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Validation and Uncertainty Quantification Methods in the DAKOTA Software Toolkit

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Outline

- Motivation
- Background
  - Risk-Informed Decision Making
  - Verification & Validation
  - Sensitivity Analysis & Uncertainty Quantification (UQ)
- DAKOTA toolkit overview
- UQ tutorial
  - Cantilever Beam example problem
  - UQ Example #1: probabilistic uncertainty
  - UQ Example #2: non-probabilistic uncertainty
- Real world UQ application:
  - Electrical component thermal response UQ study
- Summary

Acknowledgements

- Sandia National Labs colleagues:
  - Marty Pilch, Tim Trucano, Bill Oberkampf, Tom Paez, Jon Helton, Rich Hills (New Mexico State Univ.), Kevin Dowding, Vicente Romero, Laura Swiler, Mike Eldred, Monica Martinez-Canales, Patty Hough, et al.
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  - François Hemez, Ryan Maupin, Mandy Rutherford, et al.
- LLNL Colleagues:
  - Jim McEnerney, Scott Brandon, et al.
  - Frank Graziani, Charles Tong, et al.

Goals for this Briefing

- **Understand the connection between verification & validation (V&V), sensitivity analysis (SA), and uncertainty quantification (UQ).**
- **Understand the SA/UQ capabilities in the DAKOTA toolkit**
- **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.**
- **This briefing is a combination of:**
  - **Validation & UQ tutorial**
  - **DAKOTA overview**
  - **Validation & UQ example**

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

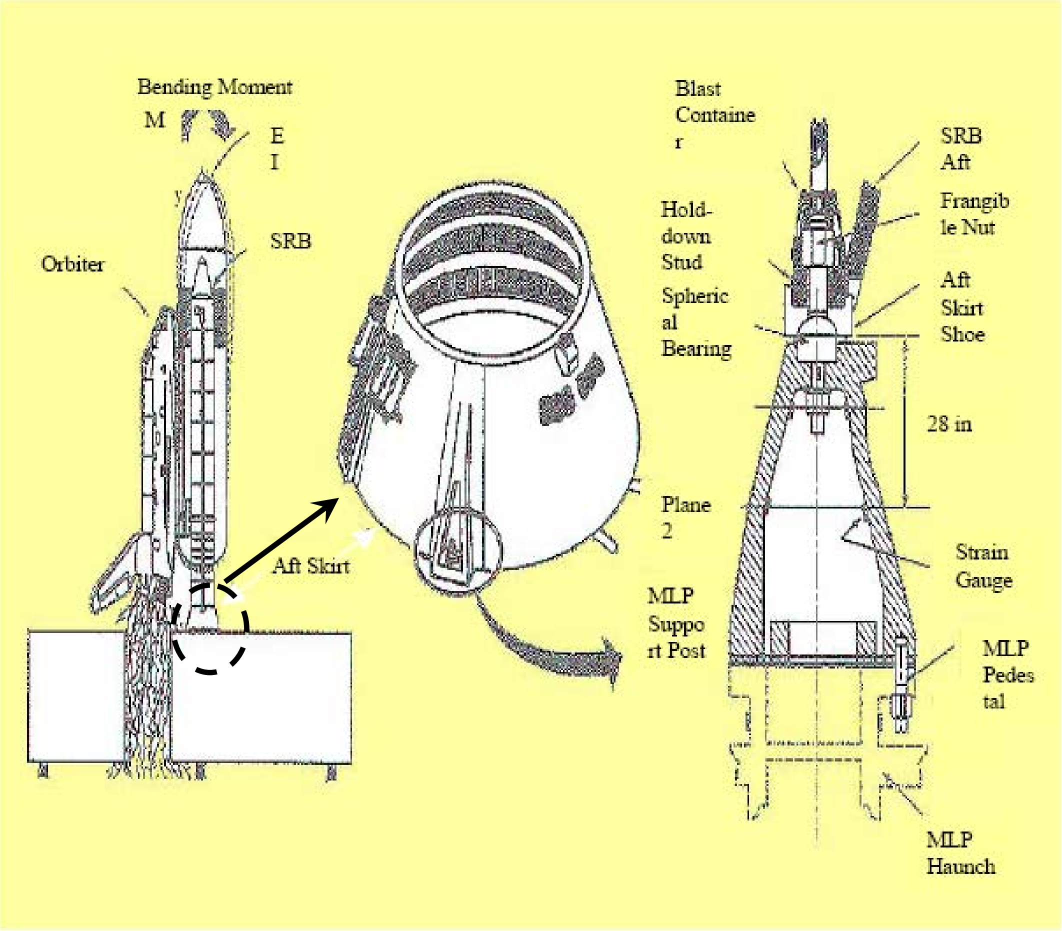
- **Risk-Informed Decision Making is based on:**
  - Verified and validated computer simulations.
  - Scientifically defensible approach to V&V, uncertainty propagation, and methods for quantifying margins and uncertainties (QMU).
    - *Uncertainty due to stochastic processes (aleatoric)*
    - *Uncertainty due to lack of knowledge (epistemic)*

- **Impact of Sandia's Verification & Validation Program:**
  - Enable <u>credible</u> computational predictions.
  - Identify most important (sensitive) uncertain/variable parameters; focus research and testing resources on these.
  - <u>Quantify</u> 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?

