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Uncertainty Quantification and Model Validation: Session Overview and Introduction

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Welcome to the UQ&MV Session

- **Purpose of this session**
  - What are Uncertainty Quantification and Model Validation?
  - How to explore the issues of UQ&MV in structural dynamics?
  - Where should we be headed?
  - How are other fields exploring UQ&MV?

- **Order of Session**
  - Ken Alvin, Sandia, “From the Middle of the Action”
  - Lisa Moore, LANL, “The Role of Statistical Sciences”
  - Anton Kast, LBNL, “Predicting Molecular Dynamics”
  - John Cafeo, GM, “Needs of Industry”
  - Mark Anderson, LANL, “The Road Ahead”

Some "Controversy-Free" Definitions

- **Test** = Physical Experiment
- **Simulation** = Numerical (computational) Experiment
- **Meta-Model** or **Response Surface** =
  Fast-running, possibly statistical model
- **Feature** = Quantity synthesized or mapped from
  experiment output
- **Cost Function or Metric** = Expression of a residue
  or "distance" between experiments

- **Verification**: Determination that computational results "solve the equations correctly"
- **Validation**: Determination that computational results resemble reality (compare simulation to test)

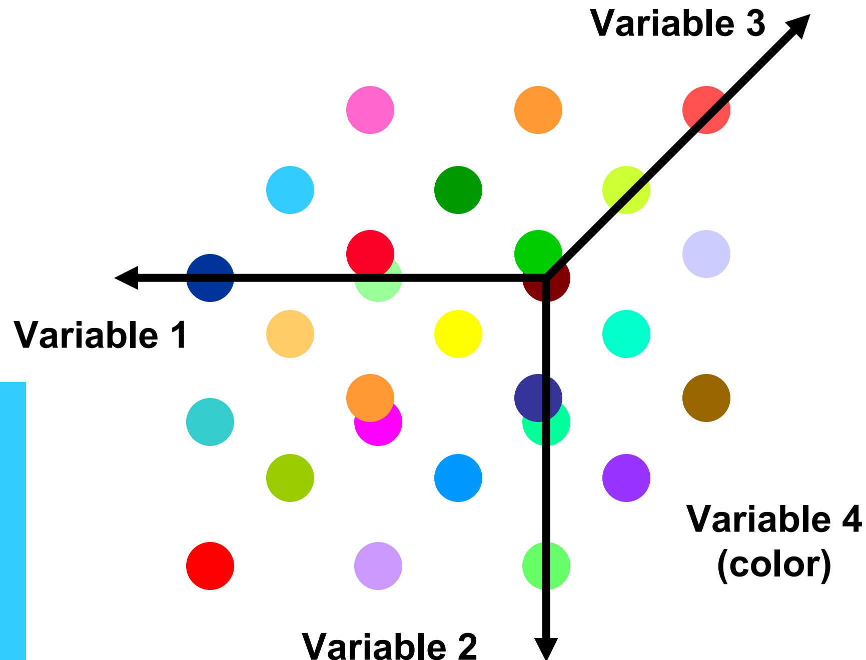
On the Threshold of Revolutionary Change

In Feb'00, LANL engineers performed an unprecedented calculation using 17.8 years of equivalent single-processor computing time over 72 hours, using nearly 4,000 ABAQUS/Explicit licenses

