

An Overview of Sensitivity Analysis and Uncertainty Quantification Methods

Anthony A. Giunta

Validation and Uncertainty Quantification Processes Dept. (01533)
Sandia National Laboratories
Albuquerque, NM

Presentation for SNL ASC Principal Investigators
13 July 2006

*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Unclassified Unlimited Release

Outline

- **Motivation**
- **Background**
 - Risk-Informed Decision Making
 - Verification & Validation
 - Sensitivity Analysis & Uncertainty Quantification (UQ)
- **Intro to Sensitivity Analysis and UQ**
 - Cantilever Beam Sensitivity Analysis
 - UQ Example #1: probabilistic uncertainty
 - UQ Example #2: non-probabilistic uncertainty
- **Real world UQ application:**
 - Electrical component thermal response UQ study
- **Summary**

Acknowledgements

- **Contributors to this talk:**

- Marty Pilch
- Paul Yarrington
- Tim Trucano
- Bill Oberkampf
- Tom Paez
- Jon Helton
- Rich Hills
- Kevin Dowding
- Vicente Romero
- Laura Swiler
- Mike Eldred
- Scott Klenke
- Monica Martinez-Canales
- Patty Hough
- John McFarland
- et al.

Motivation

- The FY07 call-for-proposals for ASC Advanced Deployment Projects will request specific information on a project's uncertainty quantification (UQ) approach.
- This briefing is intended to provide ASC AD PIs, both current and prospective, with a common background on UQ methods.
- Follow-on briefings will cover:
 - Quantification of Margins and Uncertainties (QMU)
 - DAKOTA toolkit capabilities for UQ and QMU
- My intent is NOT to turn you into statisticians, but rather to bring “statistical thinking” into your ASC engineering analysis and design studies.

Goals for this Briefing

- Understand the connection between verification & validation (V&V), sensitivity analysis (SA), and uncertainty quantification (UQ).
 - And the basic SA and UQ methods & software tools.
- Understand the difference between **aleatoric** (probabilistic) uncertainty and **epistemic** (non-probabilistic) uncertainty.
 - And how this impacts what you can and cannot learn from a UQ study.
- Know where to go for more info:
 - Dept. 1533, Dept. 1411, Dept. 8962
 - Various staff in Org. 12300, Org. 6000

Risk-Informed Decision Making for High Consequence Systems

- Sandia has many high consequence applications:
 - Nuclear weapons surety
 - Non-nuclear DOD applications
 - Infrastructure protection
 - Geological repositories for waste storage
 - Hazardous materials transportation
- Modeling and simulation (M&S) methods are a critical component in all these applications.
 - Q: How do we develop confidence in the M&S data?
 - A: Through a systematic understanding of the strengths and weaknesses of the M&S codes.
 - e.g., NNSA's Verification & Validation Program
- Goals of the Sandia V&V Program:
 - Get the right answer for the right reason.
 - Provide “best estimate + uncertainty” to decision makers.



Sandia's V&V Program Supports Risk-Informed Decision Making

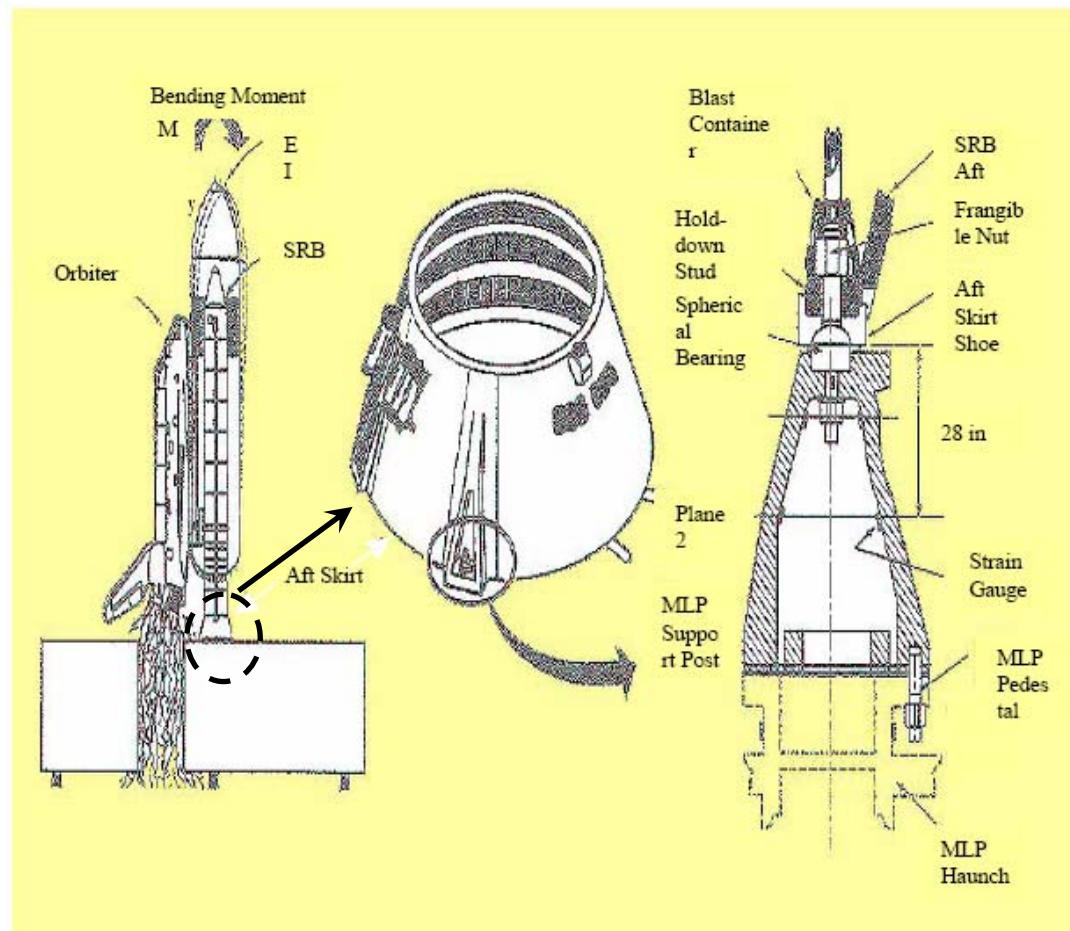
- Risk-Informed Decision Making is based on:
 - Verified and validated computer simulations.
 - Scientifically defensible approach to V&V, uncertainty propagation, and methods for quantifying margins and uncertainties (QMU).
 - *Uncertainty due to stochastic processes (aleatoric)*
 - *Uncertainty due to lack of knowledge (epistemic)*
- Impact of Sandia's Verification & Validation Program:
 - Enable credible computational predictions.
 - Identify most important (sensitive) uncertain/variable parameters; focus research and testing resources on these.
 - Quantify failure probabilities (not just expert-based assertion).
- Sandia's ASC V&V Program leverages past work in probabilistic risk analysis performed at SNL and elsewhere:
 - Nuclear reactor safety
 - Radioactive waste storage: Waste Isolation Pilot Plant

Example of Analysis w/o V&V/UQ: Space Shuttle Solid Rocket Booster Skirt

- Deterministic analysis indicates stress within allowable limit
- Skirt sometimes yields at launch
- Probabilistic analysis reveals high probability of plastic deformation due to scatter in loads and material strength

Take home messages:

1. The best deterministic analysis can yield only limited insight.
2. Neglecting or overlooking uncertainty invites problems.
(NASA: O-rings, foam debris,...)



V&V Terminology & Issues

- **Verification** – “Are we solving the equations correctly?”
 - Is our mathematical implementation of the physics model correct?
 - Code verification: Are the numerical methods in the simulation code working as expected (e.g., rate of convergence, order of accuracy, etc).
 - Solution verification: As the model is refined (e.g. # of elements, # of atoms, # of basis functions, etc), does the predicted solution (a) converge to an answer? and (b) converge to the correct answer?
- **Validation** – “Are we solving the right equations?”
 - Is the physics model sufficient for the application?
 - How much uncertainty is there in the simulation code outputs? How does this uncertainty compare to experimental data uncertainty?
 - Are there any systematic biases between simulation data and experimental data? If so, do they matter?

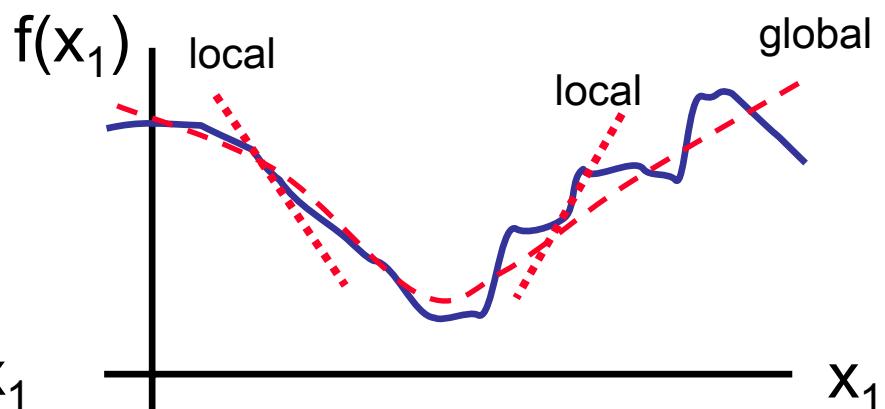
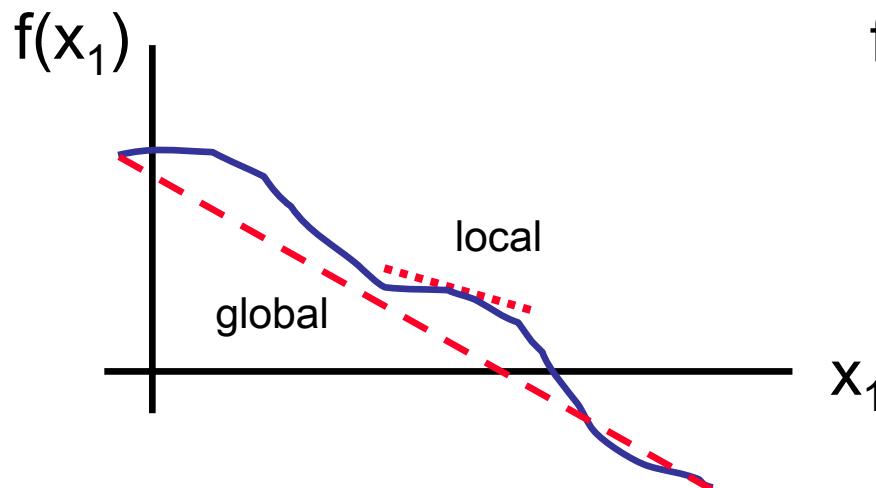
Need UQ to Answer

Sensitivity Analysis & UQ Terminology & Issues

- **Sensitivity Analysis (SA):**
 - How do my code outputs vary due to changes in my code inputs?
 - Need both “local sensitivity” and “global sensitivity” information.
 - Local sensitivity: code output gradient data for a specific set of code input parameter values
 - Global sensitivity: the general trends of the code outputs over the full range of code input parameter values (linear, quadratic, etc.)
- **Uncertainty Quantification (UQ):**
 - What are the probability distributions on my code outputs, given the probability distributions on my code inputs? **(aleatoric UQ)**
 - Estimate Probability[$f > f^*$], i.e., the probability that the system will fail
 - What are the possible/plausible code outputs? **(epistemic UQ)**
- **Quantification of margins and uncertainties (QMU):**
 - How “close” are my code output predictions (incl. UQ) to the system’s required performance level?

