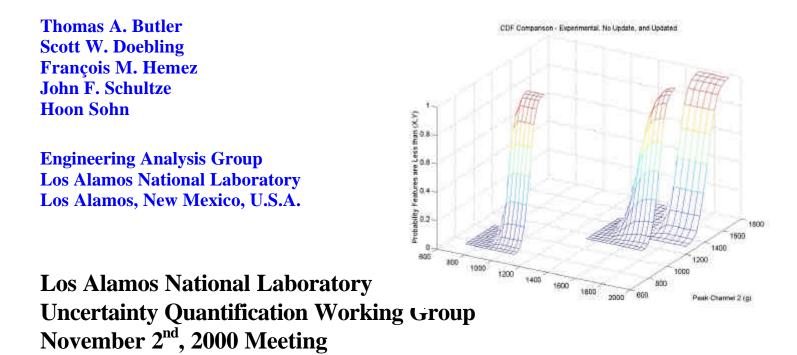
Validation of Engineering Applications at LANL^(*)



^(*) Presentation material extracted from a publication entitled "Inversion of Structural Dynamics Simulations: State-of-theart and Directions of the Research" and presented at the 25th International Conference on Noise and Vibration Engineering, Leuven, Belgium. Approved for unlimited, public release on September 5, 2000 — LA-UR-00-2562.

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OUTLINE



- Motivation
- Impact Experiment (Development of the Methodology)
- Forward Mount Impulse Experiment (ASCI Demonstration)
- Unresolved Issues & Challenges

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DEFINITION

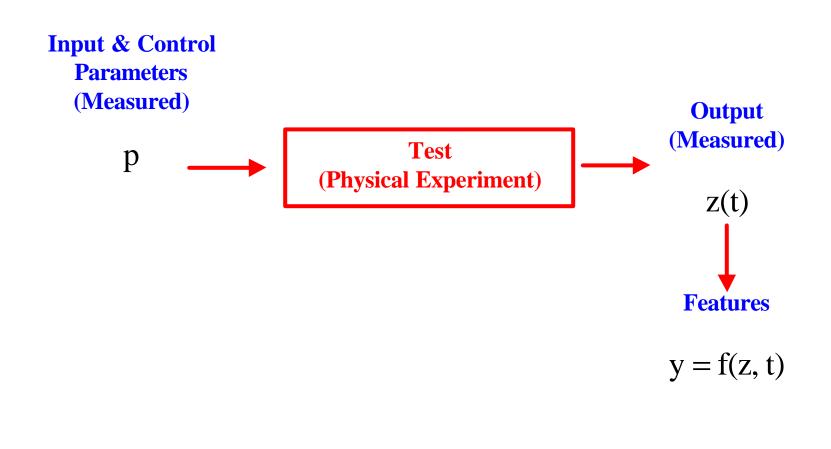
- **Test** = Physical Experiment
- Model = Numerical Experiment
- Meta-model = Fast-running, Statistical Model
- **Feature = Quantity Synthesized From the Experiment's Output**
- Test-analysis Correlation = Definition of a Residue or "Distance"
- **Cost Function** = Residue Expressed in a Particular Metric
- ... Should We Define a Common Set of Notations & Definitions?

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TEST (DEFINITION 1 OF 4)

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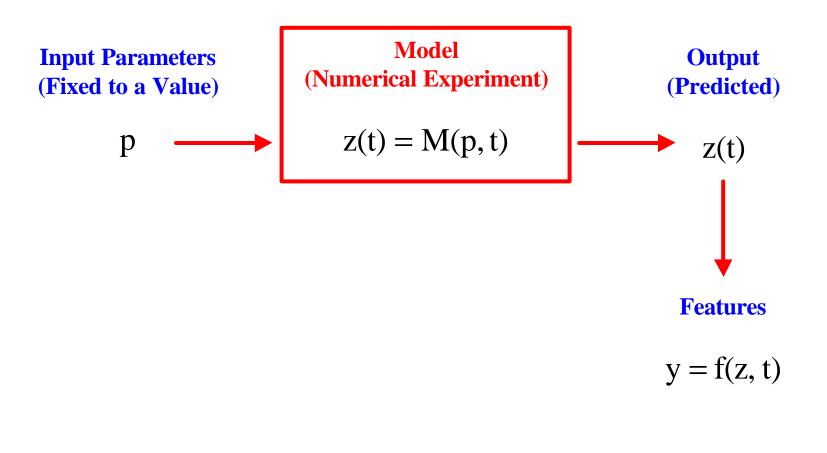


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MODEL (DEFINITION 2 OF 4)

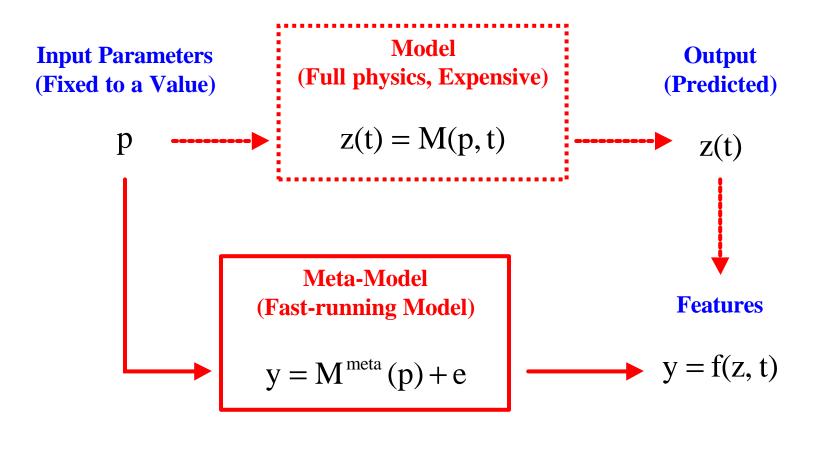
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META-MODEL (DEFINITION 3 OF 4)



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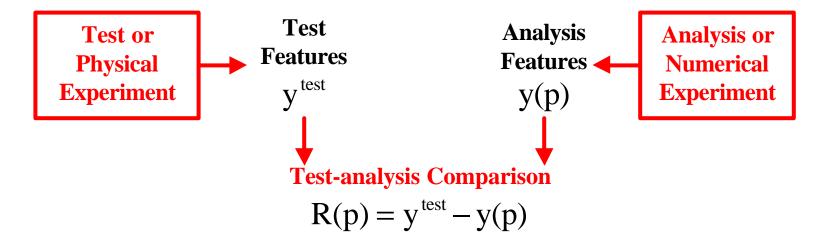
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TEST-ANALYSIS CORRELATION (DEFINITION 3 OF 4)

• Definition of a Residue or "Distance":



• Definition of a Metric or "Norm":

$$J(p) = \sum_{j=1\cdots N_{data}} \{R(p)\}^{H} [S_{RR_{j}}]^{-1} \{R(p)\} + \{p\}^{H} [S_{pp}]^{-1} \{p\}$$

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DEFINITIONS NEEDED?

- How is Uncertainty Quantification Defined?
- What Constitutes a Validated Numerical Model?
- Does it Mean That it Adequately Captures the Physics *and* the Sources of Variability/Uncertainty?
- Do We Agree on the Difference Between Validation and Verification?

• • • •

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WHAT IS UNCERTAINTY QUANTIFICATION?