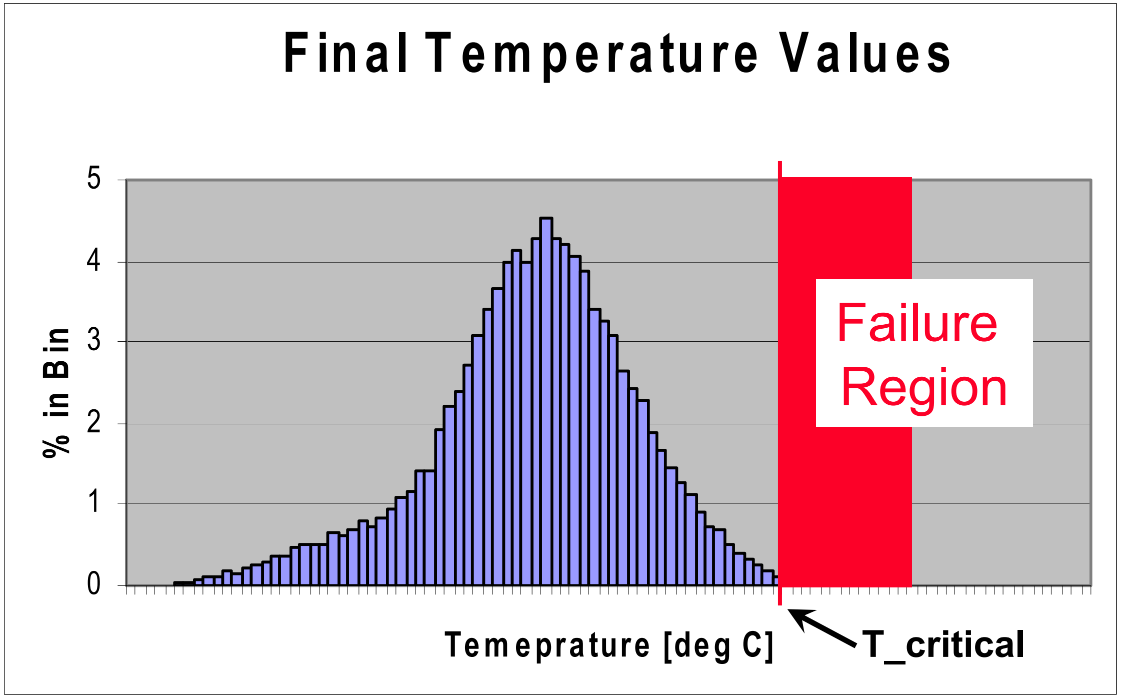
Need UQ to Answer

- **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?

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?

Example of Uncertainty Quantification



Hypothetical Example:

- Temperature = fcn($x_1,\ldots,x_N$)

-$x_1,\ldots,x_N$ 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 $x_1,\ldots,x_N$ inputs.*
  - Correlations (trends) of Temperature vs. $x_1,\ldots,x_N$.
  - Mean(T), StdDev(T), Probability(T > T_critical)

Transition from Sensitivity Analysis to UQ Studies

- A sensitivity study identifies a subset of interesting/important parameters, which likely will 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.***
  - UQ has a role in validation, and also a role in making predictions (prediction = best estimate + uncertainty).
  - 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*** } Workhorse methods
  - **Monte Carlo-type sampling methods*** } Workhorse methods
  - **Polynomial chaos methods*** } Research methods
  - **Dempster-Shafer evidence theory*** } Research methods
  - **Bayesian methods**
  - **Many others....**

**** 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.**
  - **<u>Latin hypercube sampling</u> is my method of choice,**
  - **Sampling methods can be used when there is a mix of probabilistic and non-probabilistic uncertain parameters**

What is DAKOTA? Executive Summary

- DAKOTA: Design and Analysis toolKit for Optimization and Terascale Applications
  - Under development at SNL since 1994
  - State of the art tools for performing engineering “what if” studies:
    - Uncertainty quantification, sensitivity analysis, computer model calibration, design optimization, etc.
    - Extensive support for parallel computing – PCs to supercomputers
  - Works as a “black-box” with your simulation code(s):
    - Data transferred via file read/write operations
    - Works on LINUX/UNIX, Mac OS, Windows
  - In use at SNL, LLNL, LANL, ORNL, Navy, NASA, Lockheed-Martin, 3M, Kodak, Goodyear, BMW, etc. and at numerous universities
  - Freely available worldwide via GNU General Public License
    - ~3000 downloads, approx several hundred “serious” users
  - DAKOTA team receives significant return on investment from external users:
    - Bug reports, compilations on new computer systems, suggestions for future R&D, research collaborations
  - DAKOTA enables sensitivity analysis, optimization, and uncertainty quantification w/ high-fidelity simulation tools on massively-parallel supercomputers. (http://endo.sandia.gov/DAKOTA)

What Does DAKOTA Do?

- **In many applications, we want to understand how changes in our simulation code input parameters affect the code output results.**

- **Traditional process – user changes one input at a time, runs the simulation code, and observes the change in the output.**
  - **Tried and true, but, can miss important multi-parameter interactions.**

- **Computer-aided process – DAKOTA selects the input values, runs the simulation code, collects all of the output values, and presents "data" to user.**
  - **"data" = local or global sensitivity info**
  - **"data" = optimization info (i.e., best/worst set of input values)**
  - **"data" = probability & statistical info on output values**
  - ***Then, the user decides how to proceed – new input value ranges, focus on specific input values of interest, etc.***
  - ***The user is still in control of the analysis/design process!***