Calculation Highlights

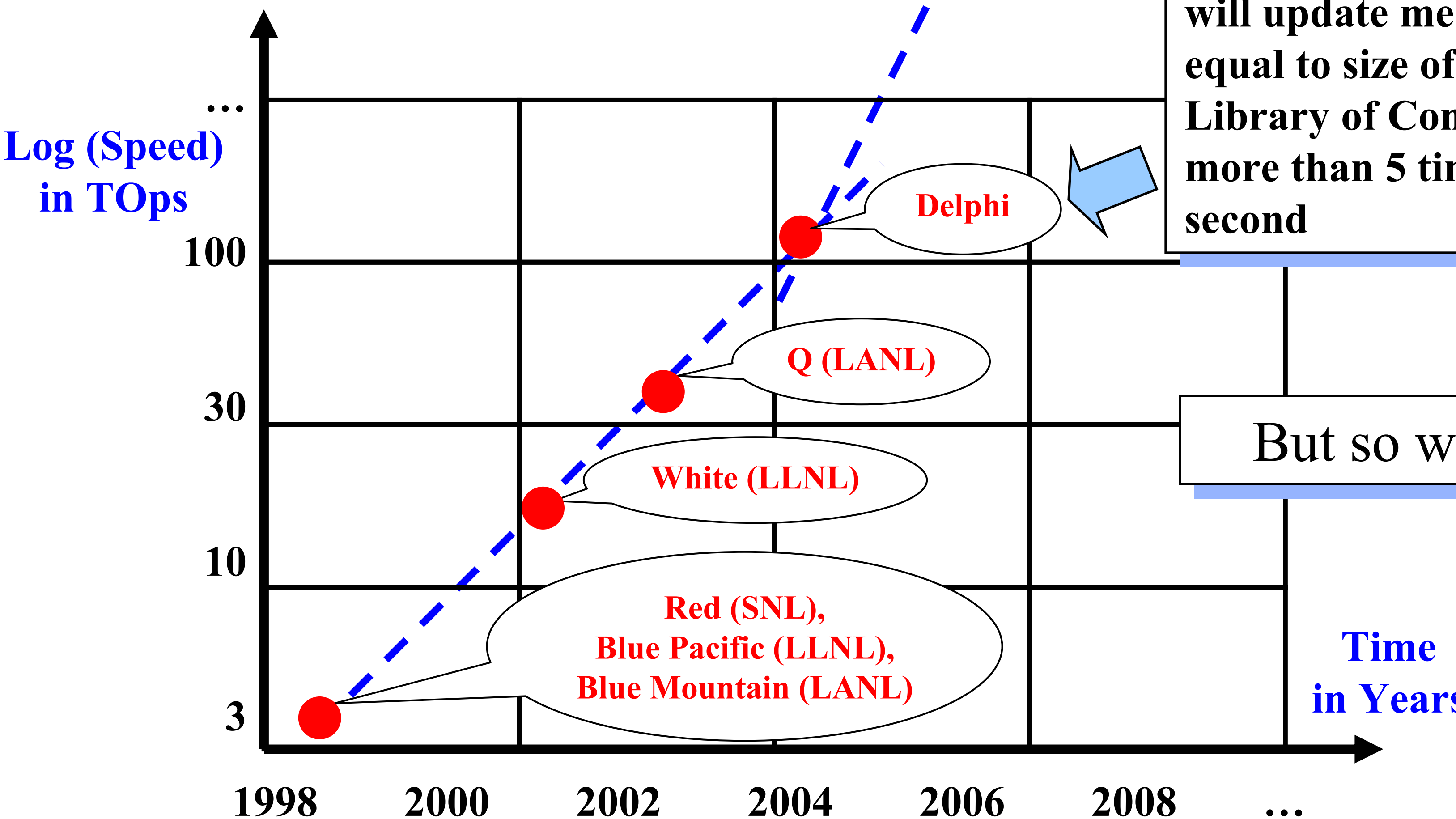
- **> 15,000 10 hour simulations**
- **~ 1.5 Million DOFs**
- **30,000 elements**
- **100 contact pairs**

Calculation was performed on 3,968 processors representing 65% utilization of a 3 Tera-Flop platform



Calculation populated a 4-D response space

On The Path Towards 100 TeraOps:



100 TeraOps machine will update memory equal to size of Library of Congress more than 5 times per second

But so what?

Harnessing TeraOps for Structural Analysis:

Beyond Computing π to Higher Precision

High-fidelity, 3D analysis is necessary to reveal multi-component interactions that are essential to understanding complex system behavior.

- In the absence of full system proof tests, must bring huge new computational resources to bear on this objective (ASCI-Advance Strategic Computing Initiative)

  Raises new challenges for Engineering Analysis:
  - **Verification of Computational Codes (ParaDYN, PRONTO3D, etc.)**
  - **Validation of Models and Modeling Techniques**
  - **Interrogation of Large Data Sets**

Model Validation is Essential to Ensure that Computational Results Resemble Reality in Some Quantifiable Way

Otherwise: Who cares what the big computer says?

Experiments: Beyond Proof Testing

- **Validation experiments must be:**
  - **SIMPLE ENOUGH to isolate the mechanical phenomena of interest**
  - **COMPLEX ENOUGH to represent the phenomena realistically**
  - **INSTRUMENTED so that the features can be measured**
  - **EXCITED over an adequate range of environments**

Beyond Proof Testing:
Analysis Predictions Guide the Experiment
Experimental Data Feed the Model

Our precious experimental resources must be focused on learning how to IMPROVE our modeling rather than PROVE whether something will break

Model Validation or Model Calibration?