- Characterization of Sources & Scenarios
- Forward Propagation
- Statistical Effects Analysis
- Characterization of the Output
- Optimization
- Characterization of "Rare" Events

- ✓ What is Uncertain?
- ✓ What Varies?
- ✓ How?
- ✓ Sampling Techniques;
- ✓ Fast Probability Integration.
- ✓ Sensitivity Study;
- ✓ Correlation Study.
- ✓ Joint Probability Density Functions;
- ✓ Higher-order Statistical Moments.
- ✓ Statistical Parameter Estimation;
- ✓ Model Improvement.
- ✓ Reliability;
- ✓ Tails of the Statistical Distributions.

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OUTLINE

• Notation & Definition



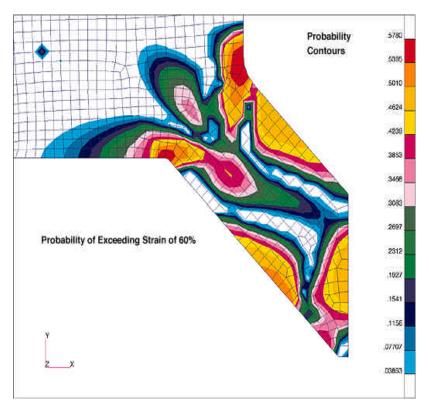
- Impact Experiment (Development of the Methodology)
- Forward Mount Impulse Experiment (ASCI Demonstration)
- Unresolved Issues & Challenges

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ASCI — ENGINEERING APPLICATIONS

- Two Main Objectives:
- Model and Predict Engineering Weapon System Performance in Normal and Hostile Stockpile-to-target Sequence (STS) Environments.
- ✓ Predict the Deformed State (Geometric, Structural, Thermal, Material Damage) of the Warhead at Detonation.^(*)

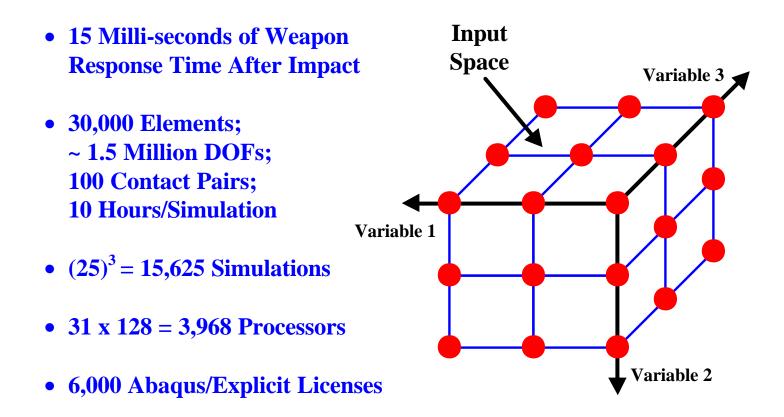


^(*) Characterization of the Deformed State at Detonation is the "Initial & Boundary Condition" for the Physics Designers.

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ASCI — ENGINEERING APPLICATIONS



• 17.8 Years of Equivalent Single-processor Computing in Just 72 Hours!

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WHERE DO WE GO FROM THERE?

• Current Achievements

 ✓ Complex Engineering Applications Can be Numerically Simulated.
 ▲ ASCI Software/Hardware Platforms.

 ✓ Stochastic Inputs Can be Propagated Through Forward Computations.
 Fast Probability Integration.

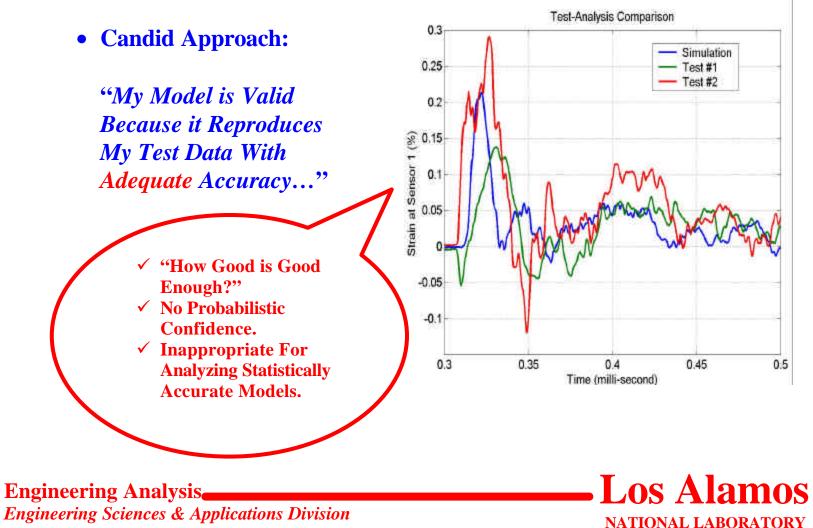
• Next ...

✓ Can We do it More Efficiently?

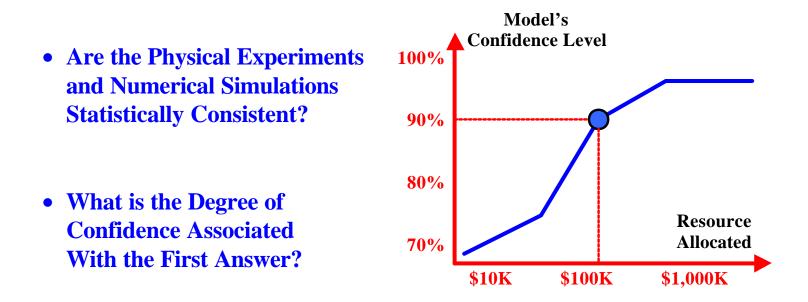
✓ Can We Assess the Predictive Quality of Our Models?

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PREDICTABILITY OF NUMERICAL MODELS



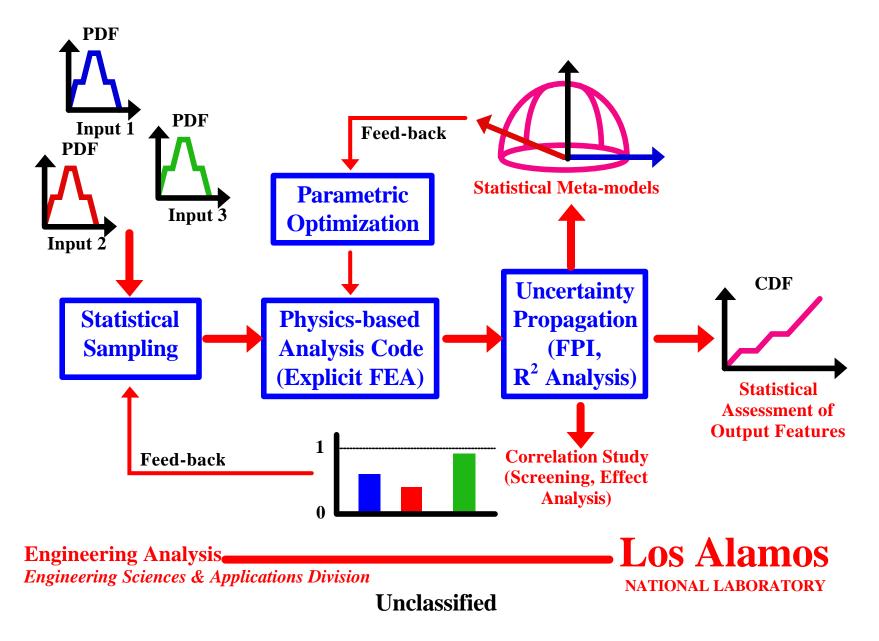
PARADIGM FOR MODEL VALIDATION



• If Additional Data Sets Are Available, by How Much Does the Confidence Increase?

