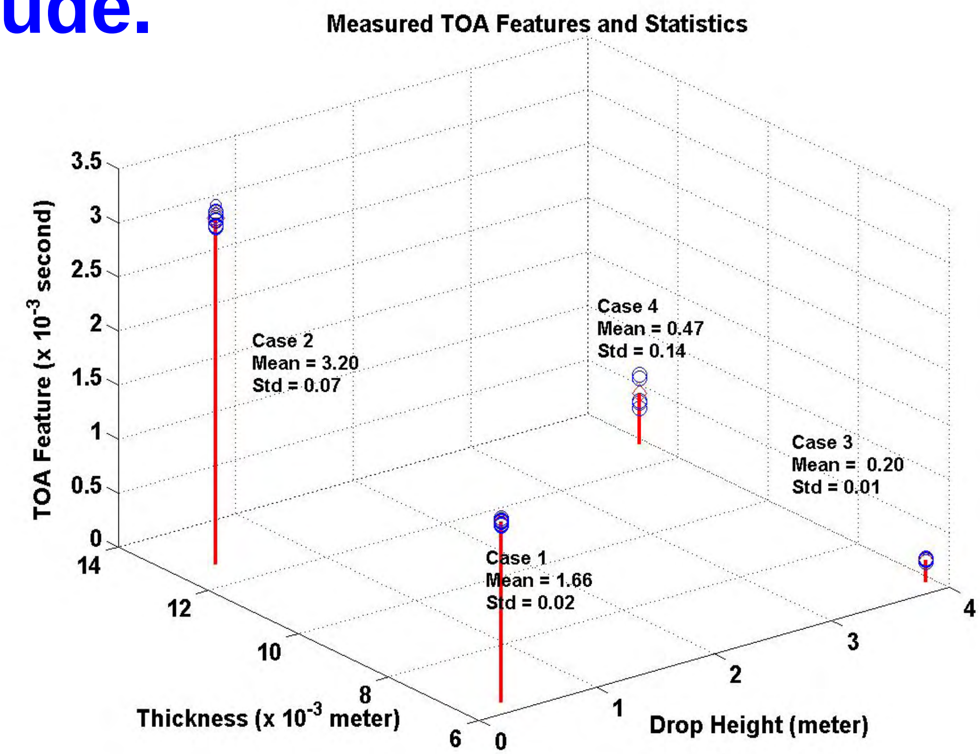




Design Space

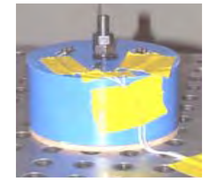


- **Predictions must be made for combinations of foam pad thickness and impact load magnitude.**

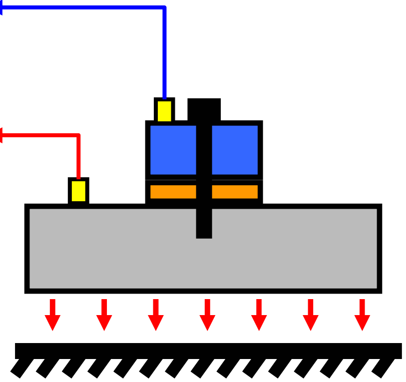


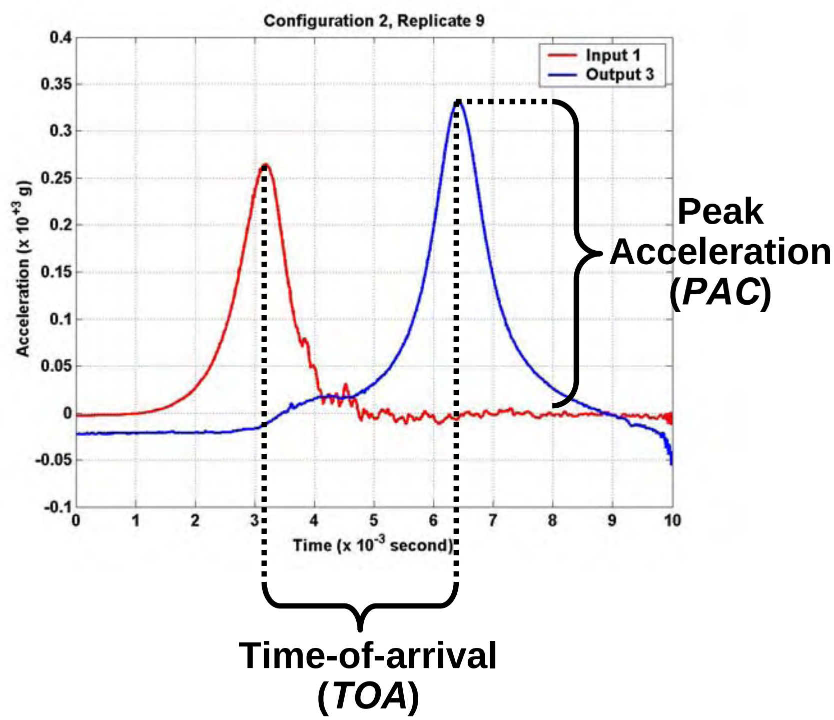
It defines a two-dimensional validation domain.

Response Features



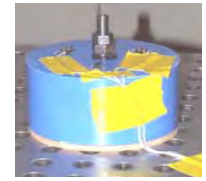
- **The two features of interest are *PAC* (peak acceleration) and *TOA* (time-of-arrival).**



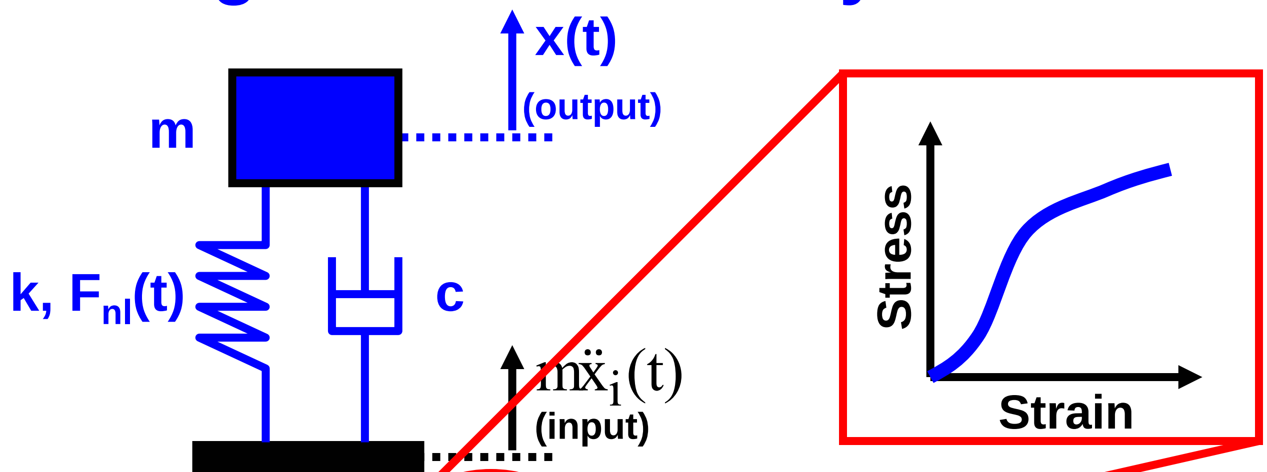


They must be predicted for all combinations of pad thickness and impact magnitude values.