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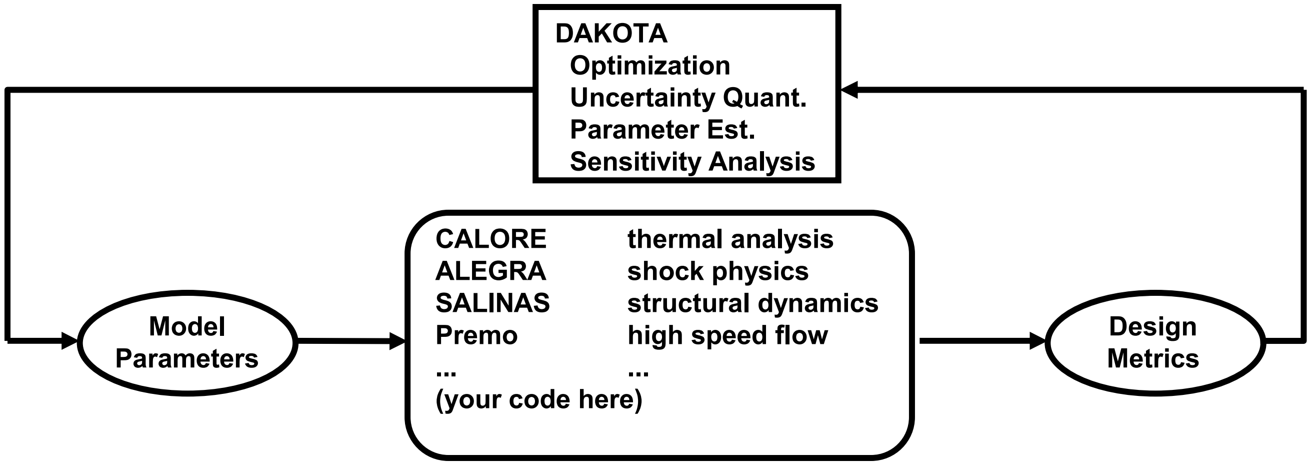
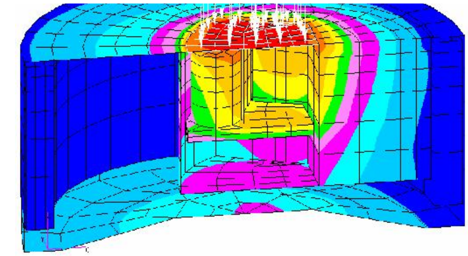
DAKOTA Overview

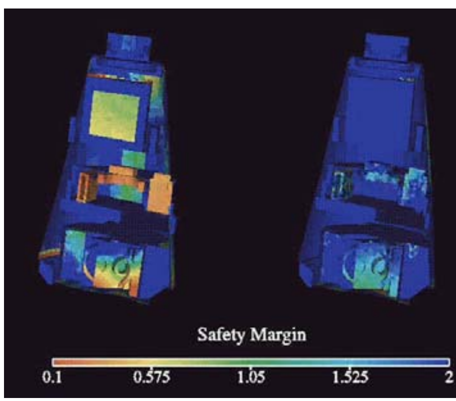


Worst Case Fire Safety



Structural Design

Nominal Optimized

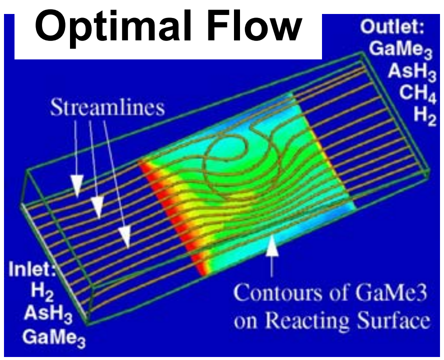


Technical themes:

- DAKOTA works with just about any simulation code.
  - Typically in "black box" mode with file reading/writing.
  - DAKOTA contains math & stats methods – no physics!
- ***Exploit large-scale/massively parallel computing platforms***
- Create and deploy state-of-the art methods for complex and expensive engineering simulations, e.g.:
  - Surrogate-based optimization & uncertainty quantification
- ***Balance research goals with production software support***

Impact:

- Internal: extensive (and growing) use within SNL
- External: DOE labs, DoD labs, NASA, commercial & academic partners



DAKOTA Core Team Members

- **SNL-NM Computational Sciences**
  - Mike Eldred (PI), Shane Brown, Laura Swiler, Brian Adams, Danny Dunlavy, Dave Gay, Bill Hart, Jean-Paul Watson, John Eddy, Scott Mitchell (manager)
- **SNL-NM Engineering Sciences**
  - Tony Giunta, Walt Witkowski, Marty Pilch (manager)
- **SNL-CA Computational Sciences**
  - Patty Hough, Monica Martinez-Canales, Tammy Kolda, Pam Williams, Josh Griffin, Heidi Ammerlahn (manager)
- ***Open to collaborations with US Government labs, corporations, and academic institutions***

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Uncertainty Quantification Example #1

- **Let's use a simple "cantilever beam" example to illustrate some basic UQ concepts.**
  - **Aleatoric (probabilistic) uncertainty**

Example: Cantilever Beam Deterministic Analysis

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

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

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

- **Deflection = (PL^3)/(3EI), stress = My/I (y = distance from neutral axis)**
- **Deflection ~ 7.2 cm for P = 100 N**
- **Yield Load = 170 N, Deflection at Yield Load ~ 12.3 cm**

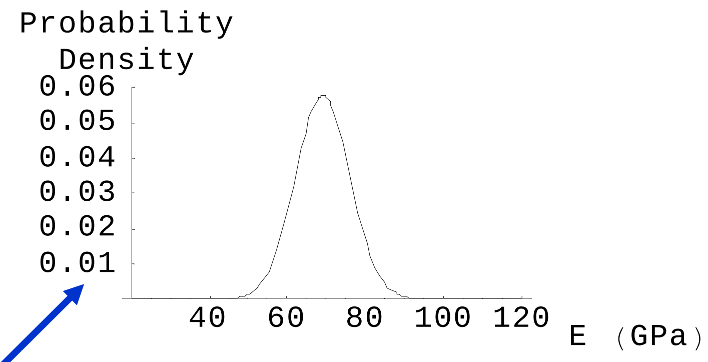
Example: Cantilever Beam UQ Analytical Approach