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STEPS OF UNCERTAINTY QUANTIFICATION



OUTLINE

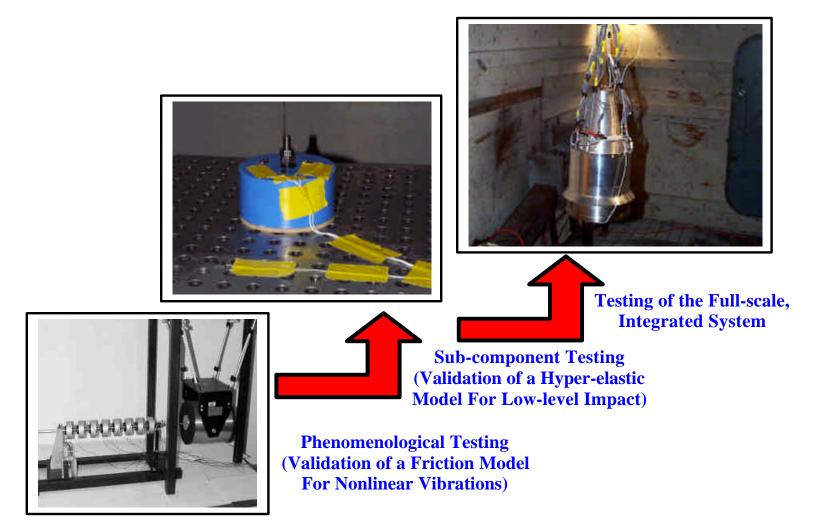
- Notation & Definition
- Motivation



- Forward Mount Impulse Experiment (ASCI Demonstration)
- Unresolved Issues & Challenges

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OVERVIEW OF MODEL VALIDATION (ESA-EA)



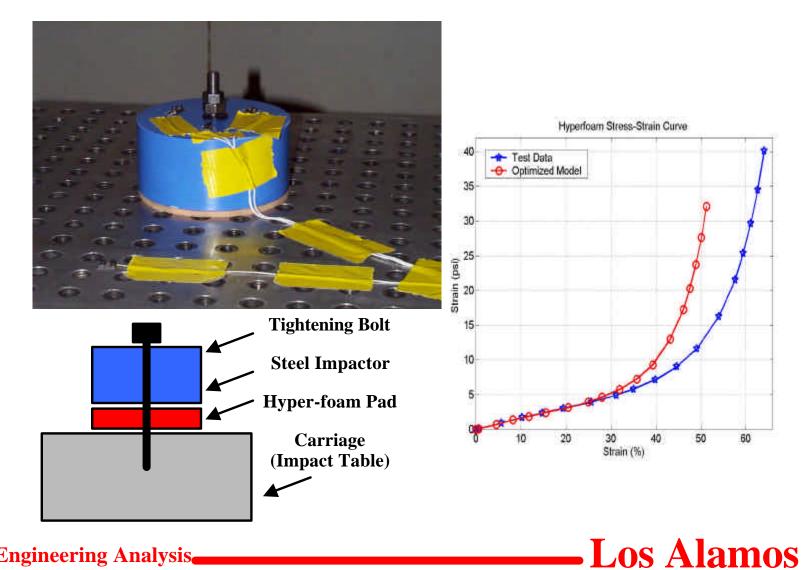
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LANL IMPACT EXPERIMENT

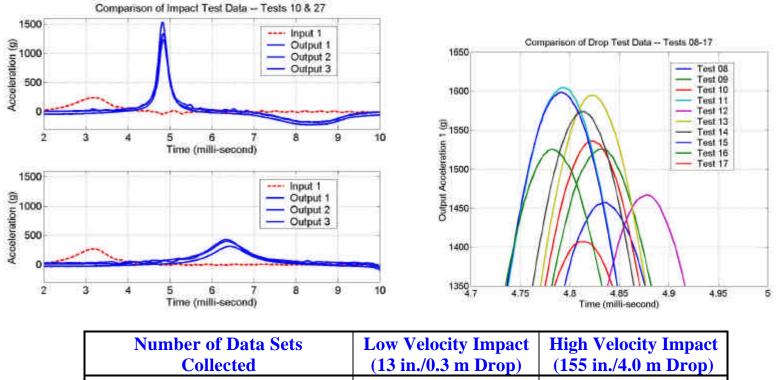


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EXPERIMENTAL VARIABILITY (LANL Impact Test)



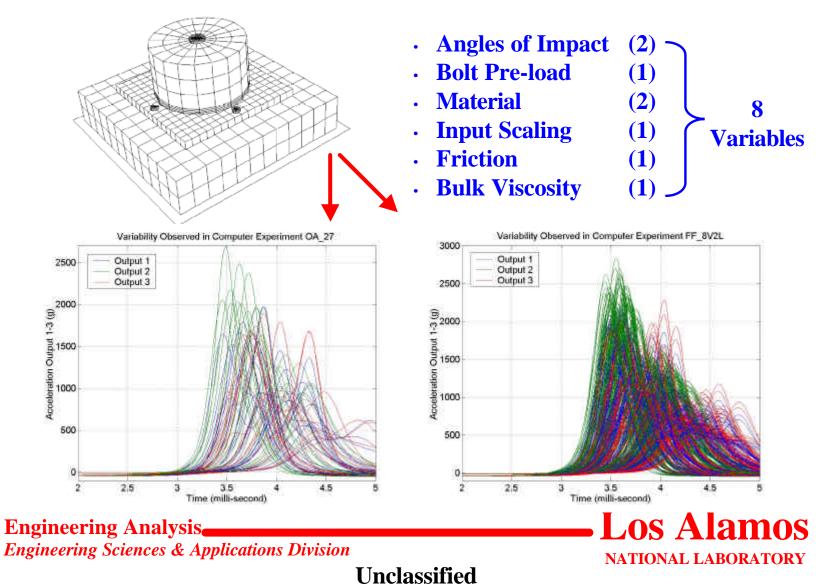
	5 Tests
Thick Layer (0.50 in/12.6 mm) 10 Tests	5 Tests
Thick Layer (0.50 in/12.6 mm)10 Tests	5 Test

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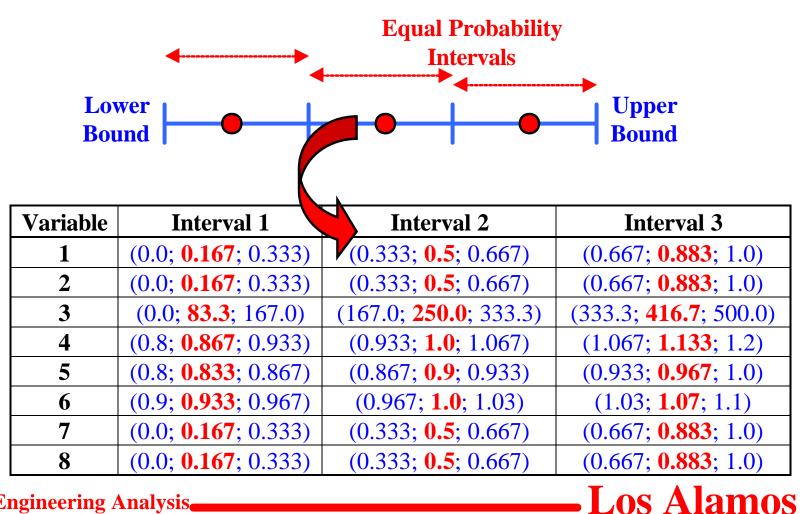
VARIABILITY OF THE NUMERICAL EXPERIMENTS