Modeling



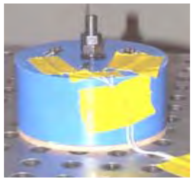
- A numerical simulation is developed to predict the output response features for various configurations of the system.



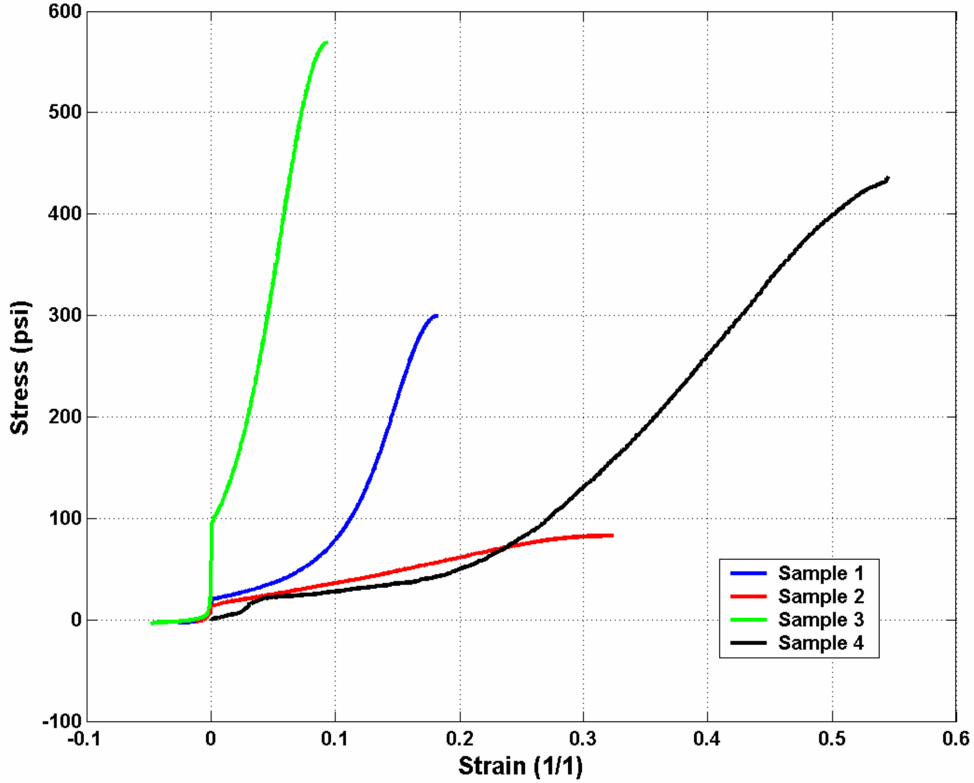
$$m\ddot{x}(t)+c\dot{x}(t)+kx(t)+F_{nl}(x)=m\ddot{x}_i(t)$$

Performing the numerical simulation is possible only after a material model has been chosen.

Uncertainty



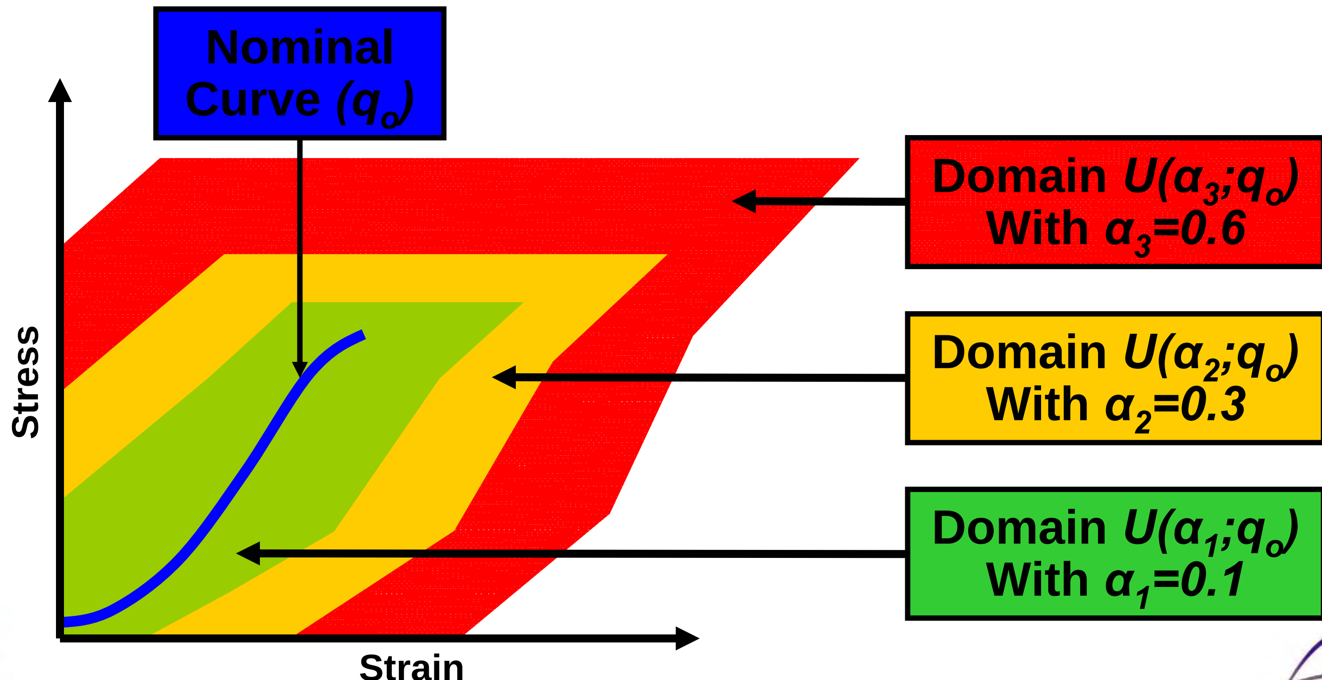
- **The main uncertainty is the constitutive behavior (or strain-stress curve) of the foam material.**