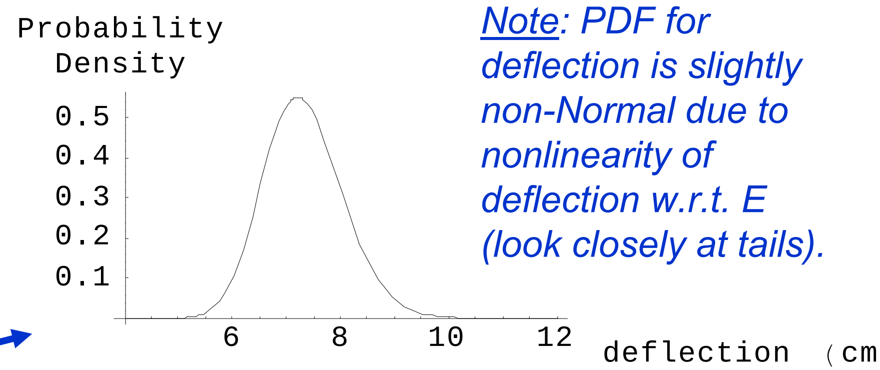
- **Length = 1 m**
- **Width = 1 cm, Height = 2 cm**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus**
  - **Mean = μ = 69 GPa**
  - **Std Deviation = σ = 6.9 GPa**

- **Deflection = PL^3/(3EI)**
- **E is Normal[μ, σ]**

- **Exact PDF of E**
- **Exact PDF of deflection**

Probability Density Functions (aka PDFs)





<u>Note</u>: 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
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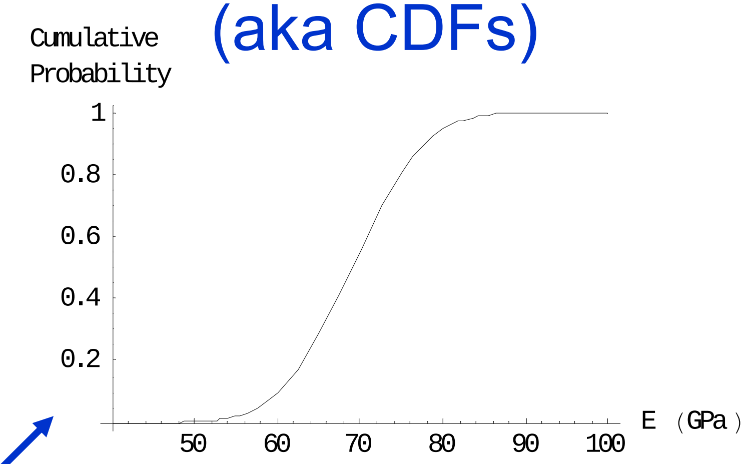
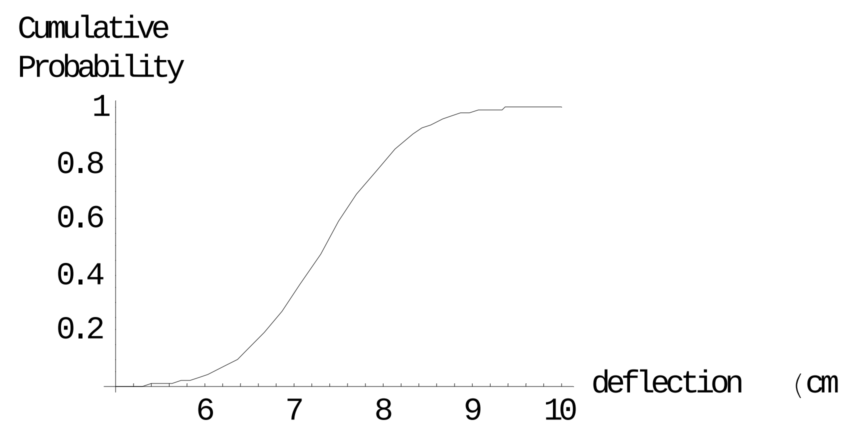
  - Std Deviation = σ = 6.9 GPa

- Deflection = PL^3/(3EI)
- E is Normal[μ, σ]

- Exact CDF of E
- Exact CDF of deflection

Cumulative Distribution Functions (aka CDFs)