(LANL Impact Test)



DESIGN OF COMPUTER EXPERIMENTS

(LANL Impact Test)



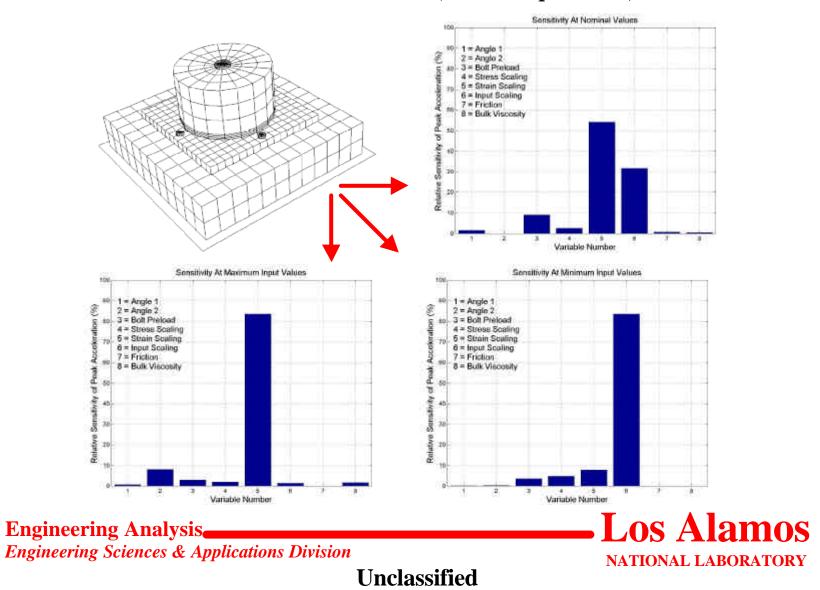
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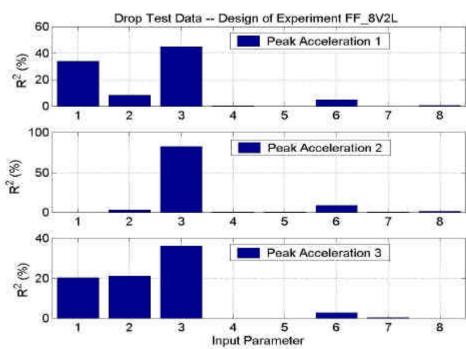
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LOCAL SENSITIVITY STUDY (LANL Impact Test)

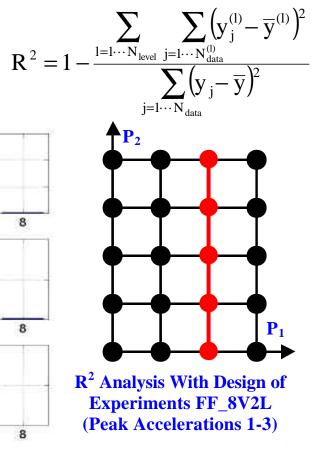


STATISTICAL EFFECTS ANALYSIS (LANL Impact Test)

• Which Variables or Combinations of Variables Best Explain the Total Variability?



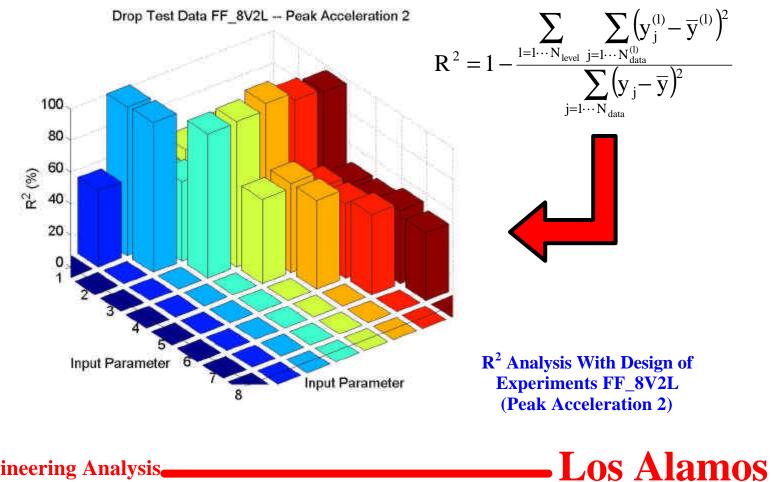
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STATISTICAL EFFECTS ANALYSIS (LANL Impact Test)

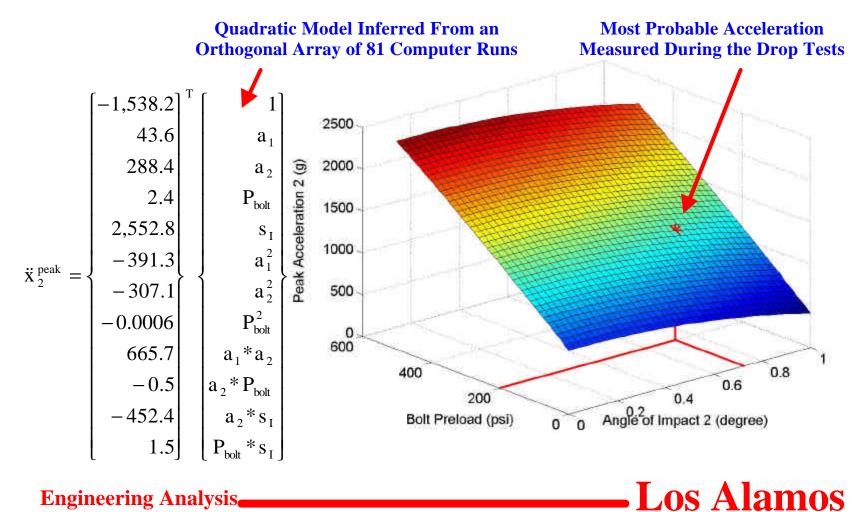


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FAST RUNNING MODELS (LANL Impact Test)