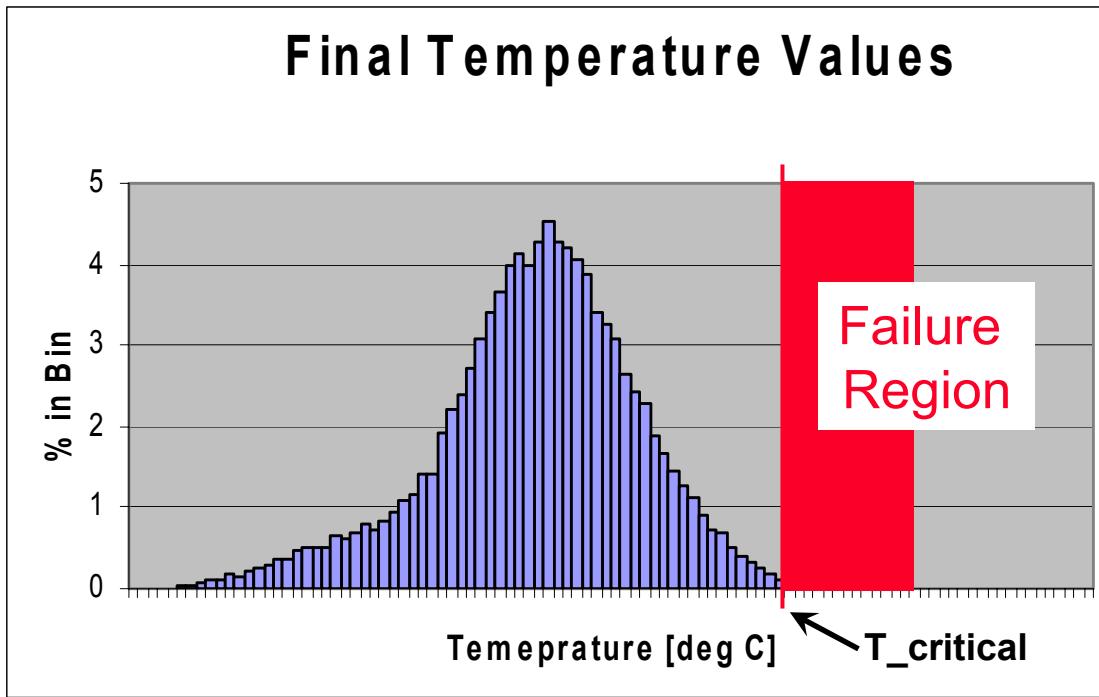
Examples of Sensitivity Analysis

Local vs. Global Sensitivity



- Sensitivity analysis examines variations in $f(x_1)$ due to perturbations in x_1
 - Local sensitivities are typically partial derivatives.
 - Given a specific x_1 , what is the slope at that point?
 - Global sensitivities are typically found via least squares.
 - What is the trend of the function over all values of x_1 ?

Example of Uncertainty Quantification



Hypothetical Example:

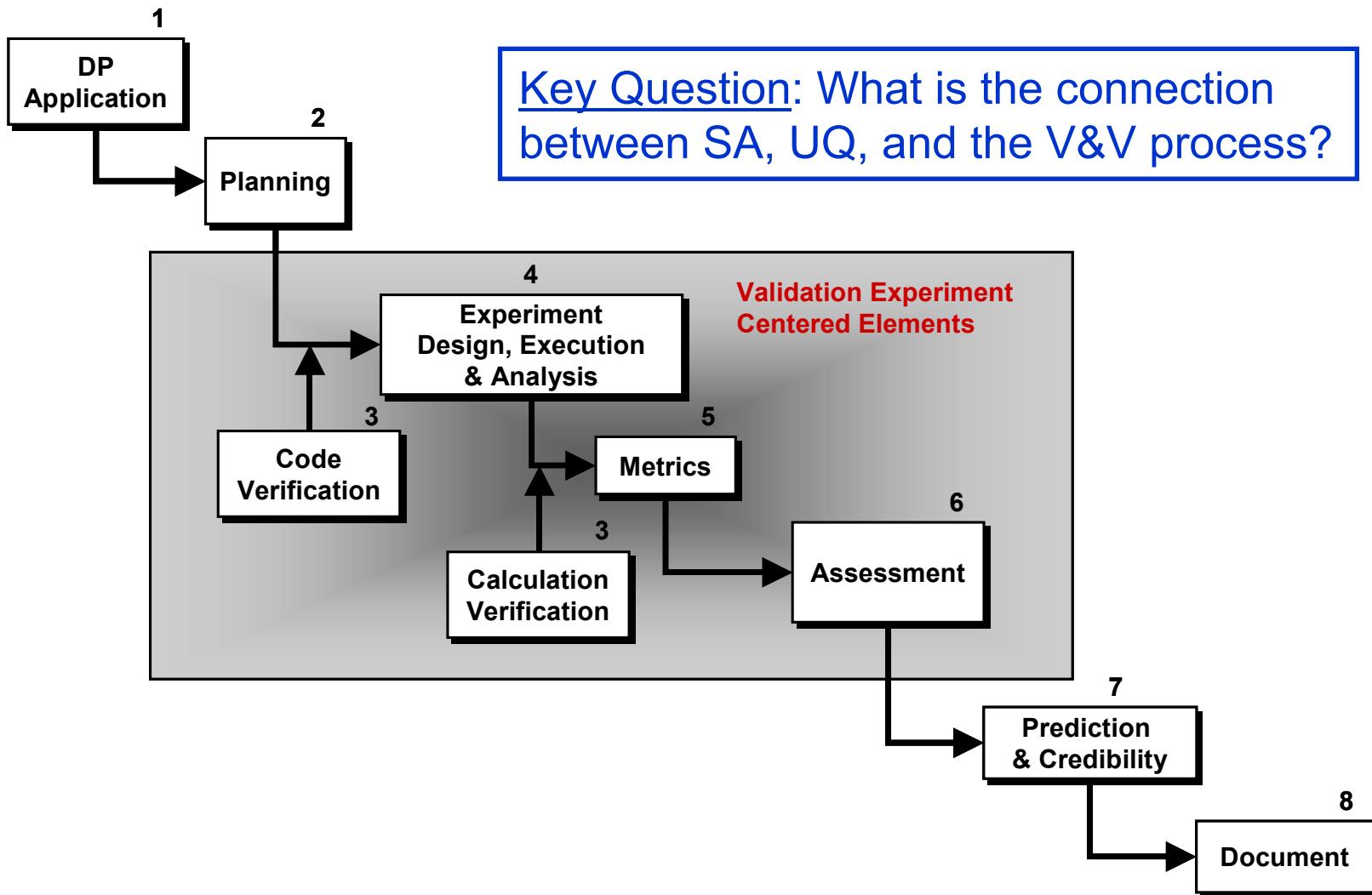
- Temperature = $fcn(x_1, \dots, x_N)$
- x_1, \dots, x_N have probability distributions
- Temperatures are computed via multiple runs of a complex simulation code (e.g., CALORE)

- UQ methods provide statistical info on the code output data:
 - Probability distribution on Temperature, given various x_1, \dots, x_N inputs.
 - Correlations (trends) of Temperature vs. x_1, \dots, x_N .
 - Mean(T), StdDev(T), Probability($T > T_{critical}$)