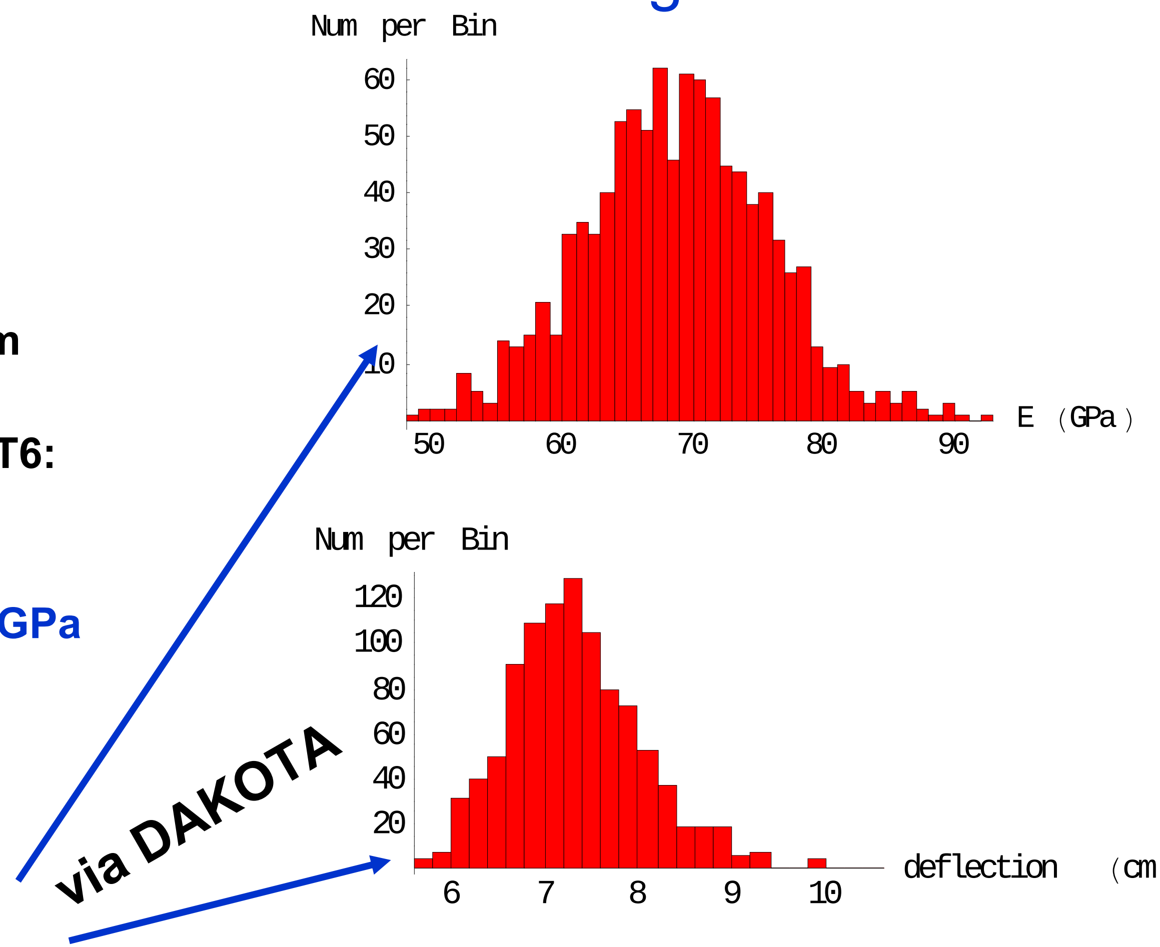
Example: Cantilever Beam UQ
Monte Carlo Sampling – Single Parameter

- **Length = 1 m**
- **Width = 1 cm, Height = 2 cm**
- **P = load = 100 N**
- **Material = Aluminum 6061-T6:**
- **E = Elastic Modulus**
  - **Mean = μ = 69 GPa**
  - **Std Deviation = σ = 6.9 GPa**

- **Deflection = PL^3/(3EI)**
- **E is Normal[μ, σ]**

- **<u>1000 random samples of E</u>**
- **<u>1000 computed deflections</u>**

Histograms



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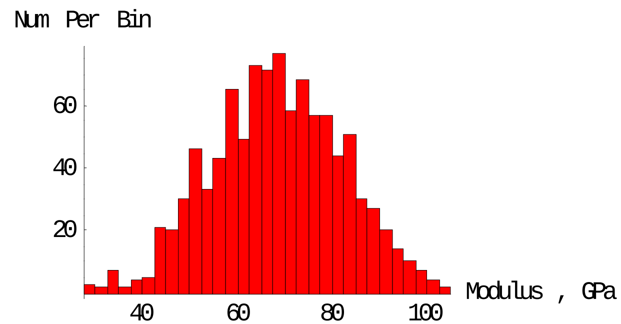
Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters

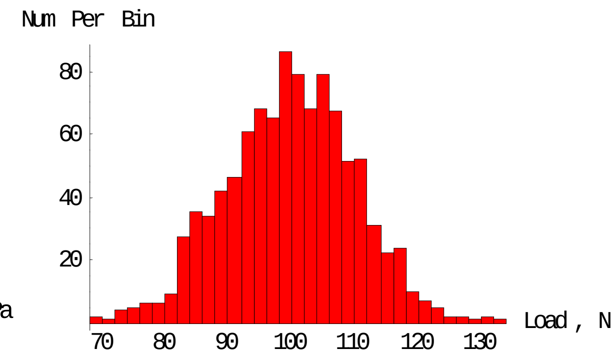
- **Now make several parameters uncertain:**

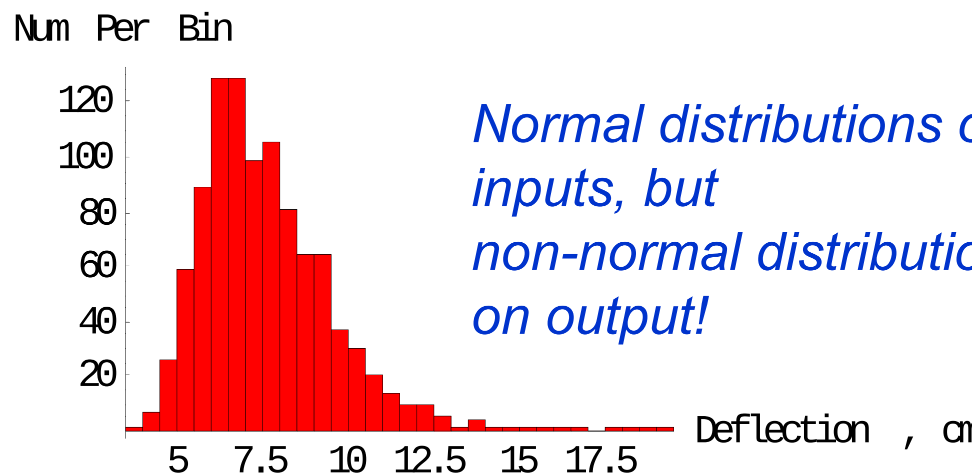
- **Deflection = PL^3/(3EI)**
- **E is Normal[69,13.8] GPa**
- **P is Normal[100,5] N**
- **L is Normal[1.0m, 1cm]**

- **1000 random samples of E, P, and L (top – for E & P)**
- **1000 computed deflections (bottom)**
- **Via DAKOTA**

Histograms







Normal distributions on inputs, but non-normal distribution on output!

Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters

- **Now make several parameters uncertain:**

- **Deflection = PL^3/(3EI)**
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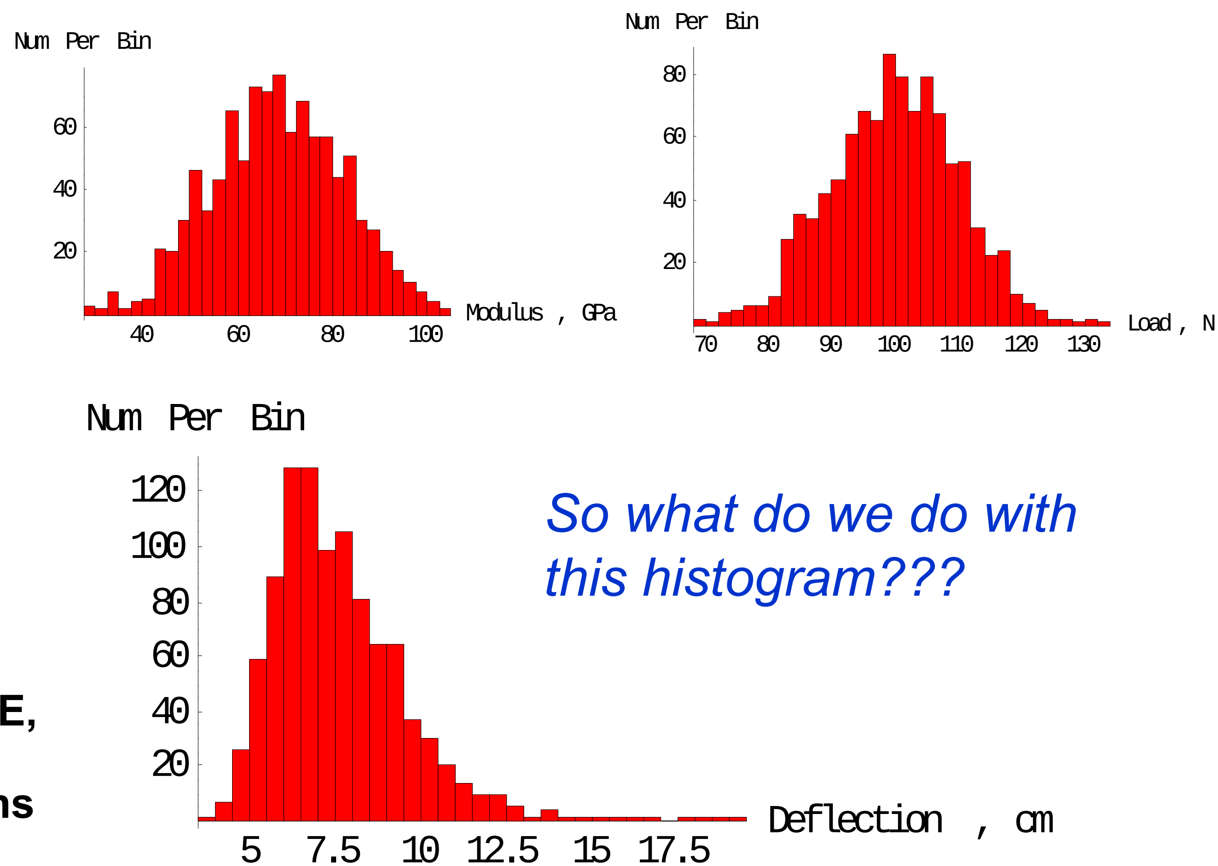
Histograms



So what do we do with this histogram???

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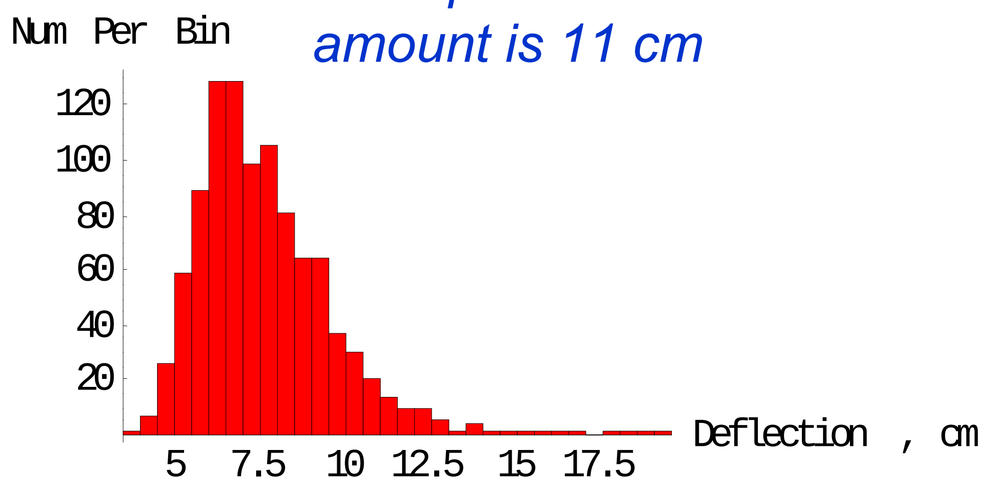
Example: Cantilever Beam UQ Monte Carlo Sampling – Multiple Parameters

- <u>**Now make several parameters uncertain:**</u>

- **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**
- <u>***DAKOTA computes these simple statistics***</u>

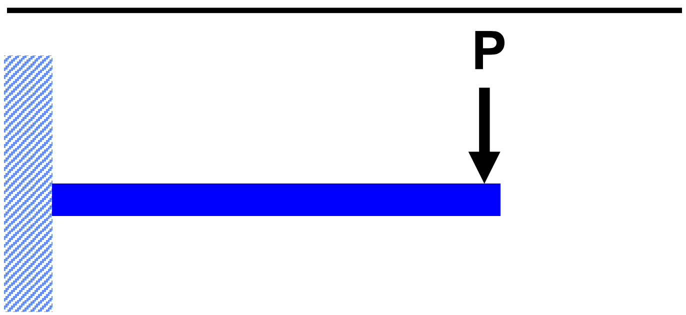
Example: "Critical" deflection amount is 11 cm



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

What if few or no points exceed limit?