- **Classical Model Updating Approach**
  - Build Model
  - Perform Test
  - Update (calibrate) parameters of model to match test data
- **Resulting model predicts (*POST*dicts) the test data, but what can we predict with certainty using this model for environments outside the test conditions? How well do we understand the mechanics?**

Model Calibration
is of limited use for an analyst to understand the adequacy of a model, but can provide insight into the conditions of a particular experiment

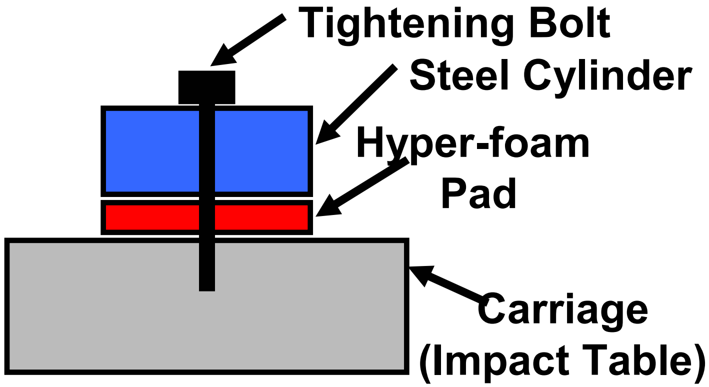
Beyond Goodness of Fit: Model Validation

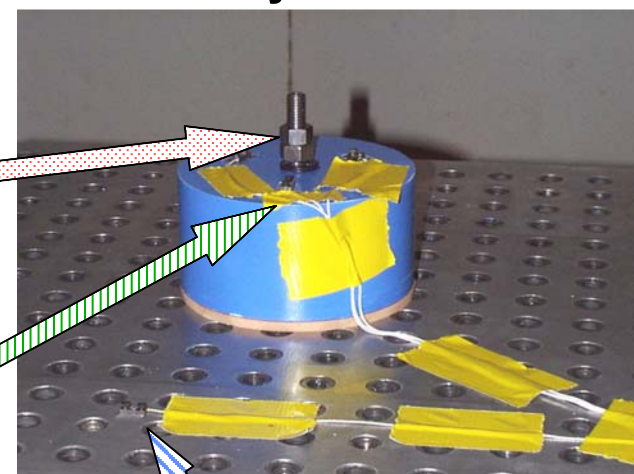
Model Validation:
Ensuring that the model adequately represents key mechanical phenomena and predicts response features of interest accurately over range of expected environments

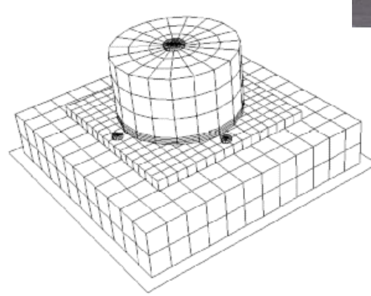
- **How is this accomplished?**
  - Selection of Validation Features
    - » Purpose of building the model --
      What are we really trying to predict, anyway?
      (Peak accelerations, modal frequency, maximum stress)
    - » How to obtain corresponding features from measured data?
  - Parameter Effects Analysis (Beyond Sensitivity Analysis)
    - » Adequacy of model form and modeling assumptions
    - » Relative importance of model parameters
    - » Key Mechanical Effects to focus on in experiment
    - » Applicability of model outside regime of existing test data

Impact Response of Polymer Foam Between Metal Components

- **Experiment: Impulse load applied to thin layer of polymer foam with steel cylinder using drop table**
- **Objective: Determine key parameters of model to predict features of measured acceleration (e.g. peak, arrival time)**
  - **Does polymer constitutive behavior vary with velocity?**







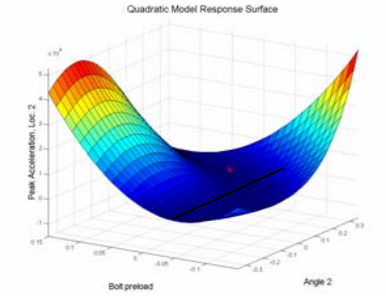
Model Validation: Main Effects Analysis

- **Main effects analysis (parameter screening)**
  - Various parameters sets selected using design of experiments (DoE) principles -- 8 parameters with 2 levels each -- sizes of 27, 81, 256 (full)
  - Main effects (linear) response surface OF PEAK G MAGNITUDE AND TIME OF ARRIVAL fit to each set of results
  - ANOVA (Analysis of Variance) techniques measured contribution of each parameter to accuracy of response surface fit
  - Only parameters with significant contribution passed the screening:
    - » Preload of bolt, Angles of impact (2), Magnitude of impact
  - Scaling of polymer constitutive relation was unimportant -- thus polymer has insignificant dependency on strain rate for this velocity regime
  - 27-run case gave as good of response surface fit as 256-run case (full factorial)
  - By comparison, sensitivity analysis gave inconsistent results depending upon assumed parameter values