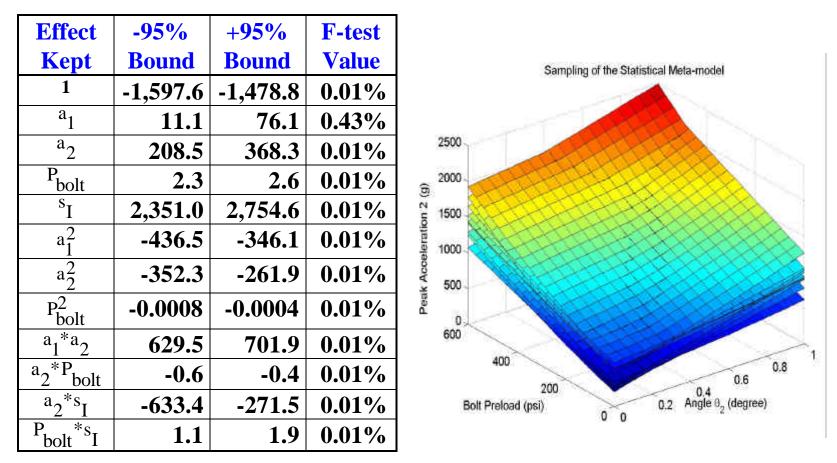


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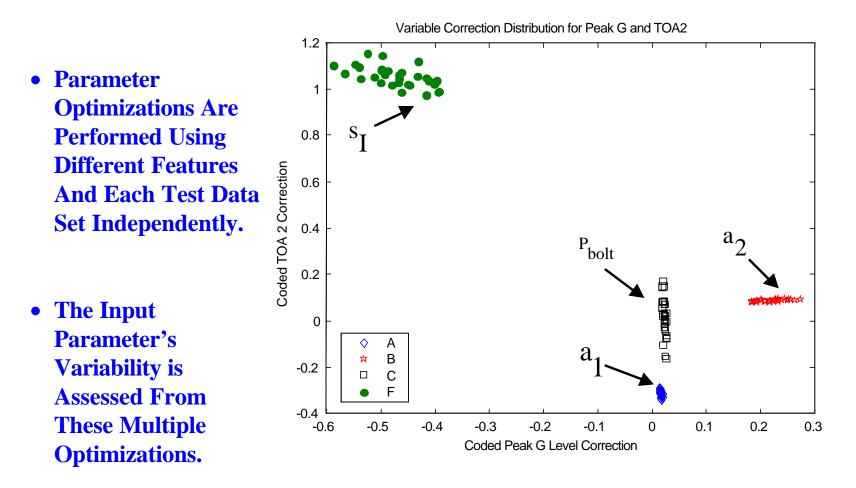
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SAMPLING OF STATISTICAL META-MODELS (LANL Impact Test)



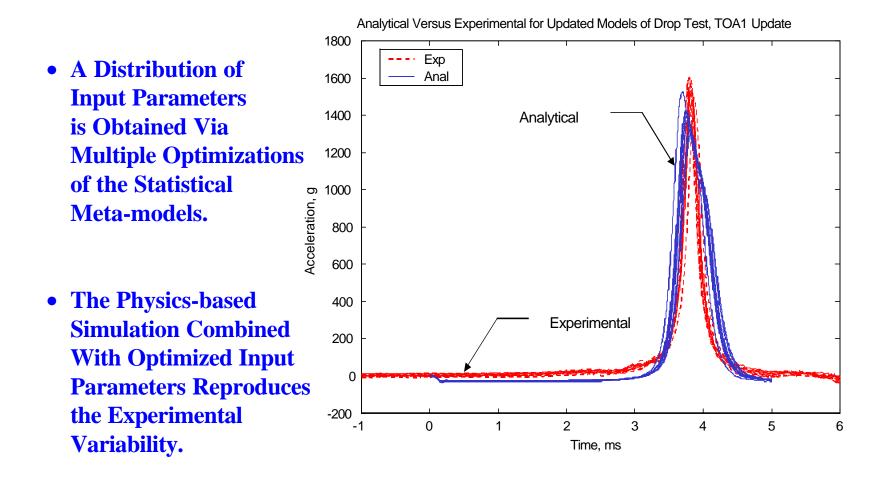
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OPTIMIZATION OF INPUT PARAMETERS (LANL Impact Test)



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PREDICTED VS. OBSERVED VARIABILITY



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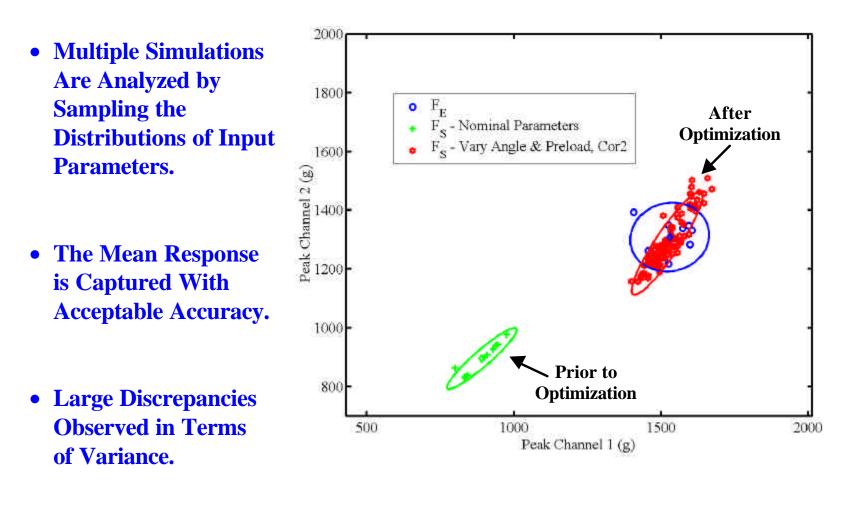
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PREDICTED VS. OBSERVED VARIABILITY

(LANL Impact Test)

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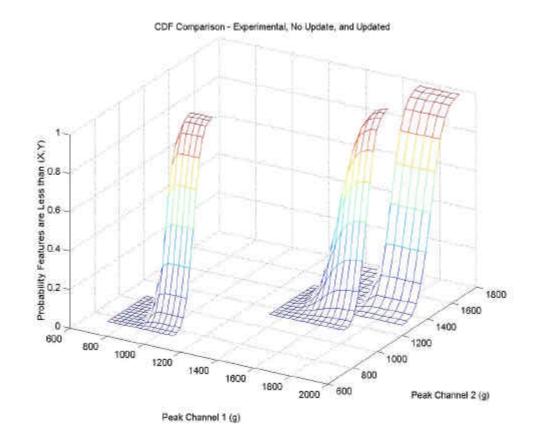
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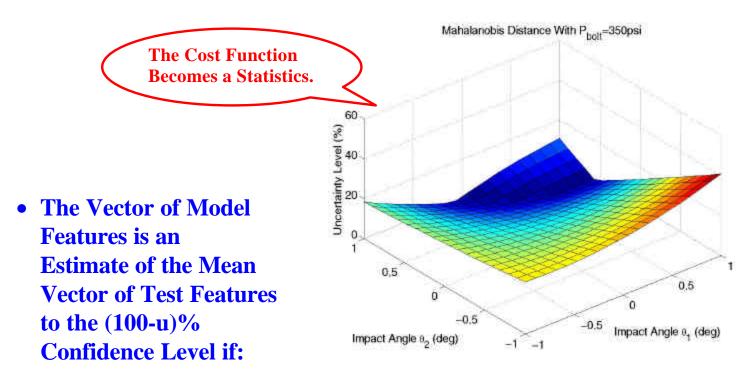
COMPARISON OF MULTIVARIATE DISTRIBUTIONS (LANL Impact Test)

- Pearson's Correlation Ratio
- Multivariate Chi² Analysis
- Kolmogorov-Smirnov Test
- Mahalanobis
 Distance
- Kullback-Leibler Relative Entropy
- ... Others?



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MAHALANOBIS DISTANCE (LANL Impact Test)



$$\left(\overline{y}^{\text{test}} - y(p)\right)^{T} \left[S_{yy}^{\text{test}}\right]^{-1} \left(\overline{y}^{\text{test}} - y(p)\right) \leq \frac{N_{y} \left(N_{s} - 1\right)}{N_{s} \left(N_{y} - 1\right)} F_{N_{y}; N_{s} - N_{y}} \left(u\right)$$
(Normal Distribution Assumed.)