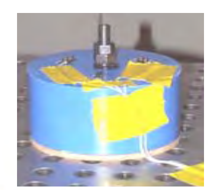


Convex Models of Uncertainty

- **Ignorance is represented by defining a family of nested, convex domains *U(α;q_o)* that "envelope" the data for a given *horizon-of-uncertainty* α.**

$$U(\alpha;q_o) = \{\text{Curves "q" such that } \|q - q_o\| \le \alpha\}, \quad \text{for } \alpha \ge 0$$



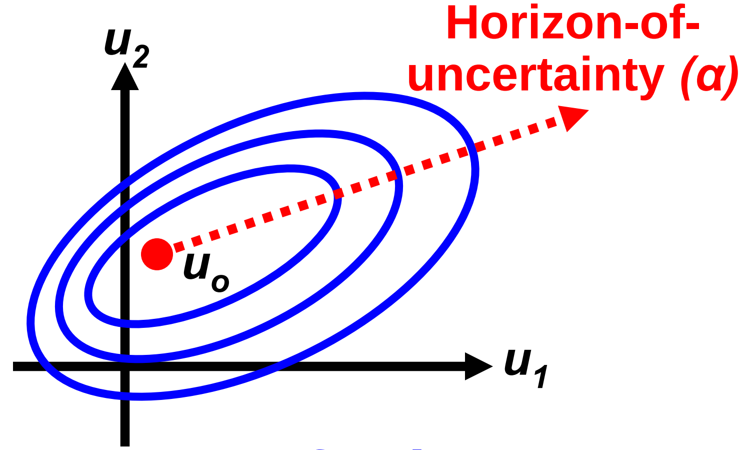


Theory of Information-gap

- **Strictly speaking, info-gap theory does not provide a mathematical representation of uncertainty.**
- **Instead of modeling uncertainty, info-gap models *ignorance*: It models the gap between what is known and what should be known in order to make an informed decision.**

Family of Nested Sets:

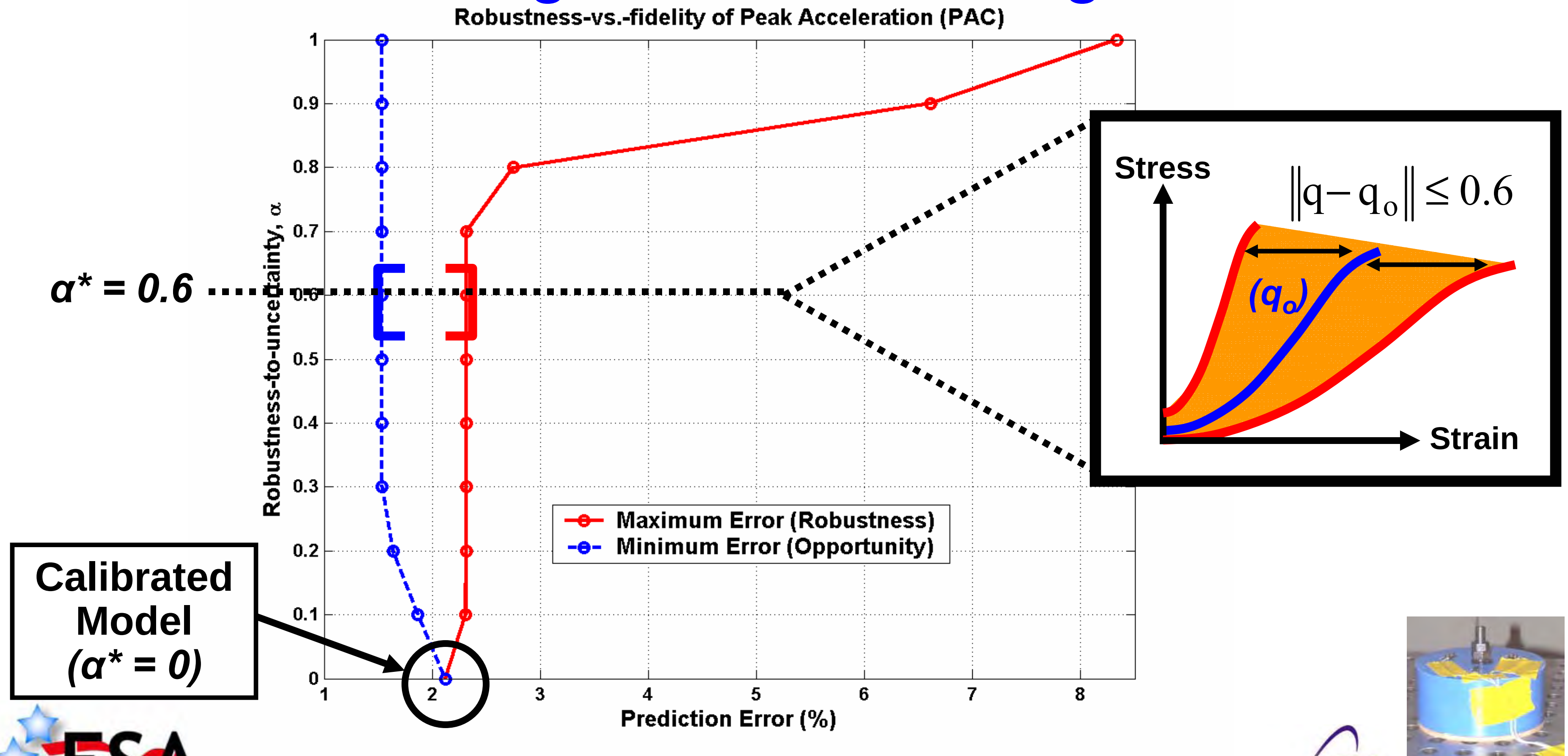
$$U(u_o;\alpha)=\left\{u\,\middle|\,(u-u_o)^T W^{-1}(u-u_o)\le\alpha\right\},\quad \alpha\ge 0$$



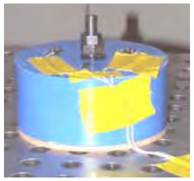
- **Info-gap models proposes a *structure* for ignorance by *clustering* uncertain events as families of nested, convex sets.**