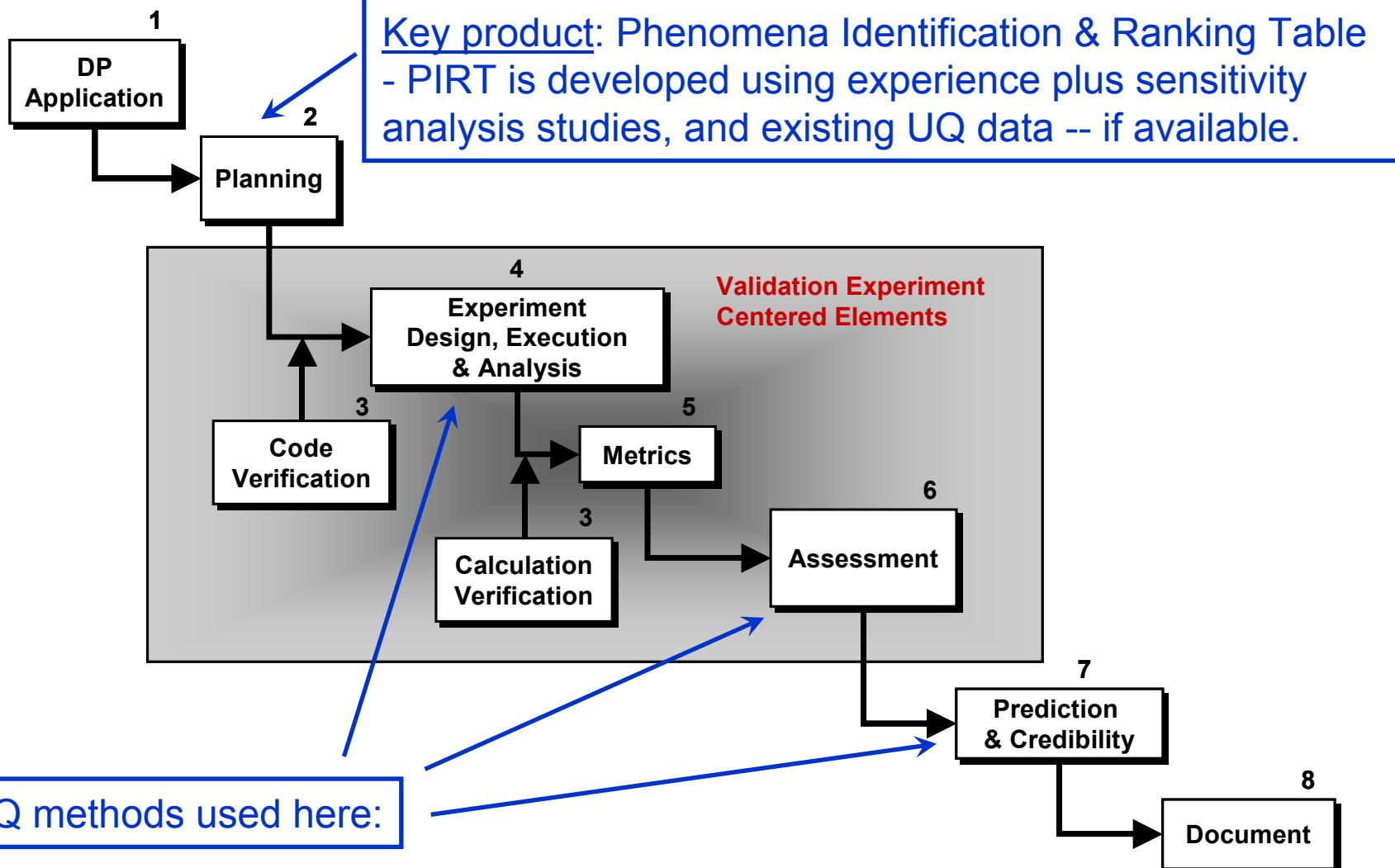
Quick Review of V&V Principles

- **What is the V&V Process?**
- **How do sensitivity analysis and UQ impact the V&V process?**

Overview of the V&V Process



Overview of the V&V Process



Reminder: What is a PIRT?

- **Phenomena Identification and Ranking Table (PIRT)**
 - identifies physical phenomena that effect performance measures over a range of specified environments
 - prioritizes each of the physical phenomena based on their impact on a performance measure over a range of specified environments
 - a table is constructed to rank the relative magnitude of importance of the physical phenomena, for a given system response measure and environment
 - the ability of the code to simulate each of the physical phenomena is ranked according to: **good**, **fair**, **poor**, or **unknown**
 - **Ranking is based on the discrepancy, if any, between the importance of each phenomenon, and the maturity of its corresponding computer model**
 - **This process is subjective, but useful for planning work and allocating resources**

Thermal Modeling PIRT (Example)

Phenomenon	Importance	Code/Model	
	Level	Adequacy	Status
<i>Conductive Heat Transfer</i>			
Material A	High	High	Good
Material B	Medium	Low	Fair (yellow)
<i>Convective Heat Transfer</i>			
Material A	Medium	High	Good
Material B	Medium	Unknown	Poor
<i>Radiative Heat Transfer</i>			
Material A	Low	High	Good
Material B	High	Low	Poor

Moving from the PIRT to Sensitivity Studies and UQ Studies

- Using the PIRT, we can make a list of the relevant parameters:
 - Experimental conditions and parameters
 - Physics parameters
 - Code algorithm parameters
- The next step is to identify what is known about each parameter:
 - Bounds?, Discrete or continuous?, Non-probabilistic or probabilistic?
- Initial sensitivity analysis studies can identify:
 - High impact parameters
 - Where to focus resources (\$, people, simulations, tests, etc.)
- Goal: Out of the O(10-100) parameters going into a simulation code, identify the most important parameters & their interactions.

Sensitivity Analysis Methods

- An abridged list of sensitivity analysis methods:

- Simple 1-parameter and multi-parameter studies*
- Importance factors*
- Scaled sensitivity coefficients
- Random sampling and correlation analysis*
- Random sampling and analysis of variance
- Variance based decomposition*
- Many others....

Workhorse
methods

*** SA capability in SNL's DAKOTA software toolkit**

- Software tools:

- DAKOTA
- Minitab statistics package (SNL site license)
- JMP statistics package (30 licenses for ASC users – contact T. Giunta)
- Mathematica
- Matlab with Statistics Toolbox
- Others (Origin, etc.)

Sensitivity Analysis Methods

- Often heard comment:
 - “Of the 30 parameters in our model, we found that parameters A, B, and C were the most important....”
- Recent experience:
 - User’s physics simulation code had approximately 100 inputs.
 - Each code run takes ~5-10 hrs on a 1-processor Linux box
 - User performed a “change one parameter at a time” sensitivity analysis study over the course of several months
 - Note: this was before I joined the project
 - User identified the 12 most important parameters out of the ~100 original parameters.
- Pros: At least he was using some type of SA method.
- Cons: Slow process. He probably missed some two-parameter interaction effects that he could have found with another SA method.

Sensitivity Analysis Example

- Let's use a simple cantilever beam example to illustrate some of these sensitivity analysis concepts.
 - Sensitivity analysis with gradients
 - Sensitivity analysis with DAKOTA's sampling methods and correlation analysis

Example: Cantilever Beam Deterministic Analysis



- $L = \text{Length} = 1 \text{ m}$
- $W = \text{Width} = 1 \text{ cm}$, $H = \text{Height} = 2 \text{ cm}$
- $I = \text{Area Moment of Inertia} = (1/12)WH^3$
- $P = \text{load} = 100 \text{ N}$
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus = 69 GPa, Yield Stress = 255 MPa (from a handbook)**

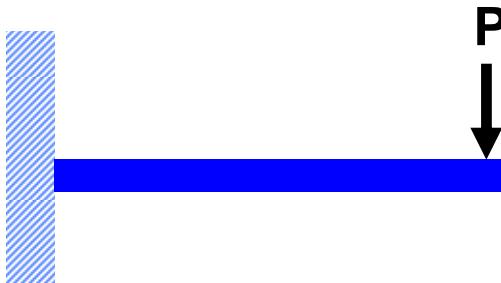
Goal:

We want to understand how deflection varies with respect to the length, width, height, load, and elastic modulus.

Beam theory: (assumes: elastic, isotropic, neglects beam mass, etc.)

- Deflection = $(PL^3)/(3EI)$, stress = My/I (y = distance from neutral axis)
- Deflection $\sim 7.2 \text{ cm}$ for $P = 100 \text{ N}$
- Yield Load = 170 N, Deflection at Yield Load $\sim 12.3 \text{ cm}$

Example: Cantilever Beam Sensitivity Analysis with Gradients



- **L = Length = 1 m**
- **Width = 1 cm, Height = 2 cm**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus = 69 GPa**
- **Deflection = $PL^3/(3EI)$**

Sensitivity Analysis of deflection (δ) vs. P, L, and E

Scaled Sensitivity Coefficients

$$\underline{\mu_x}^*(\partial\delta/\partial x)$$

$$\begin{aligned}\underline{\mu_P}^*(\partial\delta/\partial P) &= 0.0724 \\ \underline{\mu_L}^*(\partial\delta/\partial L) &= 0.217 \\ \underline{\mu_E}^*(\partial\delta/\partial E) &= -0.0724\end{aligned}$$

Notes:

1. Gradients typically computed via finite difference estimates.
2. Be wary of extrapolating trends.
3. No interaction data from this approach, but still useful.
4. *For a follow-on UQ study, maybe I'd freeze P and E at nominal values, and focus resources to study uncertainty in L.*

Example: Cantilever Beam Sensitivity Analysis with DAKOTA



- **L = Length = 1 m**
- **Width = 1 cm, Height = 2 cm**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus = 69 GPa**
- **Deflection = $PL^3/(3EI)$**

Sensitivity Analysis of deflection
(δ) vs. **P**, **L**, and **E** via random sampling over +/- 5% bounds around nominal values.

Correlation Analysis Method

1. Use DAKOTA to generate 20 random samples of L, P, E within +/-5% bounds.
2. Compute deflection for each random sample.
3. Look at partial correlation results generated by DAKOTA software.
4. Result: "L" most important parameter, but all have about equal impact.

Partial Correlation Table

	Load	Length	Modulus	Deflection
Load	.	-0.1177	-0.0753	0.2624
Length	-0.1177	.	0.2146	0.3251
Modulus	-0.0753	0.2146	.	-0.3088
Deflection	0.2624	0.3251	-0.3088	.

Moving from Sensitivity Analysis to UQ Studies

- The remaining parameters of interest will probably have some uncertainty associated with them, e.g.:
 - Lower and upper bounds (not necessarily uniform probabilities!!!)
 - Probabilistic data (vague or well-substantiated)
- *UQ is the process of propagating this uncertainty through a simulation model, and assessing the resulting uncertainty on the simulation output data.*
 - In the V&V process, UQ has a role in the “analysis,” “assessment,” and “prediction” blocks.
 - **Recall, typically we want to compute something like Probability($f > f^*$)**
- Issues:
 - There are many methods to propagate uncertainty – all requiring multiple code runs (actual time/expense are problem dependent)
 - Special methods needed for UQ with non-probabilistic parameters

Uncertainty Quantification Methods

- An abridged list of UQ methods:

- Exact analytic methods
- (Structural) reliability methods*
- Monte Carlo-type sampling methods*
- Polynomial chaos methods*
- Dempster-Shafer evidence theory*
- Bayesian methods
- Many others....

} Workhorse methods

} Research methods

*** UQ capability in SNL's DAKOTA software toolkit**

- Reliability methods are simple and cheap, but can have limited accuracy and applicability.
- Sampling methods are simple and can be expensive, but are more generally applicable.
 - Latin hypercube sampling is my method of choice,
 - Sampling methods can be used when there is a mix of probabilistic and non-probabilistic uncertain parameters

Uncertainty Quantification Example #1

- Let's return to the simple cantilever beam example to illustrate some of these UQ concepts.
 - Aleatoric (probabilistic) uncertainty

Example: Cantilever Beam Deterministic Analysis



- $L = \text{Length} = 1 \text{ m}$
- $W = \text{Width} = 1 \text{ cm}$, $H = \text{Height} = 2 \text{ cm}$
- $I = \text{Area Moment of Inertia} = (1/12)WH^3$
- $P = \text{load} = 100 \text{ N}$
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus = 69 GPa, Yield Stress = 255 MPa (from a handbook)**

Goal:

We want to understand how deflection varies with respect to the length, width, height, load, and elastic modulus.