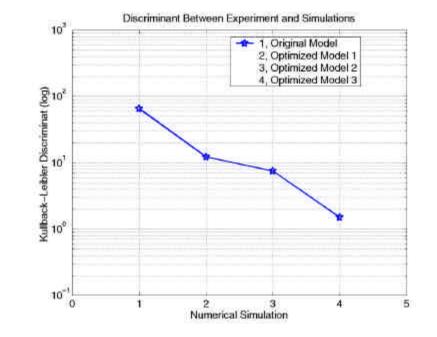
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KULLBACK-LEIBLER RELATIVE ENTROPY (LANL Impact Test)

• Expected Value of Ratio Between PDF's:

$$J(p) = E\left[log\left(\frac{f(y(p))}{f^{test}(y)}\right)\right]$$

• If PDF's Are Normally Distributed:



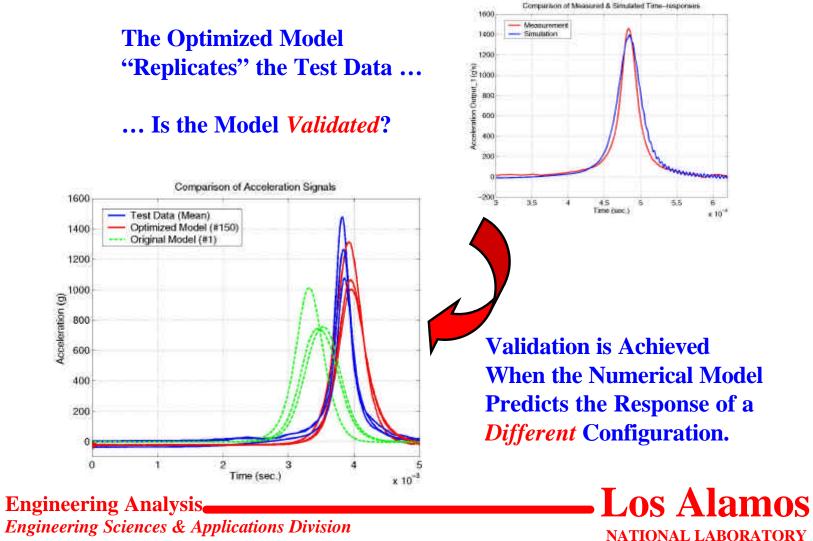
$$J(p) = \frac{1}{2} \left(\overline{y}^{\text{test}} - \overline{y}(p) \right)^{T} \left[S_{yy}^{\text{test}} \right]^{-1} \left(\overline{y}^{\text{test}} - \overline{y}(p) \right) + \frac{1}{2} \left(\text{Trace} \left(\left[S_{yy} \right] \left[S_{yy}^{\text{test}} \right]^{-1} \right) - \log \left(\frac{\det \left[S_{yy} \right]}{\det \left[S_{yy}^{\text{test}} \right]} \right) - N_{y} \right)$$

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MODEL VALIDATION (LANL Impact Test)



OUTLINE

- Notation & Definition
- Motivation
- Impact Experiment (Development of the Methodology)



- Forward Mount Impulse Experiment (ASCI Demonstration)
- Unresolved Issues & Challenges

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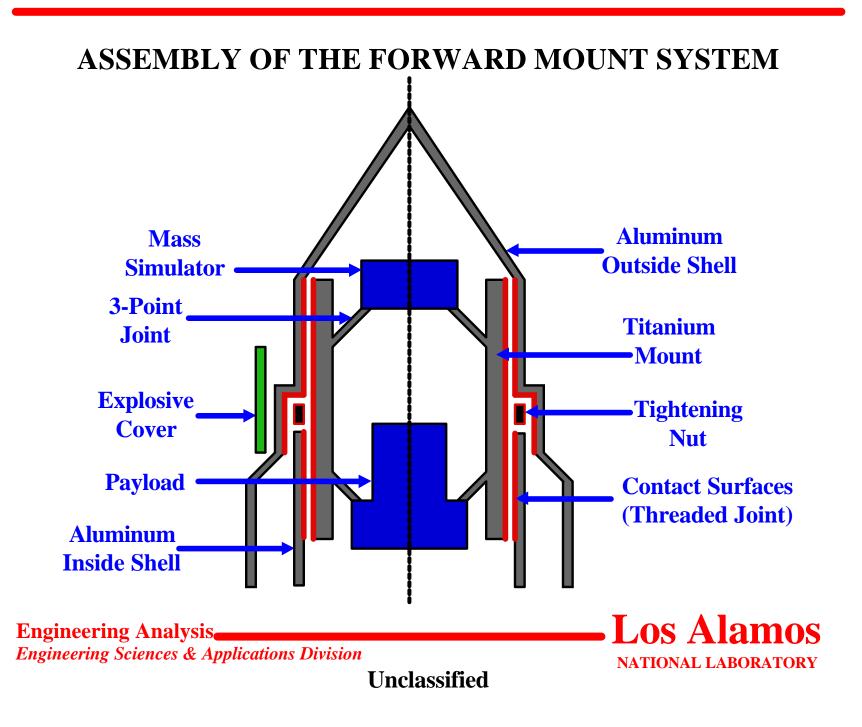
FORWARD MOUNT SYSTEM TESTS

Components:
✓ Lower Case.
✓ Forward Mount.
✓ Electronics.
✓ Retaining Nut.
✓ Upper Case.
✓ Mass Simulators.



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FORWARD MOUNT SYSTEM TESTS (Low Level Impulse Tests)

- Useful Model Validation Requires Carefully Planned Experiments:
- ✓ Well-defined Input.
- ✓ Sufficient Instrumentation For Measuring Appropriate Response Quantities.
- ✓ Test Matrix That Appropriately Varies Key Parameters.
- ✓ Data Resolution Capable of Capturing all Frequency Content of Interest.



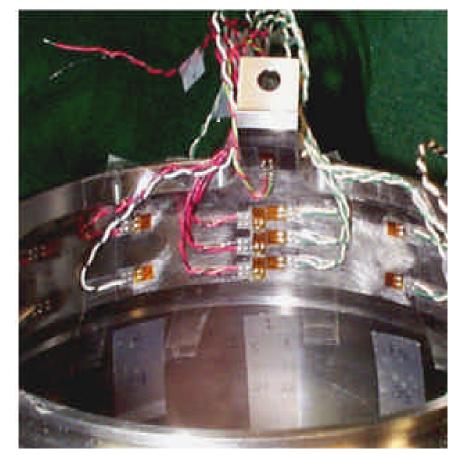
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FORWARD MOUNT SYSTEM TESTS (Instrumentation)

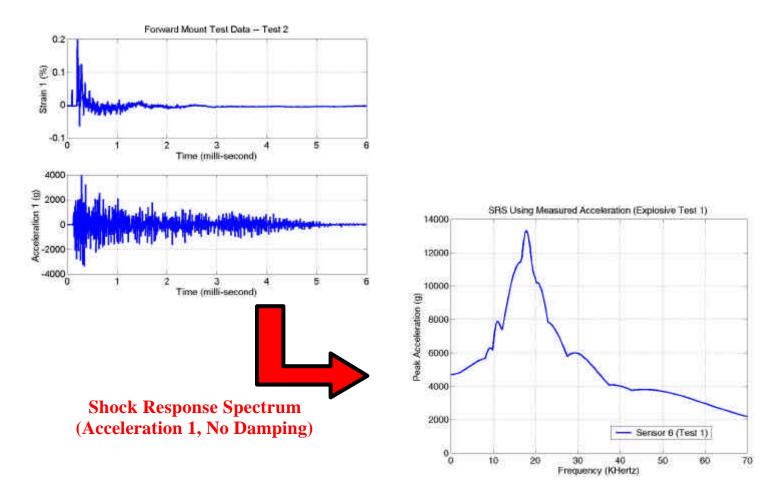
- 33 Strain Gages on Inside of Titanium Mount.
- 6 Accelerometers on Mass Simulators.
- Fiber Optic Displacement Measurement.
- High Speed Photography.
- Sampling Rate = 50 x 10⁻⁹ seconds.