Accuracy of Predictions

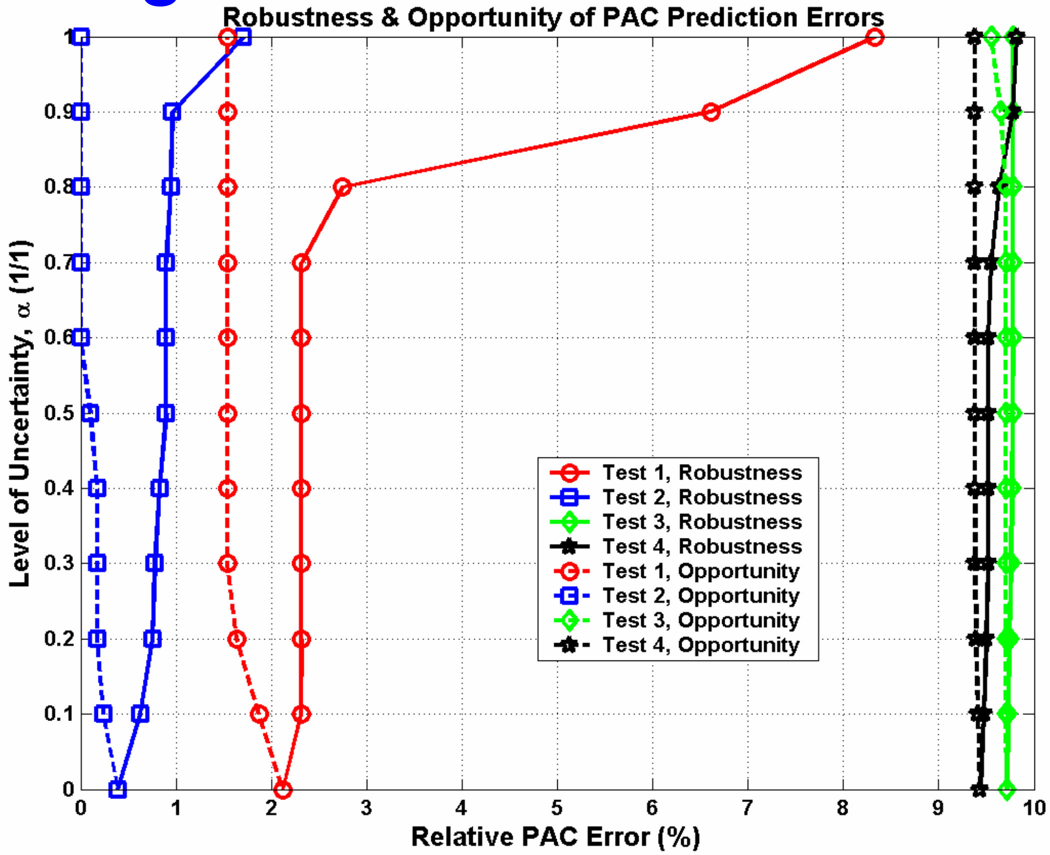
- **How accurate can *PAC* predictions be as the modeling lack-of-knowledge increases?**



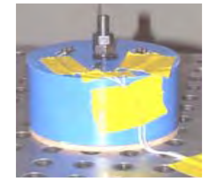
Accuracy of Predictions



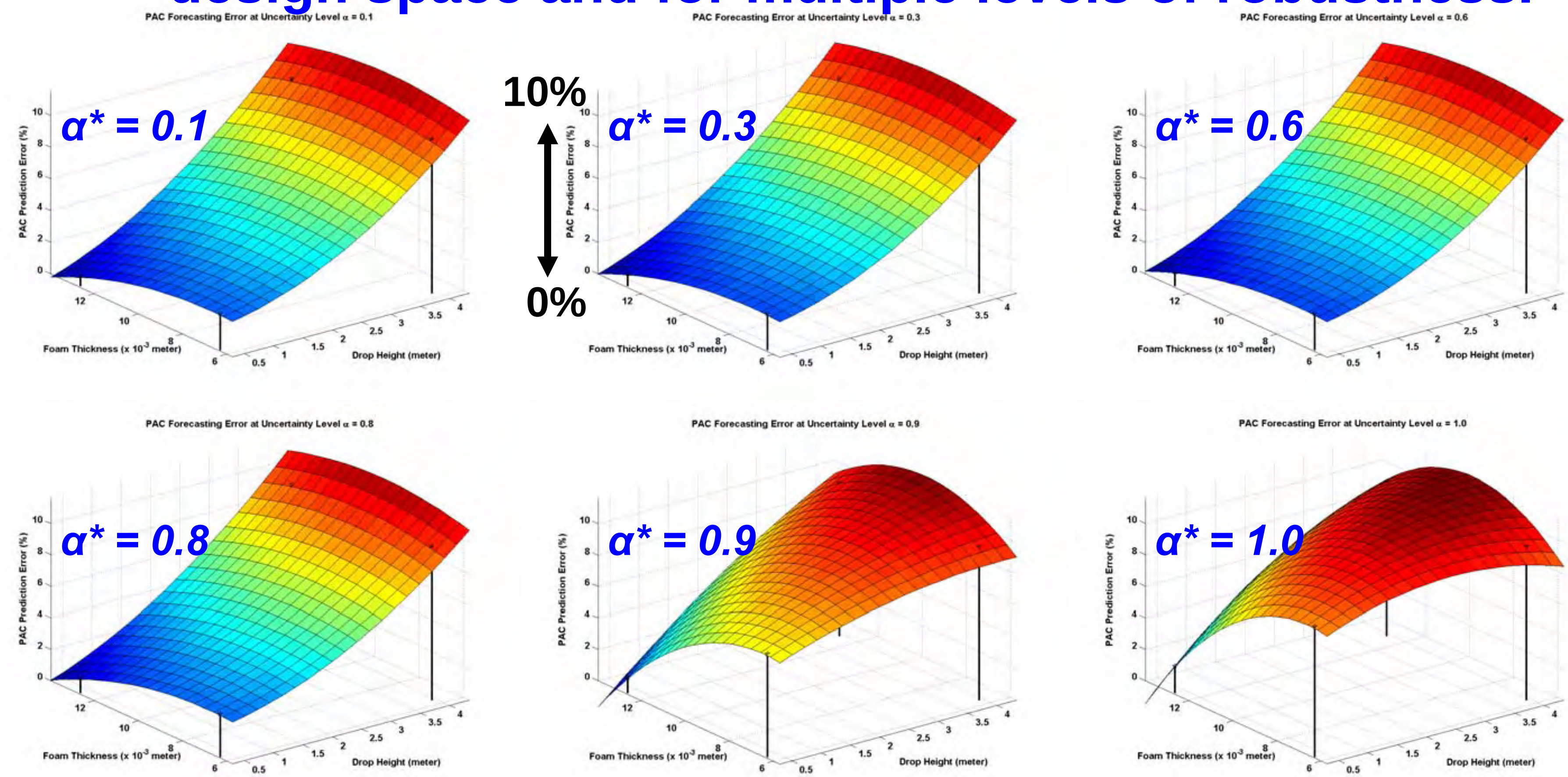
- **Robustness (R_{Max}) and opportunity (R_{Min}) for predicting the *PAC* features of Tests 1-4.**