Beam theory: (assumes: elastic, isotropic, neglects beam mass, etc.)

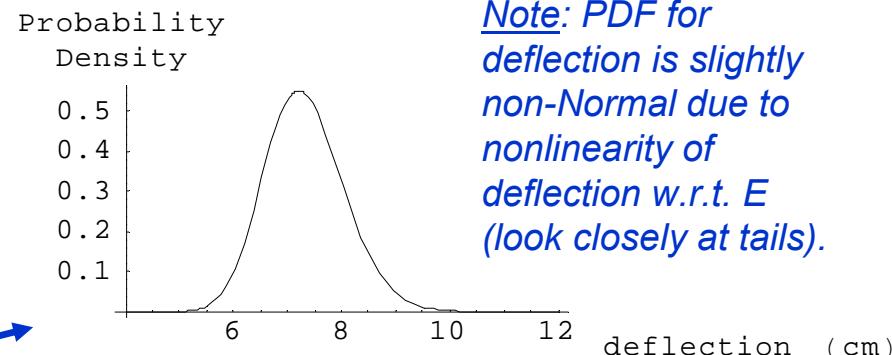
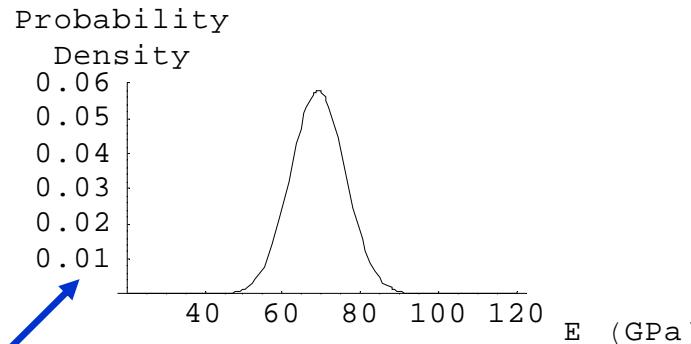
- Deflection = $(PL^3)/(3EI)$, stress = My/I (y = distance from neutral axis)
- Deflection $\sim 7.2 \text{ cm}$ for $P = 100 \text{ N}$
- Yield Load = 170 N, Deflection at Yield Load $\sim 12.3 \text{ cm}$

Example: Cantilever Beam UQ Analytical Approach



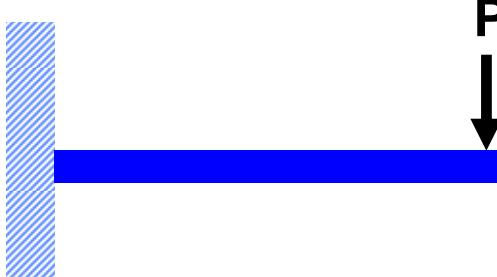
- Length = 1 m
- Width = 1 cm, Height = 2 cm
- P = load = 100 N
- Material = Aluminum 6061-T6:
- E = Elastic Modulus
 - Mean = $\mu = 69$ GPa
 - Std Deviation = $\sigma = 6.9$ GPa
- Deflection = $PL^3/(3EI)$
- E is Normal[μ, σ]
- Exact PDF of E
- Exact PDF of deflection

Probability Density Functions
(aka PDFs)



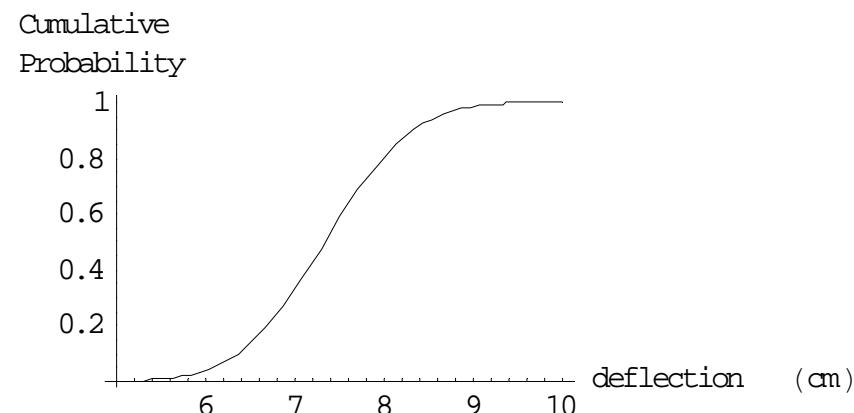
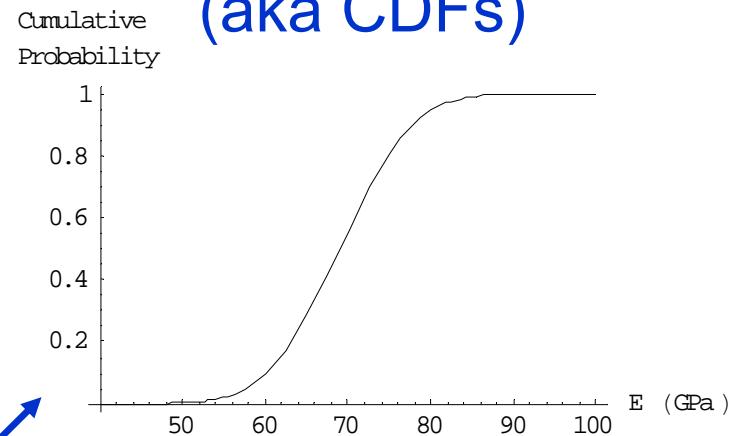
Note: PDF for deflection is slightly non-Normal due to nonlinearity of deflection w.r.t. E (look closely at tails).

Example: Cantilever Beam UQ Analytical Approach



- Length = 1 m
- Width = 1 cm, Height = 2 cm
- P = load = 100 N
- Material = Aluminum 6061-T6:
- E = Elastic Modulus
 - Mean = $\mu = 69$ GPa
 - Std Deviation = $\sigma = 6.9$ GPa
- Deflection = $PL^3/(3EI)$
- E is Normal[μ, σ]
- Exact CDF of E
- Exact CDF of deflection

Cumulative Distribution Functions
(aka CDFs)



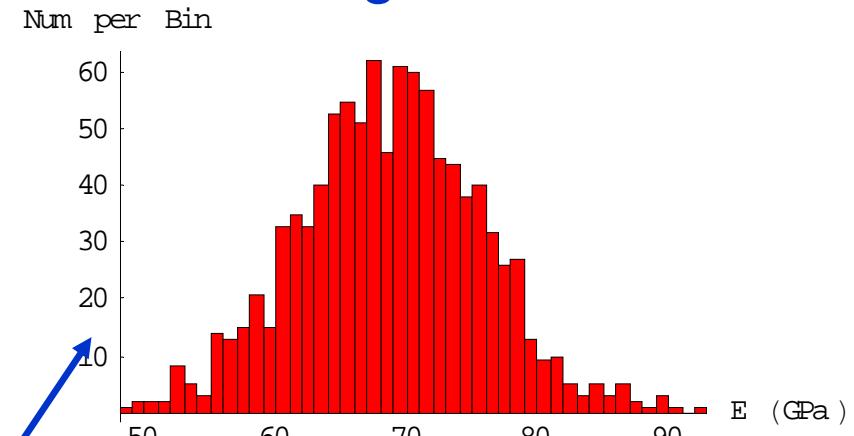
Example: Cantilever Beam UQ

Monte Carlo Sampling – Single Parameter

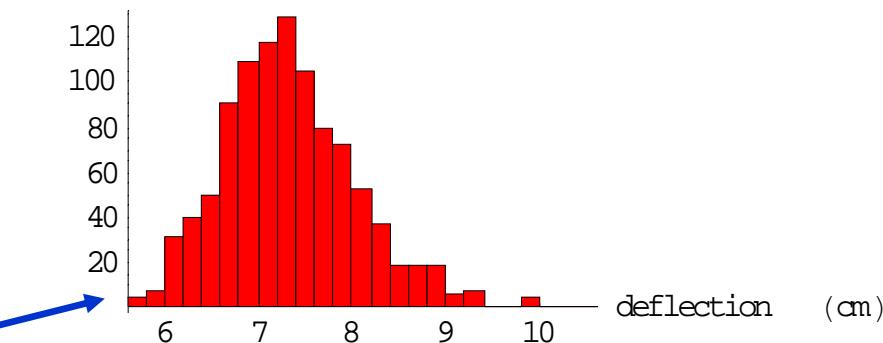


- Length = 1 m
- Width = 1 cm, Height = 2 cm
- P = load = 100 N
- Material = Aluminum 6061-T6:
- E = Elastic Modulus
 - Mean = $\mu = 69$ GPa
 - Std Deviation = $\sigma = 6.9$ GPa
- Deflection = $PL^3/(3EI)$
- E is Normal[μ, σ]
- 1000 random samples of E
- 1000 computed deflections