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TEST DATA (Forward Mount Low Level Impulse)

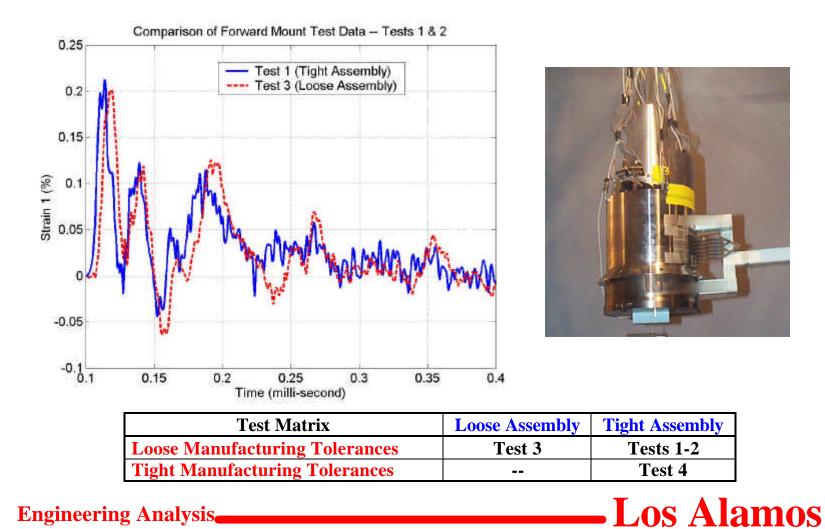


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EXPERIMENTAL VARIABILITY (Forward Mount Low Level Impulse)



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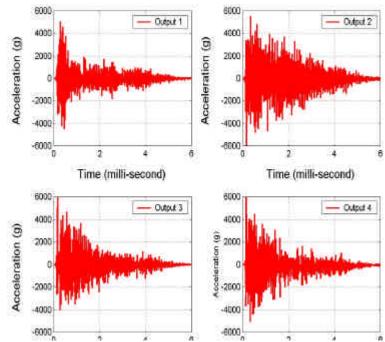
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EXPLICIT FINITE ELEMENT MODELING (W76/Mk4)

Main Features:

- ✓ Coupled Thermal-Structure
- ✓ ParaDyn (Parallel Explicit Dyna3D)
- ✓ 1.4 Million Elements
- ✓ 480 Contact Surfaces
- ✓ Over 6 Million DOF's
- ✓ Stable Time Step = 25 Nano-second
- ✓ Platform: ASCI/BlueMountain
- ✓ 504-750 Processors
- ✓ 1.3 Hour CPU/Milli-second of Response



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FEATURES FOR NONLINEAR DYNAMICS

- Karhunen-Loeve Decomposition
- Principal Component Analysis
- AR, ARX & ARMA Models
- Control Charts
- Shock Response Spectrum
- Spectral Density Function
- Joint Probability Density Function of the Output

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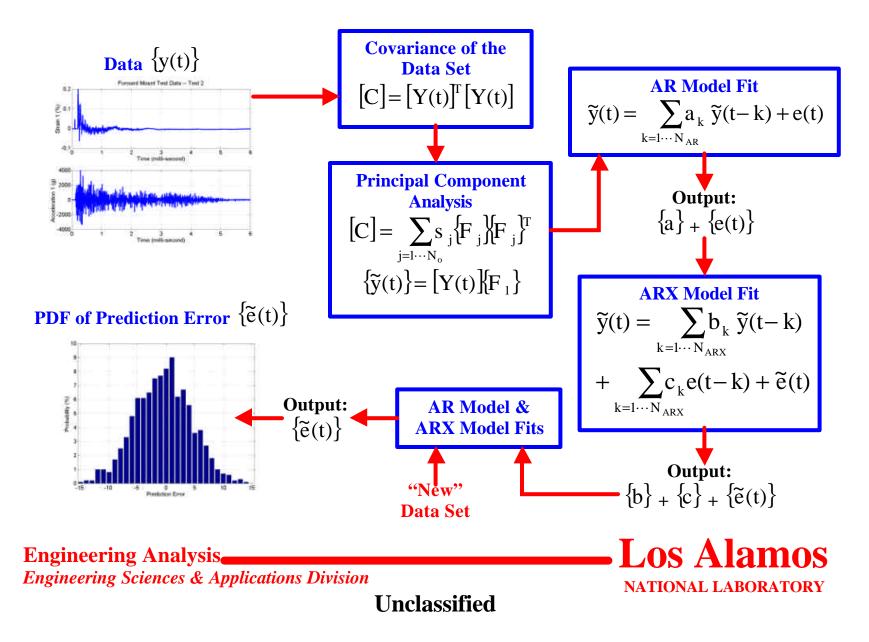
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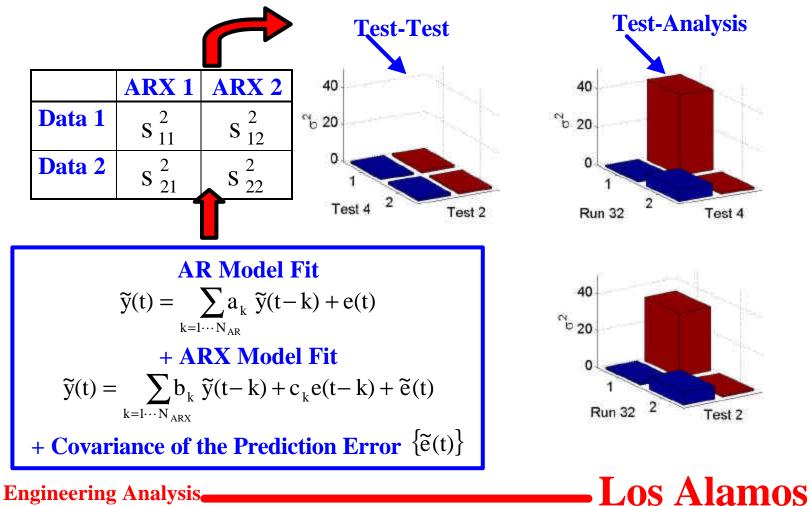


Analysis Techniques Specific to Linear Systems

PATTERN RECOGNITION



TEST-ANALYSIS CORRELATION (Forward Mount Low Level Impulse)



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LIST OF INPUT PARAMETERS (Forward Mount Low Level Impulse)

Variable Physical Influence Lower **Statistical** Upper Description Number **Guessed**? Bound Bound **Distribution Tape Pre-load** Uniform Medium 100.0 N 4,000.0 N 1 Uniform **Nut Pre-load** High 250.0 N 4,000.0 N 2 Uniform **Upper Shell Pre-load** High 250.0 N 2,000.0 N 3 **Static Friction, Al/Al** Medium 0.80 Uniform 4.00 4 **Static Friction**, Ti/Ti 0.20 2.40 Uniform Low 5 **Static Friction, Al/Ti** High 0.50 3.00 Uniform 6 **Static Friction, SS/Ti** Medium 0.20 2.40 Uniform 7 **Kinetic Friction, Al/Al** Uniform Medium 0.80 4.00 8 **Kinetic Friction, Ti/Ti** 1.80 Uniform 9 Low 0.10 Uniform **Kinetic Friction, Al/Ti** High 0.10 3.00 10 **Kinetic Friction, SS/Ti** Medium Uniform 0.10 1.80 11 **Input Signal Scaling** 1.2 Uniform Unknown 1.0 12

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New!