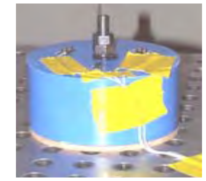
Extrapolated Accuracy (R_{Max})



- **Prediction errors are extrapolated throughout the design space and for multiple levels of robustness.**

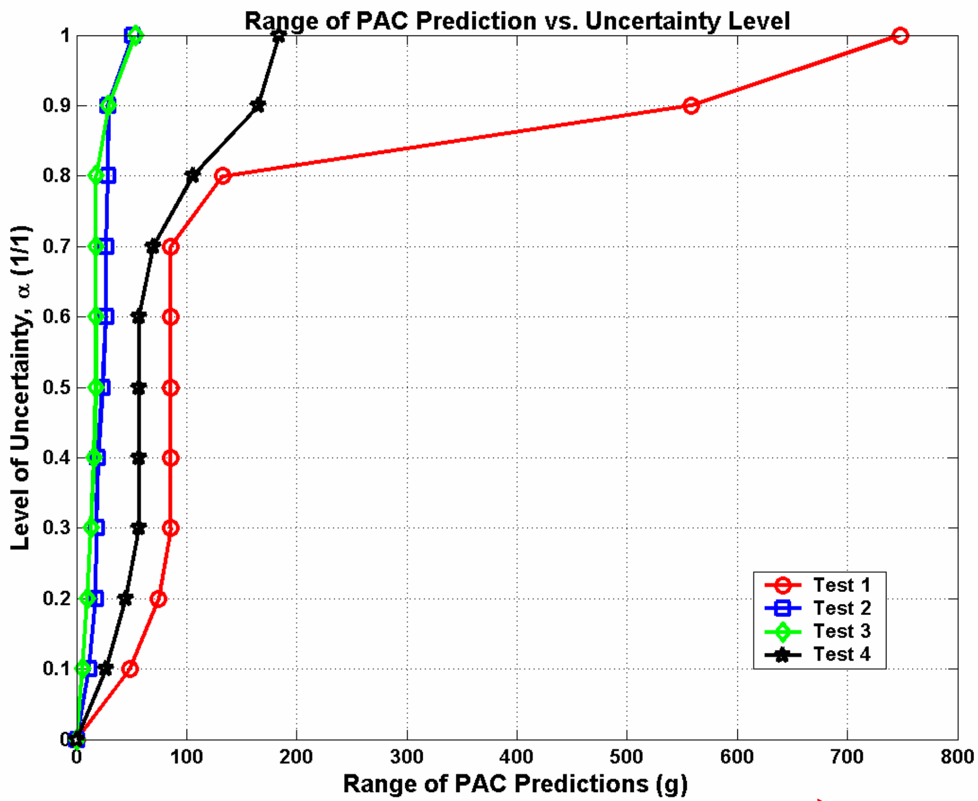


Consistency of Predictions



- The prediction looseness (or range) is calculated for multiple robustness levels α^*, at constant R_{Max}.

Robustness-to-uncertainty



Range of Predictions

Getting to "Confidence" …

- How to define a metric for the *confidence* in predictions is open research …
  - Statistical sciences only provide guidelines for the notion of confidence intervals.
  - It is reasonable to define a metric C_F as being a numerical value between zero and one.
  - Similarly, it is reasonable to state that confidence decreases when uncertainty increases.
- My metric for confidence (C_F) is defined as the opposite of *total uncertainty* (*TU*):

$$C_F = 1 - TU \quad \text{where} \quad 0 \le TU \le 1$$

Total Uncertainty (*TU*)

- **Predictions are collected in an information matrix. Information here comes in the form of intervals:**

$$H = \begin{bmatrix} TOA_{min} & PAC_{min} \\ TOA_{max} & PAC_{max} \end{bmatrix}$$

- **The information matrix is decomposed:**

$$H \overset{svd}{=} U \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} V^T$$

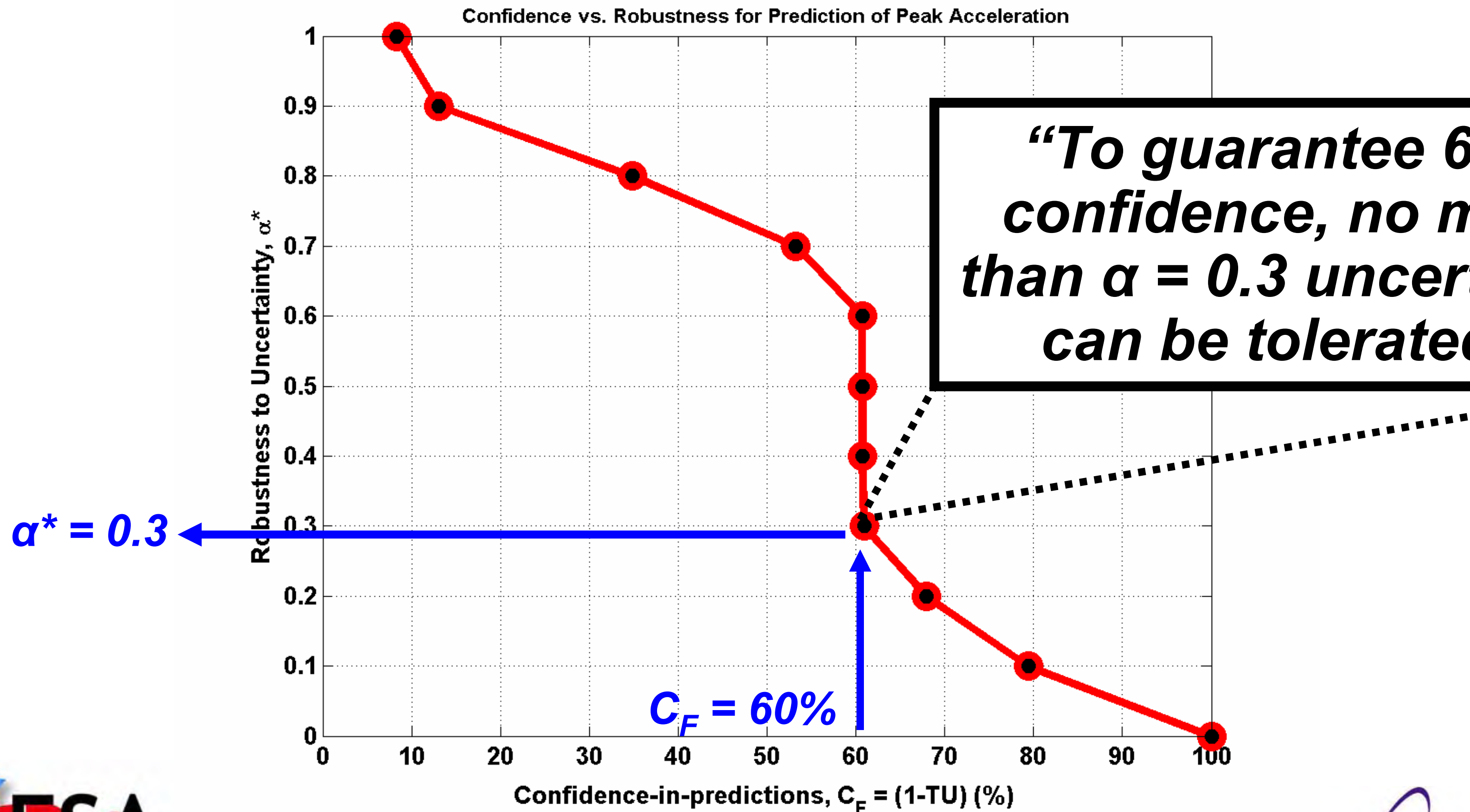
- **A metric for Total Uncertainty *(TU)* is computed:**