Histograms



Num per Bin

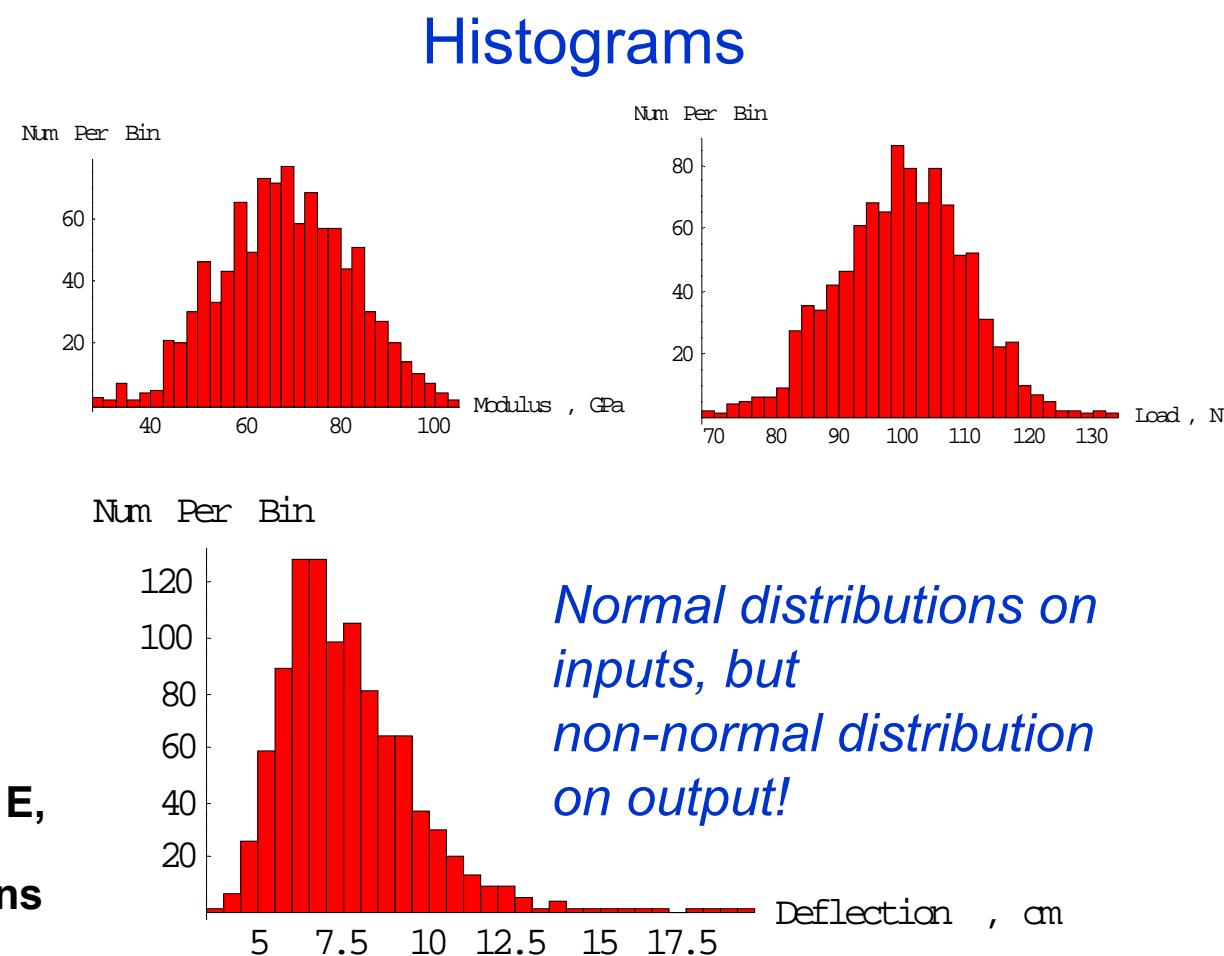


Example: Cantilever Beam UQ

Monte Carlo Sampling – Multiple Parameters



- Now make several parameters uncertain:
- Deflection = $PL^3/(3EI)$
- E is Normal[69,13.8] GPa
- P is Normal[100,5] N
- L is Normal[1.0m, 1cm]
- 1000 random samples of E, P, and L (top – for E & P)
- 1000 computed deflections (bottom)

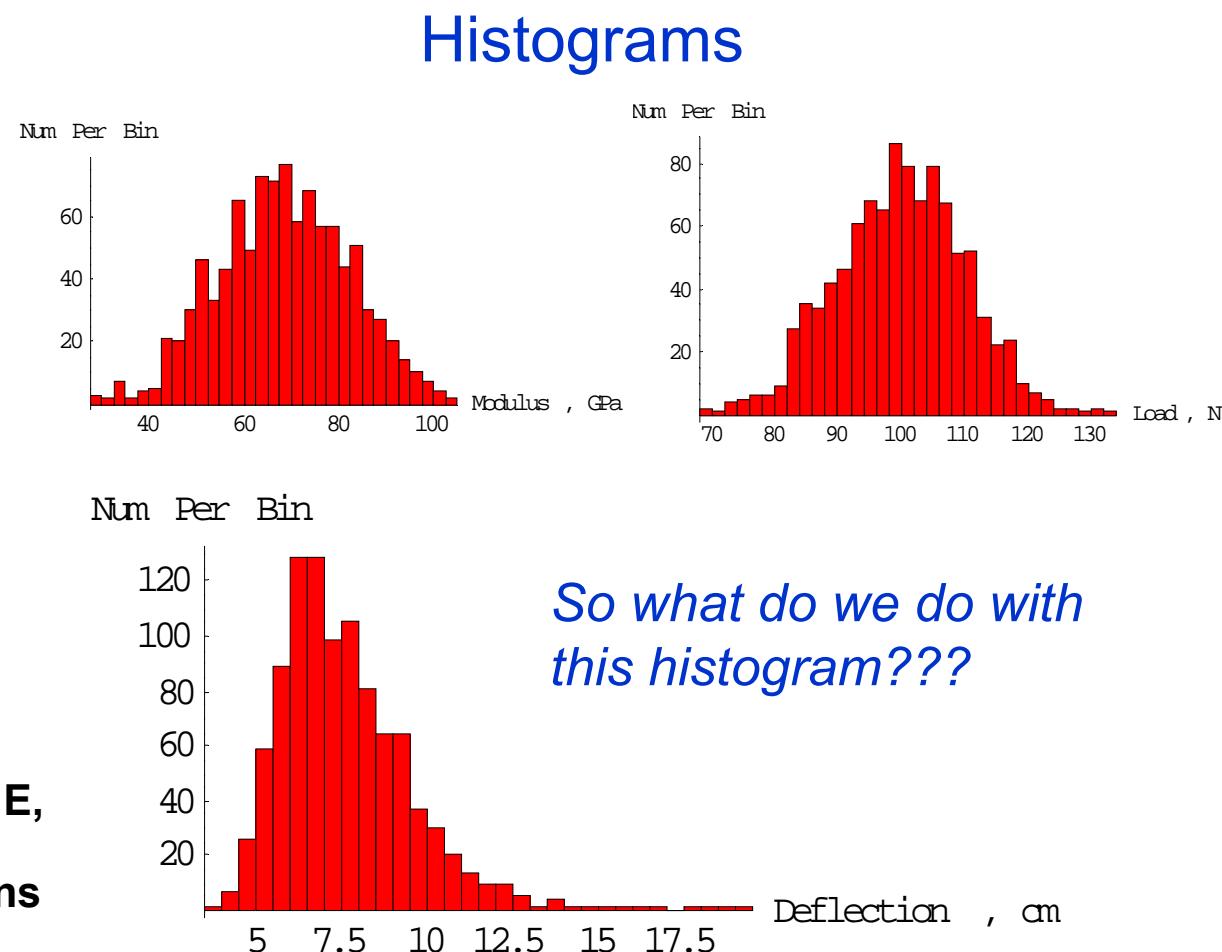


Example: Cantilever Beam UQ

Monte Carlo Sampling – Multiple Parameters



- Now make several parameters uncertain:
- Deflection = $PL^3/(3EI)$
- E is Normal[69,13.8] GPa
- P is Normal[100,5] N
- L is Normal[1.0m, 1cm]
- 1000 random samples of E, P, and L (top – for E & P)
- 1000 computed deflections (bottom)



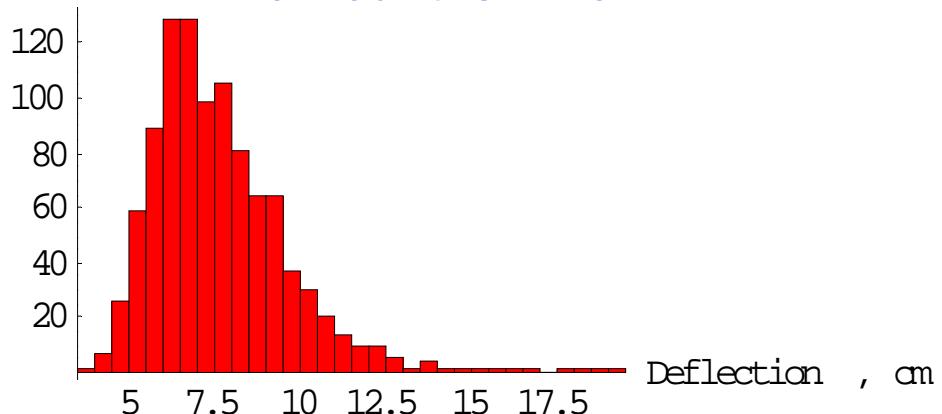
Example: Cantilever Beam UQ

Monte Carlo Sampling – Multiple Parameters



- Now make several parameters uncertain:
- Deflection = $PL^3/(3EI)$
- E is Normal[69,13.8] GPa
- P is Normal[100,5] N
- L is Normal[1.0m, 1cm]
- 1000 random samples of E, P, and L
- 1000 computed deflections
- DAKOTA computes these simple statistics

Num Per Bin



Example: “Critical” deflection amount is 11 cm

Estimate failure probability as # of samples with deflection > 11 cm , e.g.
 $P_{fail} \sim 52/1000 = 0.052$
(plus, can also estimate P_{fail} uncertainty)

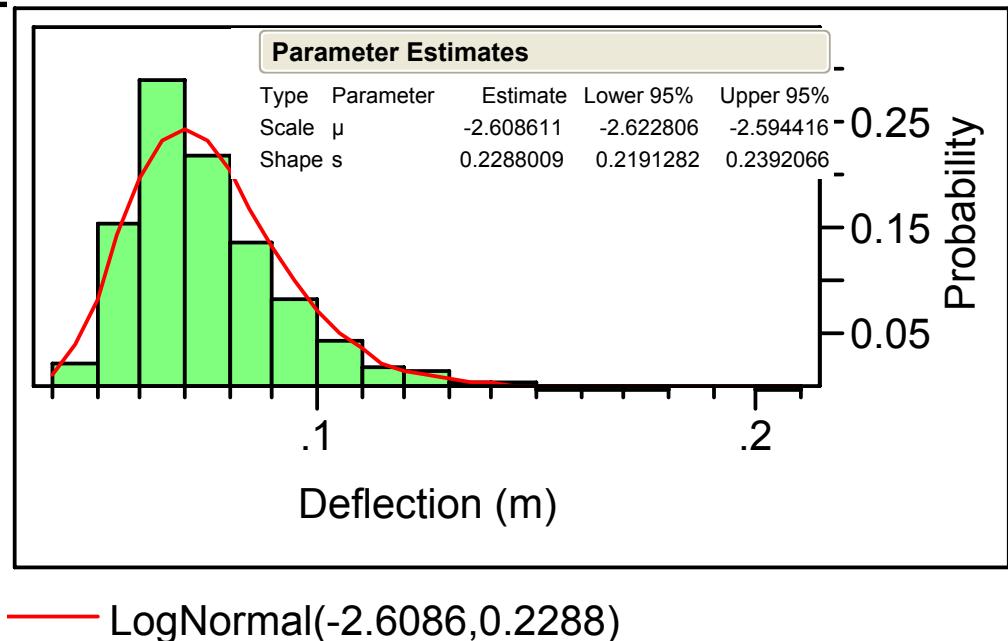
What if few or no points exceed limit?