TAGUCHI ORTHOGONAL ARRAY — OA_32

- The Matrix of Experiments is Full Rank.
- Main (Linear) Effects of the Input-Output Model Are Kept Uncorrupted From Second Order Effects (No Aliasing).

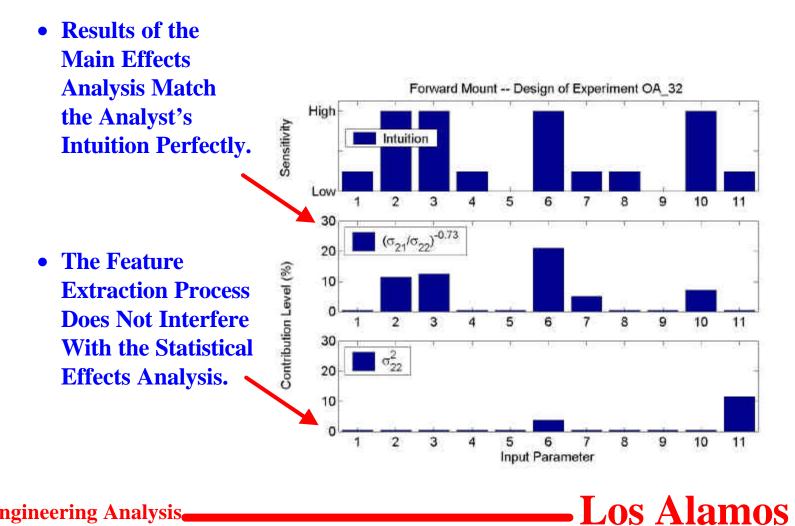
			(For	war	d Me	ount	Low	, Lei	vel I	три	lse)	
	Run	1	2	3	4	5	6	7	8	9	10	11
	1	20	10	10	0.8	0.2	0.5	0.2	0.8	0.1	0.1	0.1
	2	220	10	10	0.8	0.2	3.0	0.2	0.8	1.8	3.0	0.1
	3	15	220	10	0.8	0.2	3.0	2.4	0.8	0.1	0.1	1.8
	4	220	220	10	0.8	0.2	0.5	2.4	0.8	1.8	3.0	1.8
of	5	20	15	120	0.8	0.2	3.0	2.4	4.0	1.8	0.1	0.1
	6	220	10	115	0.8	0.2	0.5	2.4	4.0	0.1	3.0	0.1
s is	7	15	215	125	0.8	0.2	0.5	0.2	4.0	1.8	0.1	1.8
	8	220	215	125	0.8	0.2	3.0	0.2	4.0	0.1	3.0	1.8
	9	20	10	10	4.0	0.2	0.5	2.4	4.0	1.8	3.0	1.8
	10	220	10	10	4.0	0.2	3.0	2.4	4.0	0.1	0.1	1.8
	11	15	220	10	4.0	0.2	3.0	0.2	4.0	1.8	3.0	0.1
	12	220	220	10	4.0	0.2	0.5	0.2	4.0	0.1	0.1	0.1
	13	20	15	120	4.0	0.2	3.0	0.2	0.8	0.1	3.0	1.8
	14	220	10	115	4.0	0.2	0.5	0.2	0.8	1.8	0.1	1.8
r)	15	15	215	125	4.0	0.2	0.5	2.4	0.8	0.1	3.0	0.1
e	16	220	215	125	4.0	0.2	3.0	2.4	0.8	1.8	0.1	0.1
	17	20	10	10	0.8	2.4	0.5	0.2	4.0	0.1	3.0	1.8
ıt	18	220	10	10	0.8	2.4	3.0	0.2	4.0	1.8	0.1	1.8
	19	15	220	10	0.8	2.4	3.0	2.4	4.0	0.1	3.0	0.1
Kept	20	220	220	10	0.8	2.4	0.5	2.4	4.0	1.8	0.1	0.1
	21	20	15	120	0.8	2.4	3.0	2.4	0.8	1.8	3.0	1.8
	22	220	10	115	0.8	2.4	0.5	2.4	0.8	0.1	0.1	1.8
	23	15	215	125	0.8	2.4	0.5	0.2	0.8	1.8	3.0	0.1
d	24	220	215	125	0.8	2.4	3.0	0.2	0.8	0.1	0.1	0.1
	25	20	10	10	4.0	2.4	0.5	2.4	0.8	1.8	0.1	0.1
ts	26	220	10	10	4.0	2.4	3.0	2.4	0.8	0.1	3.0	0.1
`	27	15	220	10	4.0	2.4	3.0	0.2	0.8	1.8	0.1	1.8
j).	28	220	220	10	4.0	2.4	0.5	0.2	0.8	0.1	3.0	1.8
	29	20	15	120	4.0	2.4	3.0	0.2	4.0	0.1	0.1	0.1
	30	220	10	115	4.0	2.4	0.5	0.2	4.0	1.8	3.0	0.1
	31	15	215	125	4.0	2.4	0.5	2.4	4.0	0.1	0.1	1.8
	32	220	215	125	4.0	2.4	3.0	2.4	4.0	1.8	3.0	1.8

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INPUT-OUTPUT MAIN EFFECTS ANALYSIS (Forward Mount Low Level Impulse)



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Unclassified

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OUTLINE

- Notation & Definition
- Motivation
- Impact Experiment (Development of the Methodology)
- Forward Mount Impulse Experiment (ASCI Demonstration)



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SPECIFIC QUESTIONS & ISSUES (1/2)

- How Can We Compare Data Sets?
 - ✓ Are There Features of Choice Adopted by Statisticians or Others?
- Are There Techniques Available For Hypothesis Testing of Multivariate Distributions?
- Can We Sample the Input Parameter Space Most Efficiently?
- We Need to Understand Better Techniques For Designing Experiments.

✓ How to Fold-over a Design of Experiment?
✓ How to Make Use of Runs Already Completed?
✓ How to Add One Variable to an On-going Analysis?

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SPECIFIC QUESTIONS & ISSUES (2/2)

- Is Our Approach For Translating Variability Observed on the Output in Terms of Statistical Distributions on the Input Correct?
- Are There Techniques Available For Optimizing the Variance of a Distribution?
- Are There Techniques Available For Replacing the Predictions of a Statistical Meta-model by Ensemble Averages?

✓ How Can a Meta-model be Sampled?

• We Need to Understand Better the Differences Between Theories Available For Modeling Uncertainty.

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CONCLUSION

- The Need For Model Validation and Uncertainty Quantification is Rapidly Growing and Expanding.
- Dealing With Nonlinear Systems and Uncertainty is Going to Be Very Expensive, NO MATTER WHAT YOU DO.
- Experience May Be Gained From Learning What is Being Achieved in Other Scientific Communities.

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