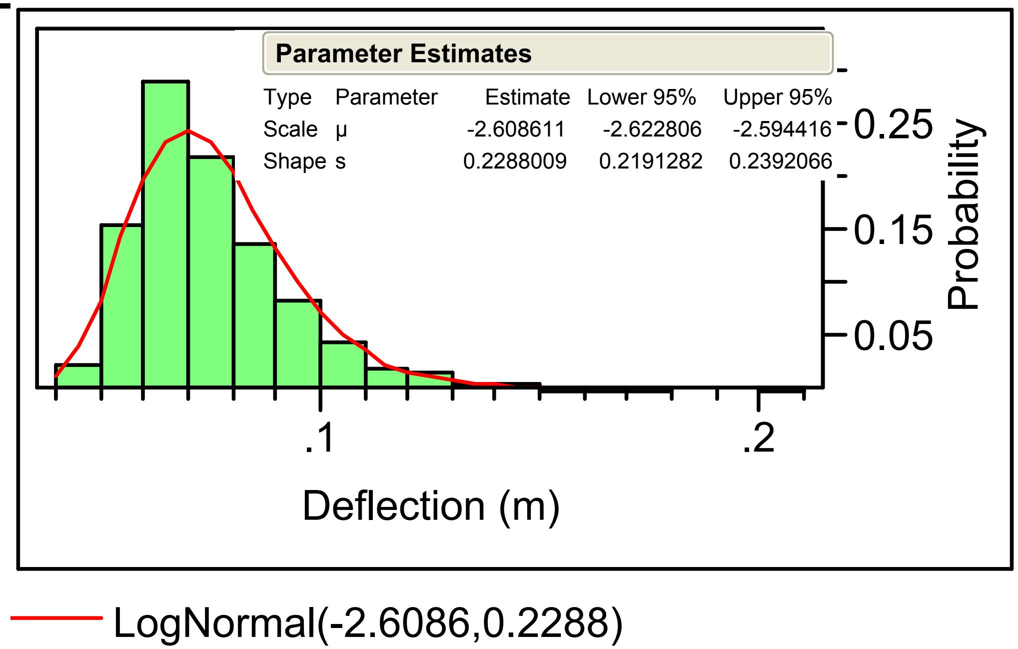
Example: Cantilever Beam UQ
Monte Carlo Sampling – Multiple Parameters



- <u>**Now make several parameters uncertain:**</u>

- **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**
- <u>***Use JMP, Minitab, or other statistics software***</u>



Fit a probability distribution function to the histogram & estimate P_{fail} values:
Prob(δ > 11 cm) ~ 0.04
Prob(δ > 21.8 cm) ~ $1.0e^{-6}$
(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 <u>epistemic</u> uncertainty:**

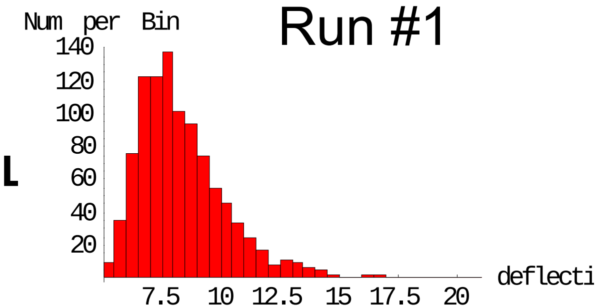
- **Deflection = PL^3/(3EI)**
- **<u>E is Normal[69, 13.8] GPa</u>**
- **<u>L is in [0.97, 1.03] m</u>**
- **<u>P is in [85, 115] N</u>**

- **1000 random samples of E for <u>each</u> instance of P and L (via DAKOTA)**

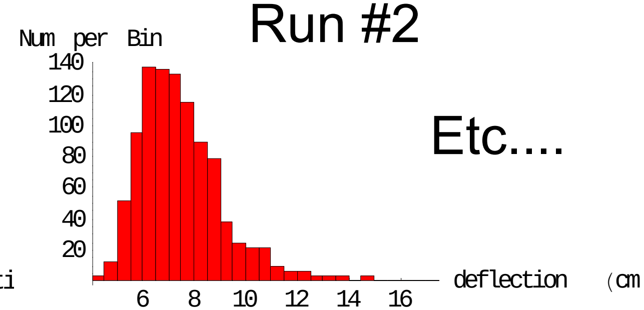
- **<u>Report range of failure probability estimates to decision maker, including the worst-case failure probability.</u>**

<u>Approach</u>:
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



Run #2



Etc....