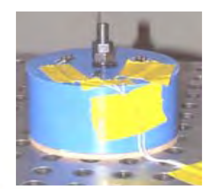
$$TU = \frac{\left(\sigma_1^2 + \sigma_2^2\right)}{\left(PAC_{max}^2 + TOA_{max}^2\right)} - 1$$

- **The key point is that the *TU* metric is, by definition, bounded between zero and one.**

Confidence in Predictions

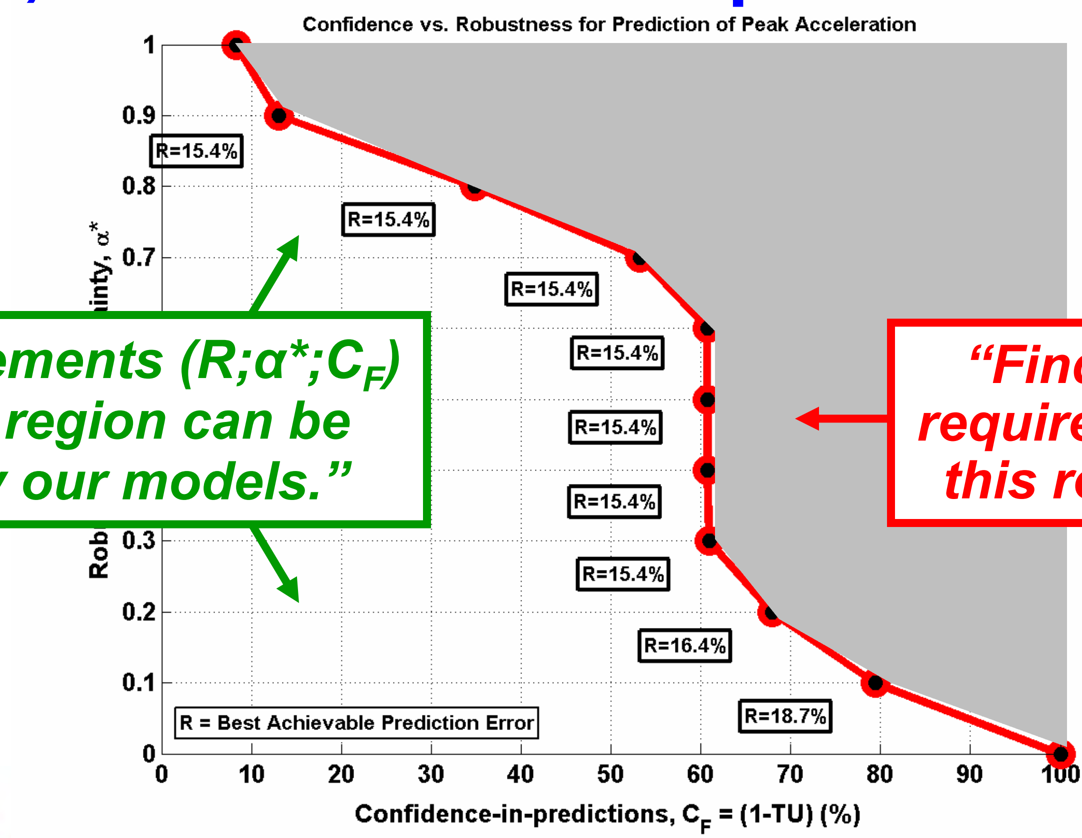
- How confident can we be in the predictions as a function of increasing robustness?





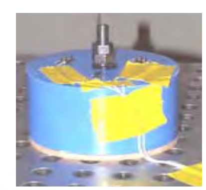
Where is the "Myth"?

- **Can simulations provide arbitrary levels of fidelity-to-data *R*, robustness-to-uncertainty *α**, and confidence-in-predictions C_F?**