For Parameter Screening:
Main effects analysis gave much more useful results than sensitivity analysis

Model Validation: Parameter Optimization

- **Coupled effects analysis (parameter screening)**
  - **More levels on fewer parameters (4V4L, 5V3L)**
  - **Develop quadratic response surface (meta-model) using full-factorial runs (256, 243 respectively)**

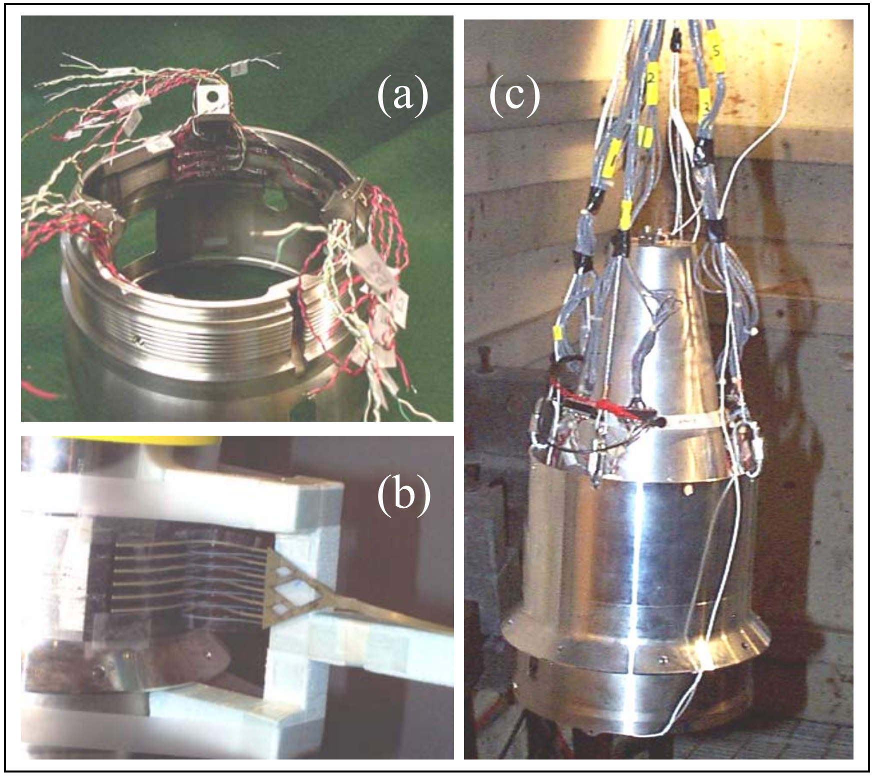


  - **Parameters optimized such that distances between measured features and simulated features were minimized (using quadratic meta-model)**
  - **Optimized model parameter values improved time history prediction of model, as well as providing a bound on experimental variability**

For Parameter Optimization:
Fits to various experimental repetitions gave indication of variability in test runs

Beyond Toy Problems: Impulsive Loading of a Threaded Joint

- **Experiment: Apply impulse load to outside of test assembly using explosive charge strips.**
- **Objective: Predict acceleration and strain response of locations on structure, including propagation of shock across threaded joint. Select appropriate measures to validate model.**
- **Main effects analysis indicates that preloads and friction in joints are key parameters, but...**
- **Many physically meaningful features, based on both time and frequency-domain signals, have been investigated**
- **Still have not found a feature that is amenable to accurate main effects analysis (good fitting of response surface)**



Threaded Interface Component (a), Explosive Charge Strips (b), Assembly in Test Configuration (c)

Relationship of Analysis and Experiments is Changing...

- **Primary Objective of ASCI is to "replace system-level proof tests"**
- **Far from replacing experiments, more complex computational techniques have a *higher reliance* on experimentation for reality check and understanding of mechanics**
- **Need more experiments in those regimes where we CAN acquire data with reasonable cost**

But they must still be friends