Example: Cantilever Beam UQ

Monte Carlo Sampling – Multiple Parameters



- Now make several parameters uncertain:
- Deflection = $PL^3/(3EI)$
- E is Normal[69,13.8] GPa
- P is Normal[100,5] N
- L is Normal[1.0m, 1cm]
- 1000 random samples of E, P, and L
- 1000 computed deflections
- Use JMP, Minitab, or other statistics software



Fit a probability distribution function to the histogram & estimate P_{fail} values:

$Prob(\delta > 11 \text{ cm}) \sim 0.04$

$Prob(\delta > 21.8 \text{ cm}) \sim 1.0e^{-6}$

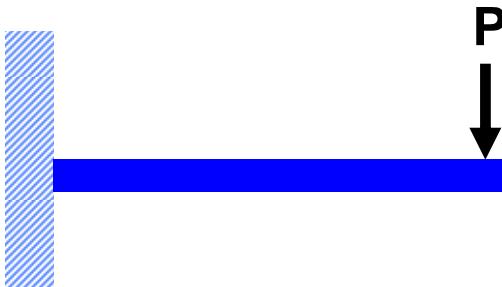
(note: there is uncertainty on the lognormal parameters!)

Uncertainty Quantification Example #2

- What happens in the UQ study if some or all of the parameters have epistemic (non-probabilistic) uncertainty?
- This is an active research area:
 - Bayesian methods
 - Dempster-Shafer methods
 - Interval methods, etc.
- Approach used in WIPP and Nuclear Reg. Comm. studies:
 - “2nd order sampling” methods
 - Epistemic parameters define “possible” scenarios.
 - Aleatoric parameters give probability estimates within each scenario.
 - Result: yields a collection of failure probability estimates, but user cannot know which scenario is most likely.

Example: Cantilever Beam UQ

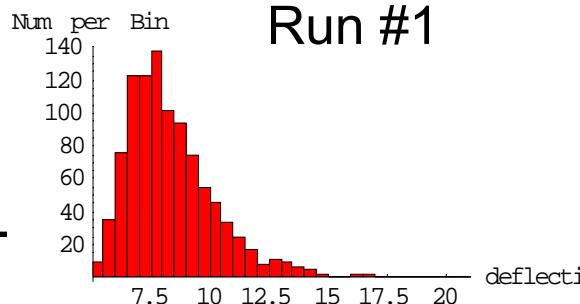
Monte Carlo Sampling – Multiple Parameters



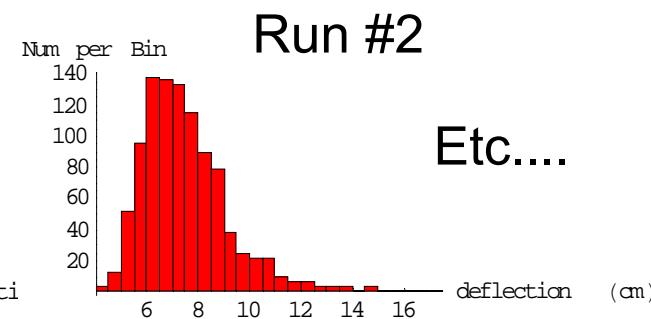
- Now make two parameters have epistemic uncertainty:
- Deflection = $PL^3/(3EI)$
- E is Normal[69, 13.8] GPa
- L is in [0.97, 1.03] m
- P is in [85, 115] N
- 1000 random samples of E for each instance of P and L
- Report range of failure probability estimates to decision maker, including the worst-case failure probability.

Approach:

1. Randomly choose a Load and a Length from their respective intervals.
2. Perform Monte Carlo (or Latin hypercube) sampling over the Elastic Modulus PDF
3. Compute probability deflection > 11 cm
4. Return to step 1 and repeat until computational budget limit reached.



Run #1: $P_{fail} \sim 0.043$



Etc....

Run #2: $P_{fail} \sim 0.055$

Real-World ASC UQ Application

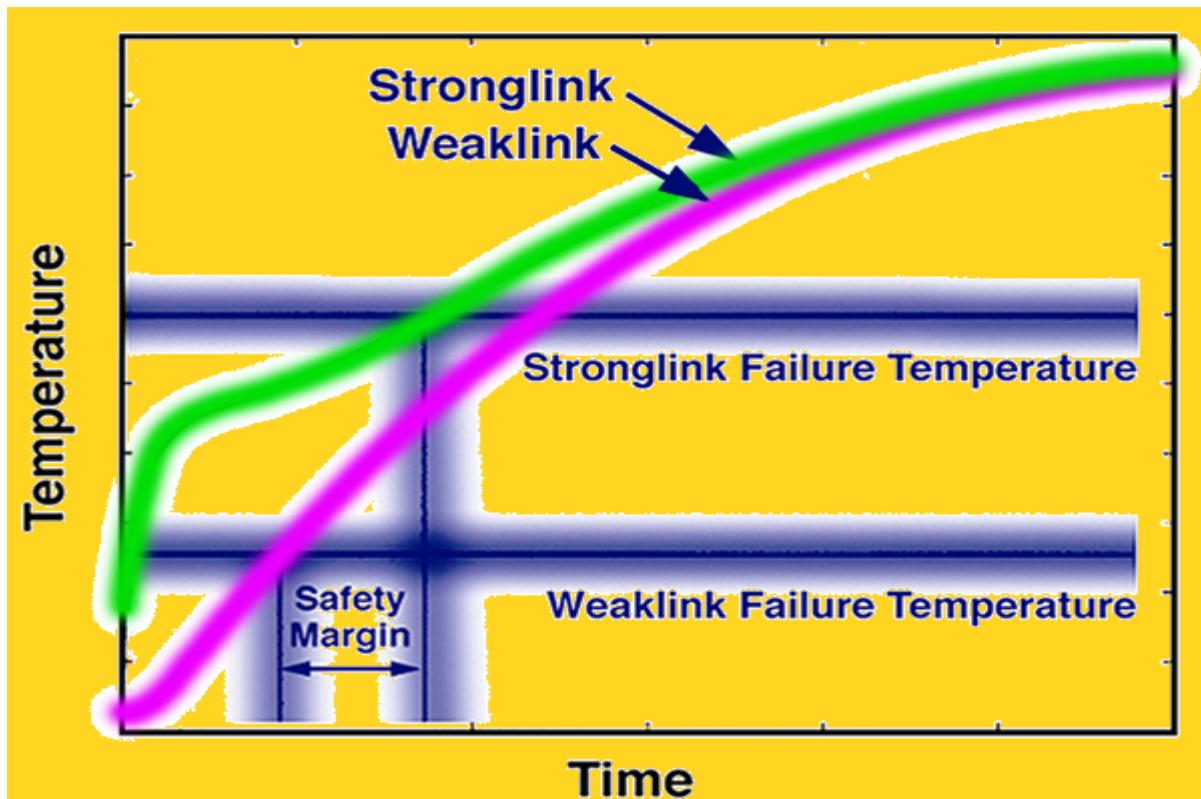
- **UQ study on the thermal response of an electrical component in a fire.**

Example: Thermal Response UQ Study

- **Background information:**
 - Electrical component has two safety components: weak link and strong link
 - Safety requirements dictate that weak link must fail before strong link (this is the “thermal race”)
- **Typical real-world UQ issues are present in this study:**
 - Cannot afford $O(10^6)$ high fidelity simulations.
 - We have a mix of epistemic and aleatoric uncertainties.
 - Q: How can we obtain probability data on system performance with only $O(10^1-10^2)$ code runs?
 - A: We have to do something other than brute-force sampling for UQ.

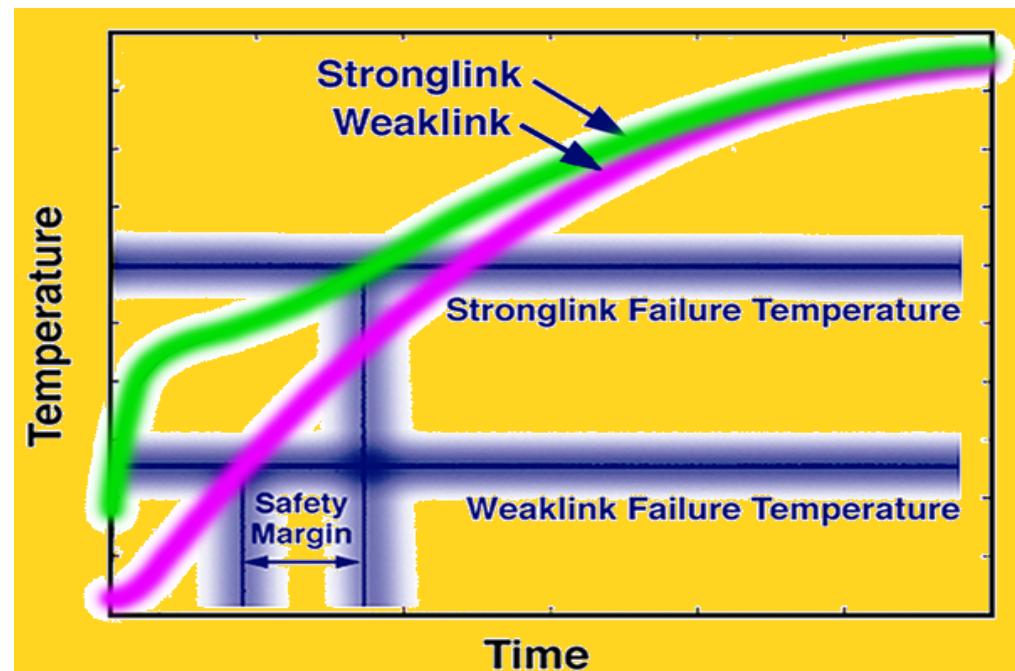
Example: Thermal Response UQ Study

- Application: electrical component in a hydrocarbon fuel fire due to an accident.
 - Thermal race study: weak link (WL) must fail before strong link (SL) for assured safety.
 - Questions:
 - How much margin (time) is in the WL/SL system?
 - How uncertain is the margin estimate?