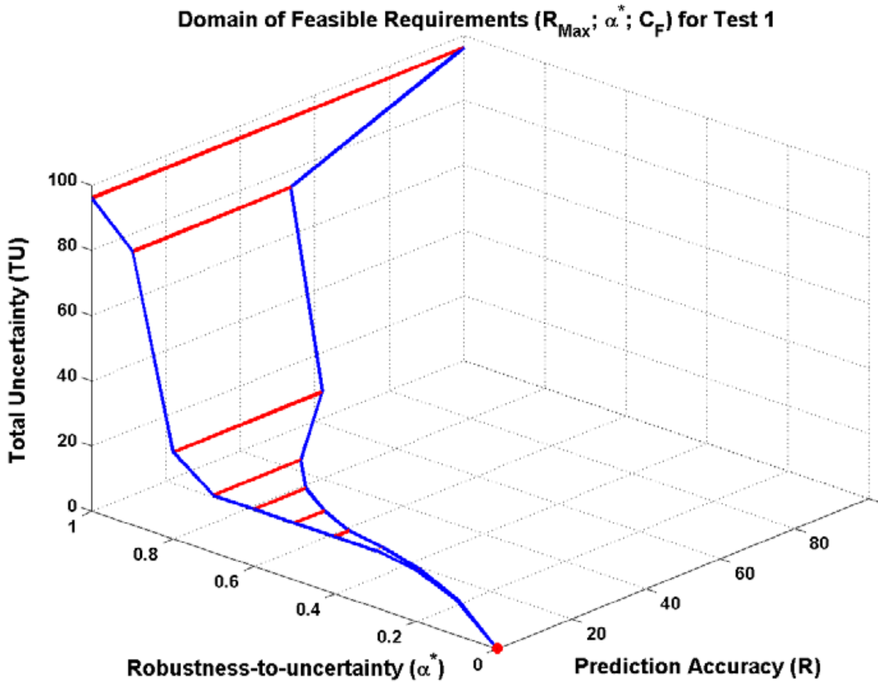
"Requirements (R;α;C_F) in this region can be met by our models."*

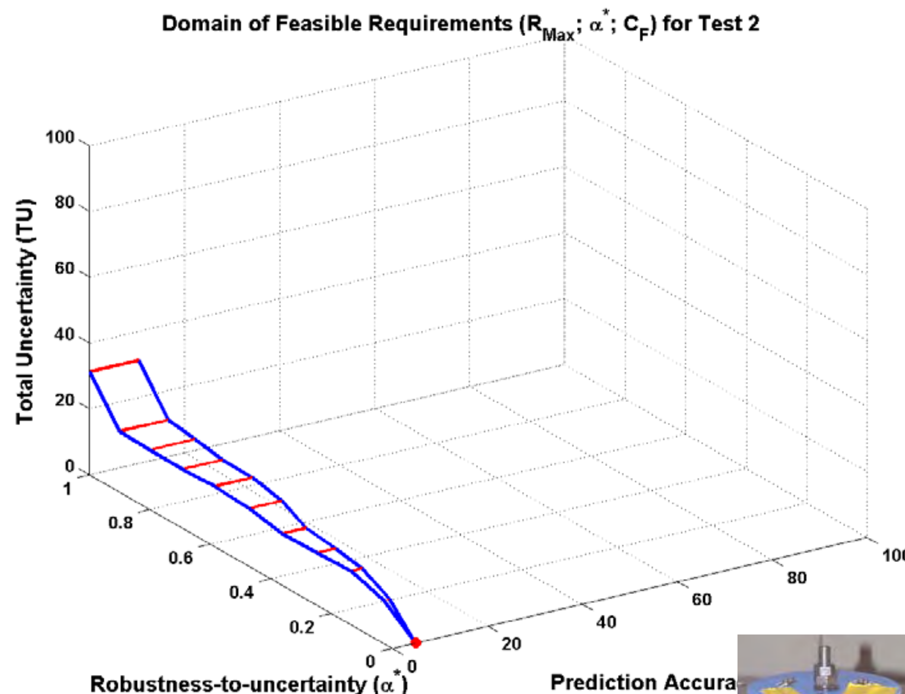
"Finding models with requirements (R;α;C_F) in this region is a MYTH!"*

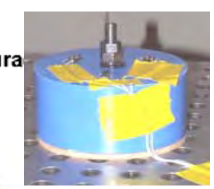


Feasible Requirements $(R;\alpha^*;C_F)$

- **Attainable requirements $(R;\alpha^*;C_F)$ of fidelity-to-data, robustness-to-uncertainty, confidence in prediction for Tests 1 & 2 (low drop height).**