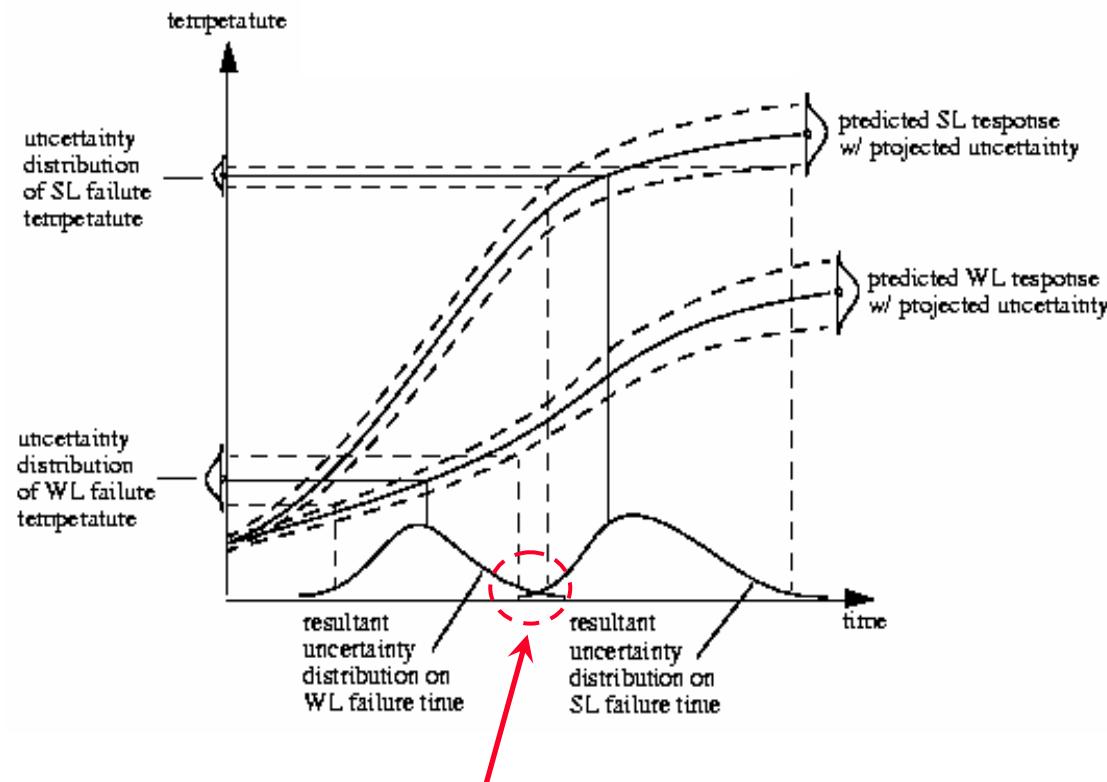
Thermal Response UQ Study: Issues

- Have epistemic uncertainty in temperature vs. time curves due to uncertainty in WL/SL model:
 - Recall: epistemic = “No PDF”
 - Material properties, initial and boundary conditions, etc.
- Have both aleatoric and epistemic uncertainty in WL and SL failure temperatures.
 - Recall: aleatoric = “Has a PDF”
 - Failure temperature follows a known distribution type (this is the aleatoric part), but the attributes of the distribution are not certain (this is the epistemic part).



Thermal Response UQ Study: Issues

- Have epistemic uncertainty in temperature vs. time curves due to uncertainty in WL/SL model:
 - Recall: epistemic = “No PDF”
 - Material properties, initial and boundary conditions, etc.
- Have both aleatoric and epistemic uncertainty in WL and SL failure temperatures.
 - Recall: aleatoric = “Has a PDF”
 - Failure temperature follows a known distribution type (this is the aleatoric part), but the attributes of the distribution are not certain (this is the epistemic part).

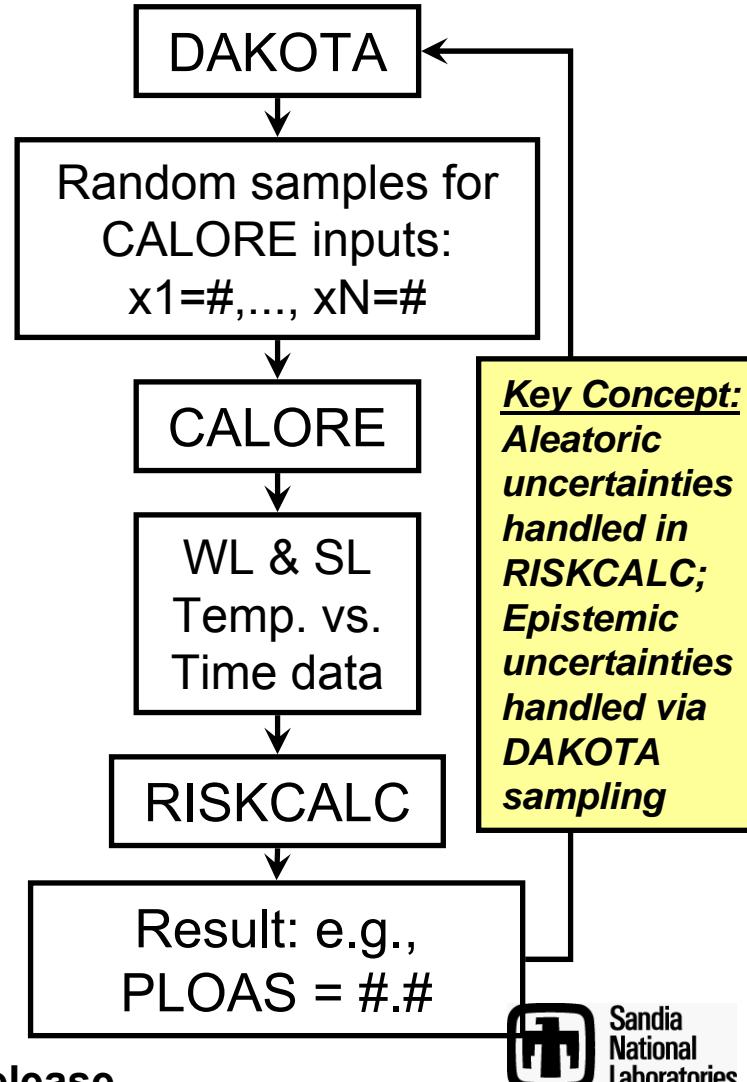


Probability of failure given by amount of tail overlap.

Thermal Response UQ Study: Approach

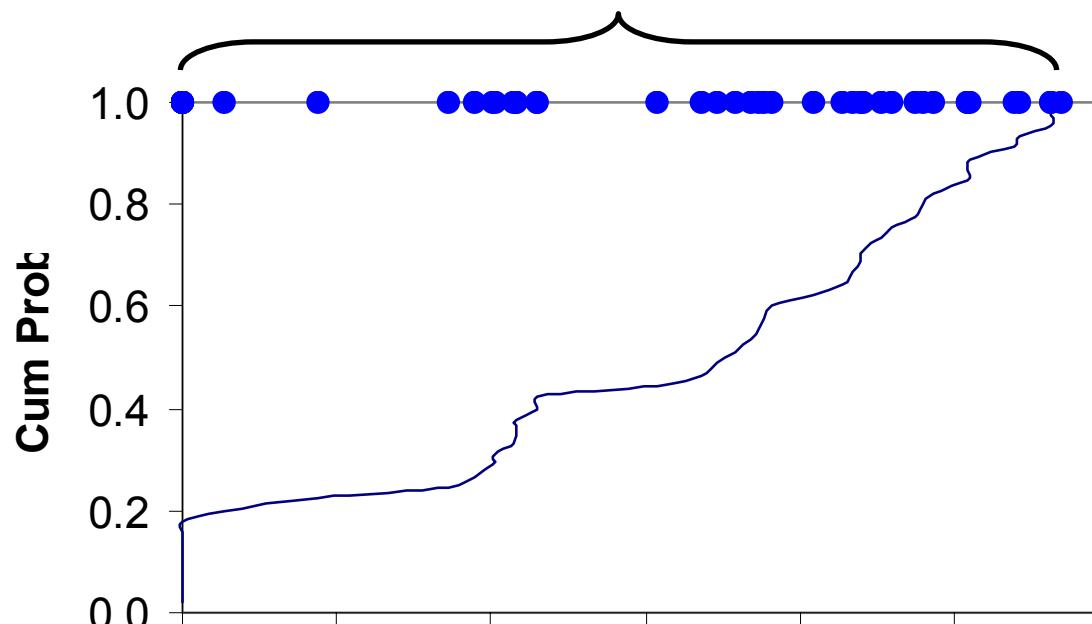
(PLOAS = Probability of Loss of Assured Safety)

- **Uncertainty:**
 - 28 thermal modeling parameters - epistemic
 - 3 component failure parameters with uncertainty in means and standard deviations – aleatoric & epistemic
 - CALORE model resolution parameters also investigated
- **CALORE thermal simulations on ASCI-Red**
 - 100 processors per simulation
 - ~20 hours (real-time) per sim. (for ~30 min of data)
 - Finite element model: 374K TET elements, 73.5K nodes (this is the “small” model for UQ study)
- **UQ Approach:**
 - DAKOTA + CALORE to generate an ensemble of Temp.-vs.-time data:
 - Latin hypercube sampling over bounds for 28 epistemic parameters: 45 CALORE runs completed
 - For each CALORE run, compute a PLOAS value (probability SL fails before WL) via RISKCALC code.
 - **Result: Ensemble of PLOAS estimates.**
 - **Note: this process is embarrassingly parallel.**



Thermal Response UQ Study Predicts Probability of Loss of Assured Safety

Note: All PLOAS estimates are possible, but we don't know which one is most probable.



Results:

PLOAS required to be $\leq 10^{-6}$

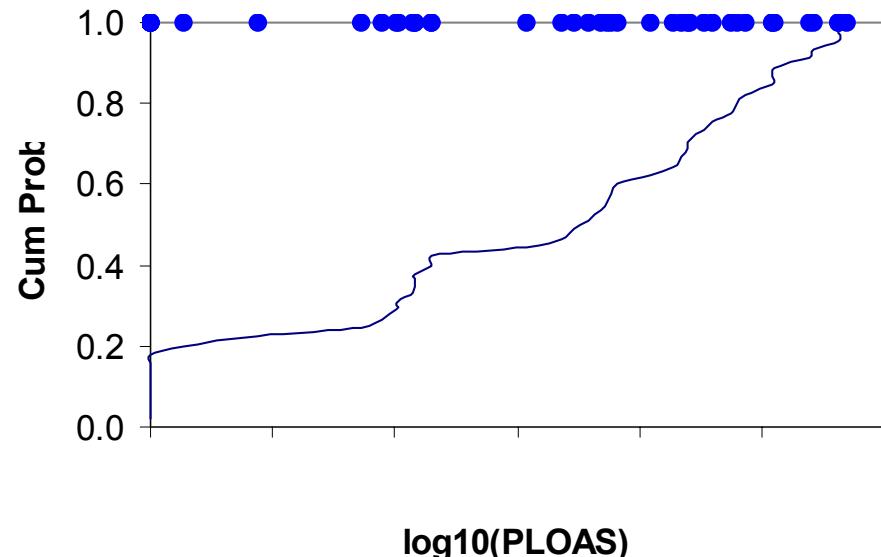
Margin = $10^{-6}/\text{PLOAS}_{\max}$

$\log_{10}(\text{PLOAS})$

Thermal Response UQ Study Predicts Probability of Loss of Assured Safety

- So what would we tell a decision maker about PLOAS?
 - The plot shows our best estimates of possible PLOAS values.
 - The requirement is **PLOAS <= 10⁻⁶**
 - The worst-case PLOAS estimate is **PLOAS_{max}**
 - The PLOAS margin is **10⁻⁶/PLOAS_{max}**

This is an example of “best estimate + uncertainty”.



Conclusion Slides

- **Summary**
- **Points of contact**

Summary: UQ Applications in Sandia Mission Areas

- Sandia's engineering practices are evolving to include UQ concepts to enable risk-informed design.
- Risk-informed design leverages past work on analysis of low-probability and high-consequence systems:
 - Waste Isolation Pilot Plant (WIPP)
 - Nuclear Regulatory Commission (NRC) studies on reactor safety
- Programmatic front:
 - Partner statisticians with engineers on projects.
 - Educate engineers on basic statistical methods and relevant topics, e.g., V&V, sensitivity analysis, UQ, QMU.
- Technical front:
 - Employ UQ methods that accommodate both probabilistic (aleatoric) and non-probabilistic (epistemic) uncertainty.
 - Employ existing software tools: both in-house (DAKOTA) and commercial.
 - **Perform UQ within the time/simulation run budget of the study.**
 - **Produce “best estimate + quantified uncertainty” for our customers.**

Closing Remarks

- Sensitivity analysis and UQ are key components of ASC verification & validation studies:
 - Also, SA and UQ have much utility outside of ASC applications
 - Must discriminate between **epistemic** (non-probabilistic) uncertainty and **aleatoric** (probabilistic) uncertainty.
 - *Just assuming that every uncertain parameter has a normal distribution is not acceptable engineering practice.*
- Sandia has software tools (DAKOTA, JMP, Minitab, etc.) and experts that can help you use these tools in SA and UQ studies.
 - Training in these software tools is available (by SNL staff, online “webinars”, multi-day courses)
 - Must be a partnership, with SA/UQ experts collaborating on your projects, i.e., not just SA/UQ experts running your code.

Points of Contact

- **Programmatic:**

- [Marty Pilch \(1533\)](#)

[SNL ASC V&V Program Manager](#)

- **Technical – SNL/NM:**

- [Tony Giunta \(1533\)](#)
 - [Bill Oberkampf \(1533\)](#)
 - [Jon Helton \(1533\)](#)
 - [Tom Paez \(1533\)](#)
 - [Tim Trucano \(1411\)](#)
 - [Mike Eldred \(1411\)](#)
 - [Laura Swiler \(1411\)](#)
 - [Brian Rutherford \(12337\)](#)
 - [Experienced Staff - V. Romero, K. Dowding, A. Urbina, R. Field, J. Red-Horse, R. Hogan, D. Dobranich, A. Brundage, C. Glissman, F. Dempsey, T. Simmermacher, S. Tieszen, R. MacKinnon, G. Rice, M. Kerschen, T. Brown, et al.](#)

UQ & sensitivity analysis, V&V topics, DAKOTA applications
Epistemic UQ, V&V methods & applications
Epistemic UQ, sensitivity analysis
UQ, statistical methods, V&V methods & applications
V&V topics, UQ & QMU methods & future directions
UQ methods research, DAKOTA R&D
UQ/SA, Bayesian methods, DAKOTA applications
Statistical analysis methods

- **Technical – SNL/CA:**

- [Monica Martinez-Canales \(8962\)](#) UQ, V&V, statistical design of experiments
 - [Patty Hough \(8962\)](#) UQ, V&V, statistical design of experiments
 - [Genetha Gray \(8962\)](#) UQ, V&V, statistical design of experiments
 - [Steve Margolis \(8962\)](#) DAKOTA applications (esp. running DAKOTA on SNL Linux clusters)
 - [Experienced Staff – J. Dike, B. Kistler, E. Marin, M. Chiesa, M. Jew, C. Lam, B. Owens, et al.](#)

References

- AIAA (1998), "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations," American Institute of Aeronautics and Astronautics, AIAA-G-077-1998, Reston, VA.
- Box, G. E. P., W. G. Hunter and J. S. Hunter (1978), *Statistics for Experimenters*, John Wiley, New York.
- Coleman, H. W. and W. G. Steele, Jr. (1999), *Experimentation and Uncertainty Analysis for Engineers*, John Wiley, New York.
- Cullen, A. C. and H. C. Frey (1999), *Probabilistic Techniques in Exposure Assessment: A Handbook for Dealing with Variability and Uncertainty in Models and Inputs*, Plenum Press, New York.
- Ditlevsen, O. and H. O. Madsen (1996), *Structural Reliability Methods*, John Wiley.
- Dowding, K. (2001), "Quantitative Validation of Mathematical Models," ASME International Mechanical Engineering Congress Exposition, New York.

References (continued)

- Easterling, R. G. (2001), "Measuring the Predictive Capability of Computational Models: Principles and Methods, Issues and Illustrations," Sandia National Laboratories, SAND2001-0243, Albuquerque, NM.
- Hasselman, T. K. (2001), "Quantification of Uncertainty in Structural Dynamic Models," *Journal of Aerospace Engineering*, Vol. 14, No. 4, 158-165.
- Helton, J. C., and F. J. Davis (2001), "Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems," Sandia National Laboratories, SAND2001-0417, Albuquerque, NM.
- Helton, J. C., and F. J. Davis (1999), "Sampling-Based Methods for Uncertainty and Sensitivity Analysis," Sandia National Laboratories, SAND99-2240, Albuquerque, NM.
- Hills, R. G. and T. G. Trucano (2002), "Statistical Validation of Engineering and Scientific Models: A Maximum Likelihood Based Metric," Sandia National Laboratories, SAND2001-1783, Albuquerque, NM.
- Montgomery, D. C. (2000), *Design and Analysis of Experiments*, John Wiley.

References (continued)

- Morgan, M. G. and M. Henrion (1990), *Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*, Cambridge University Press, Cambridge, UK.
- Oberkampf, W. L., S. M. DeLand, B. M. Rutherford, K. V. Diegert and K. F. Alvin (2002), "Error and Uncertainty in Modeling and Simulation," *Reliability Engineering and System Safety*, Vol. 75, No. 3, 333-357.
- Oberkampf, W. L. and T. G. Trucano (2002), "Verification and Validation in Computational Fluid Dynamics," *Progress in Aerospace Sciences*, Vol. 38, No. 3, 209-272.
- Oberkampf, W. L., T. G. Trucano, and C. Hirsch (2003), "Verification, Validation, and Predictive Capability," Sandia National Laboratories, SAND2003-3769, Albuquerque, NM (to appear in *ASME Applied Mechanics Reviews*).
- Oberkampf, W. L. and M. F. Barone (2004), "Measures of Agreement Between Computation and Experiment: Validation Metrics," 34th AIAA Fluid Dynamics Conference, AIAA Paper No. 2004-226, Portland, OR.

References (continued)

- Rutherford, B. M. and K. J. Dowding (2003), "An Approach to Model Validation and Model-Based Prediction--Polyurethane Foam Case Study," Sandia National Laboratories, SAND2003-2336, Albuquerque, NM.
- Taylor, J. R. (1997), *An Introduction to Error Analysis: The study of uncertainties in physical measurements*, University Science Books, Sausalito, CA.
- Trucano, T. G., M. L. Pilch, and W. L. Oberkampf (2002), "General Concepts for Experimental Validation of ASCI Code Applications," Sandia National Laboratories, SAND2002-0341, Albuquerque, NM.
- Urbina, A. and T. L. Paez (2001), "Statistical Validation of Structural Dynamics Models," Annual Technical Meeting & Exposition of the Institute of Environmental Sciences and Technology, Phoenix, AZ.
- Wilson, G. E. and B. E. Boyack (1998), "The Role of the PIRT in Experiments, Code Development and Code Applications Associated With Reactor Safety Analysis," *Nuclear Engineering and Design*, Vol. 186, No. 1-2, pp. 23-37

Extra Vugraphs

Common UQ Pitfall:

(Cannot have PDF on results if no PDFs on inputs!)

The “Model”

$$Y = A^B$$

Indisputable

$$A = [0, 2]$$

Only Bounds Are Known

$$B = [1, 3]$$

Only Bounds Are Known

How do you interpret the results?

(a) Y as a probability distribution?

(b) Y bounded by (0,8)?