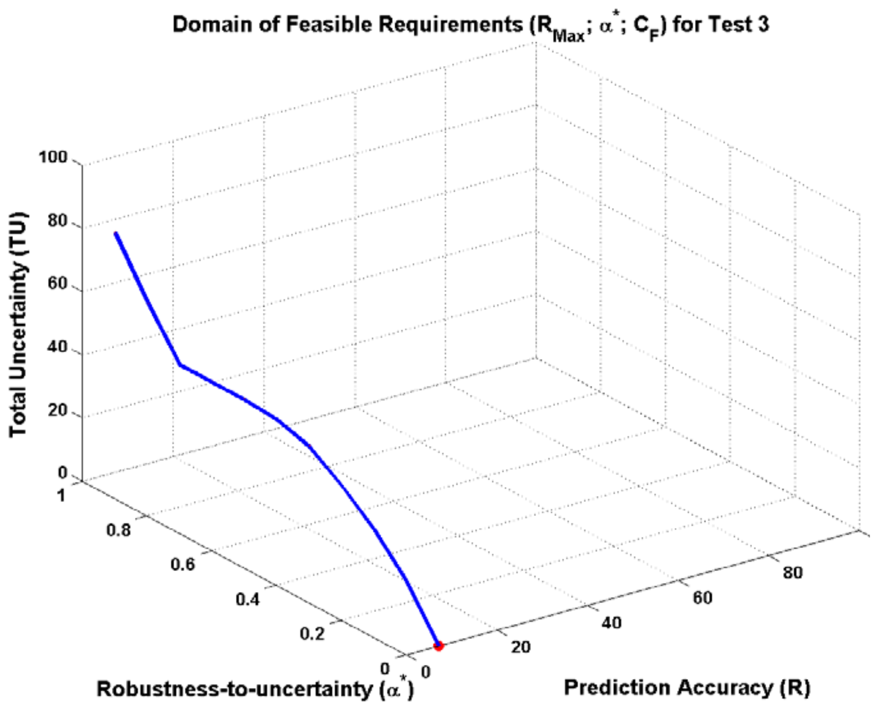


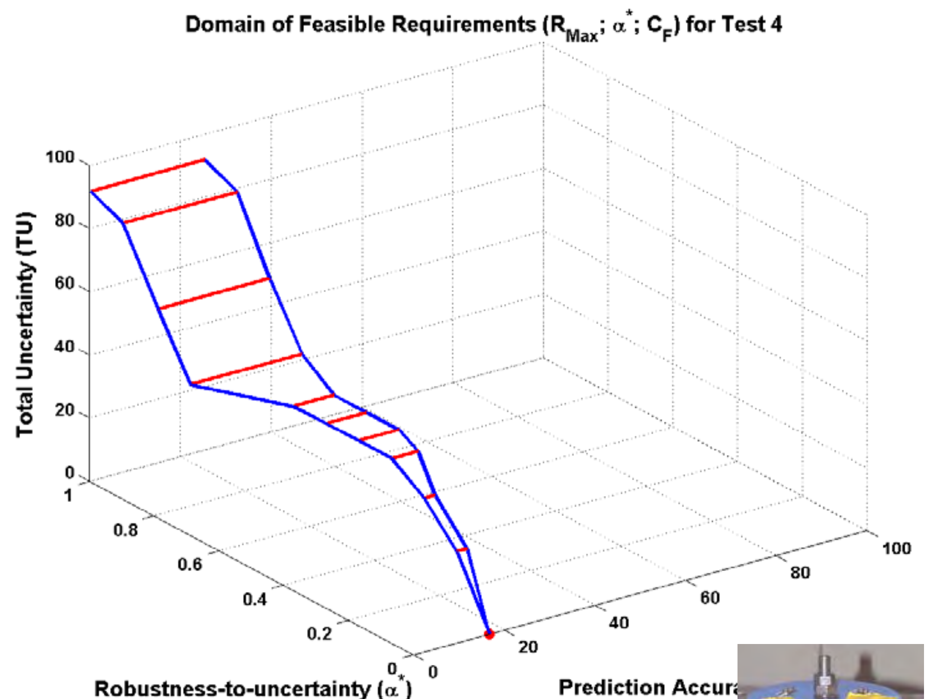


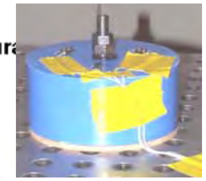
Note: Values of the Mahalanobis *R* metric are normalized to [0;1]. *α and *TU* are scaled between zero and one.**

Feasible Requirements *(R;α*;C_F)*

- **Feasible requirements (*R*;*α**;C_F) of fidelity-to-data, robustness-to-uncertainty, confidence in prediction for Tests 3 & 4 (high drop height).**

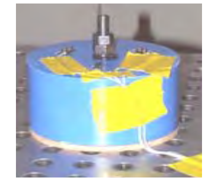




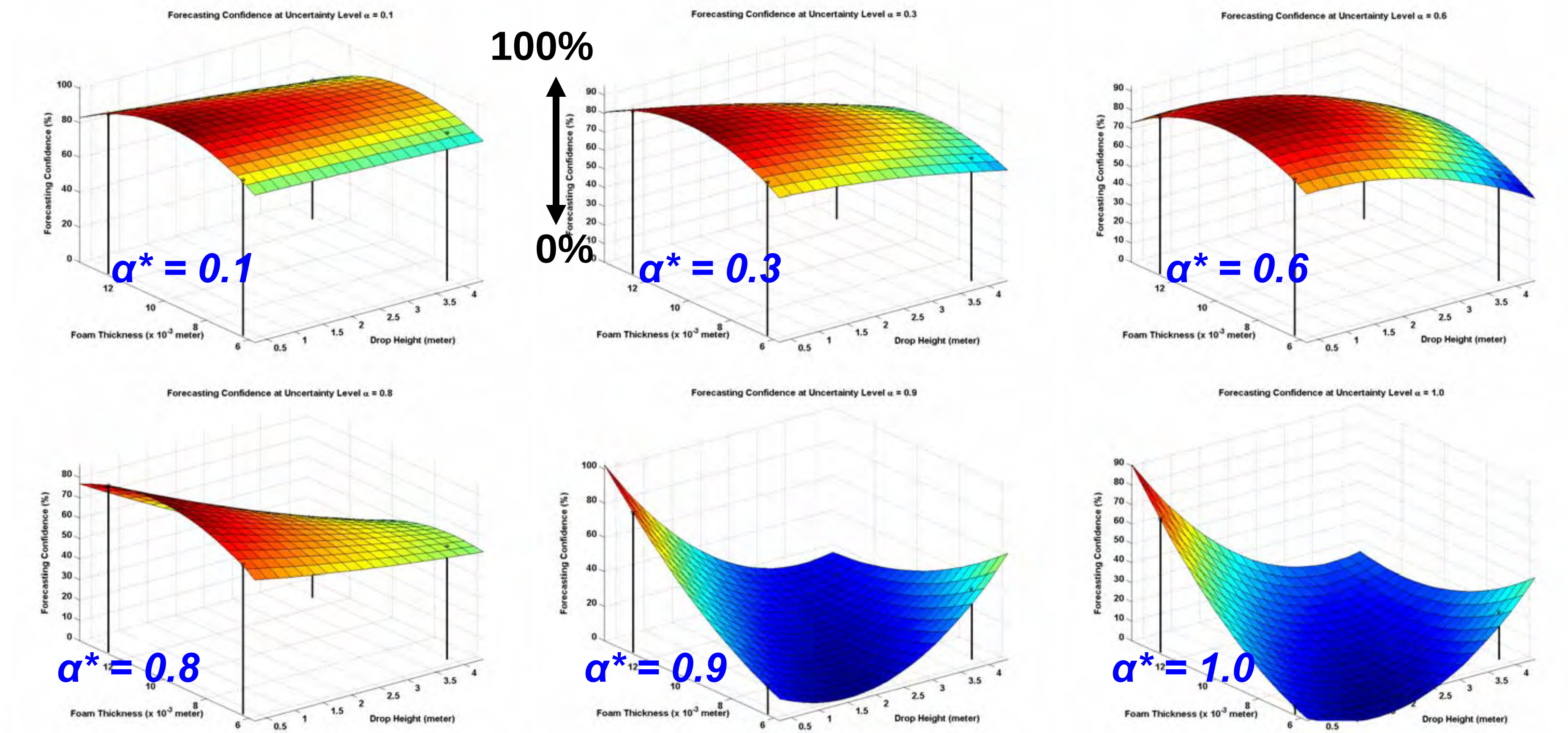


Note: Values of the Mahalanobis *R* metric are normalized to [0;1]. *α and *TU* are scaled between zero and one.**

Extrapolated Confidence (C_F)



- Confidence-in-predictions of *TOA* and *PAC* features is extrapolated throughout the design space.



Conclusion

- **To demonstrate *credibility*, the objectives of robustness-to-uncertainty, fidelity-to-data and confidence-in-prediction must be explored.**
- **These three objectives may be *antagonistic*.**
- **Calibrating models for improving their fidelity to data reduces the robustness to uncertainty and lack-of-knowledge.**
- **Studying these trade-offs is important to understand the strengths and weaknesses of our models, and allocate resources through cost-benefit analysis.**