Run #1: P_{fail} ~ 0.043

Run #2: P_{fail} ~ 0.055

Real-World 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”)

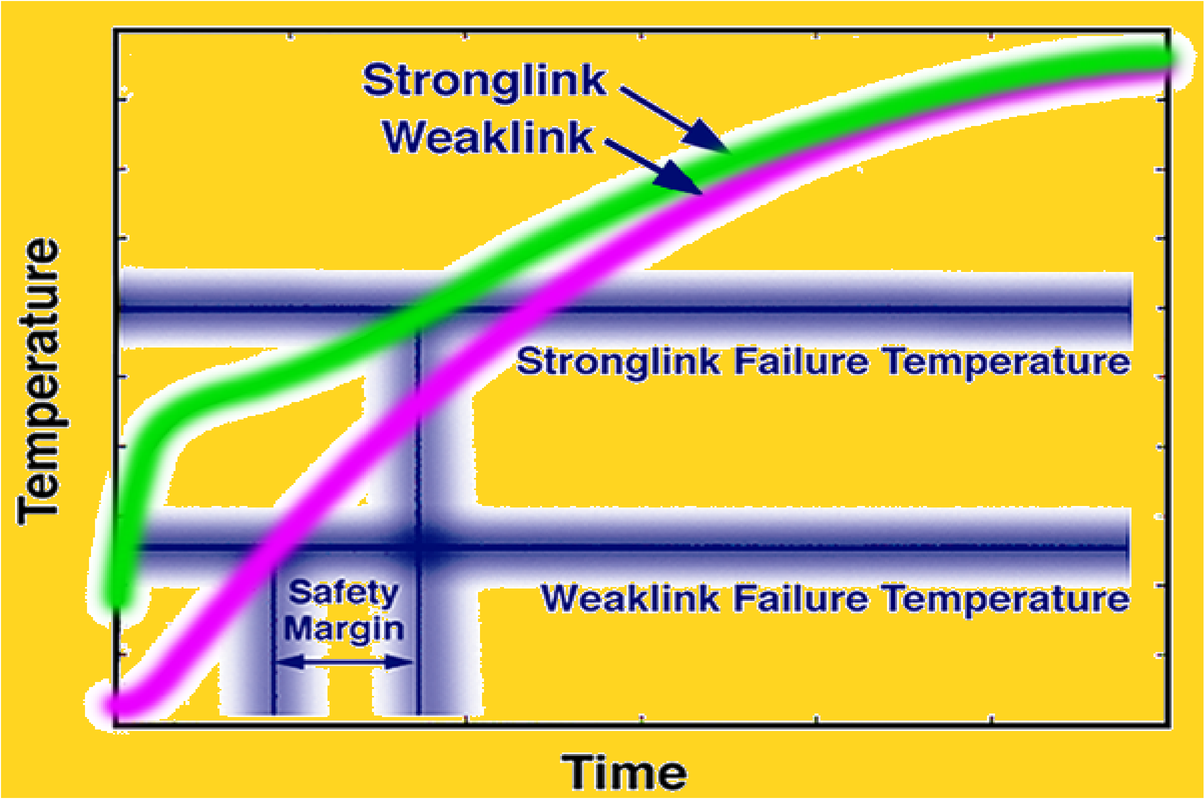
- Typical real-world UQ issues are present in this study:
  - Cannot afford O(10^6) high fidelity simulations.
  - We have a mix of epistemic and aleatoric uncertainties.
  - Q: How can we obtain probability data on system performance with only O(10^1-10^2) code runs?
  - A: We have to do something other 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:**

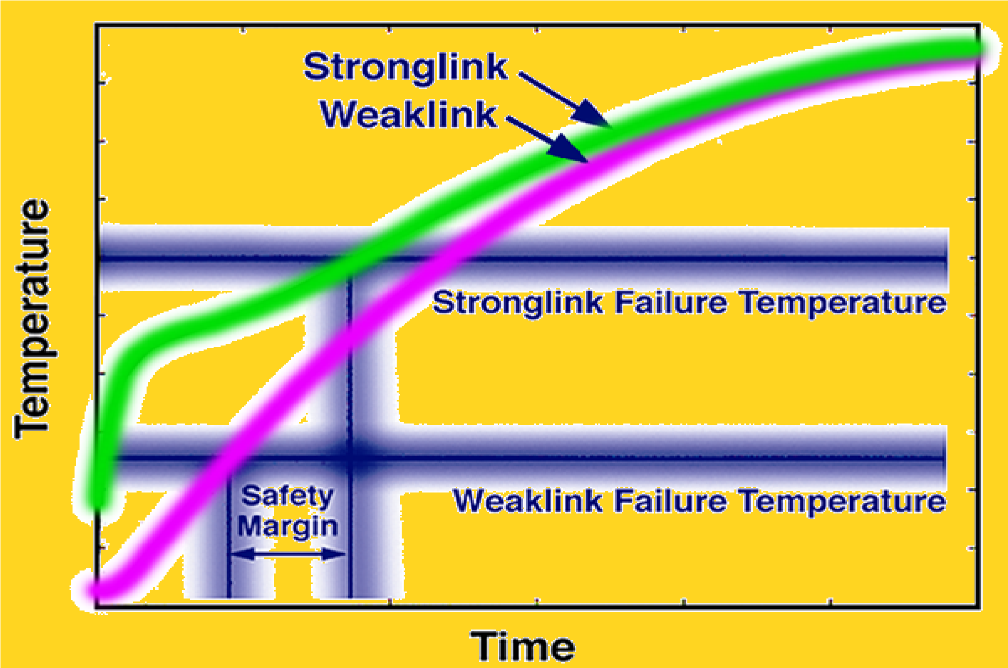
    How much margin (time) is in the WL/SL system?

    How uncertain is the margin estimate?



Thermal Response UQ Study: Issues

- Have <u>epistemic uncertainty</u> in temperature vs. time curves due to uncertainty in WL/SL model:
  - Recall: epistemic = “No PDF”
  - Material properties, initial and boundary conditions, etc.
- Have <u>both aleatoric and epistemic uncertainty</u> 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

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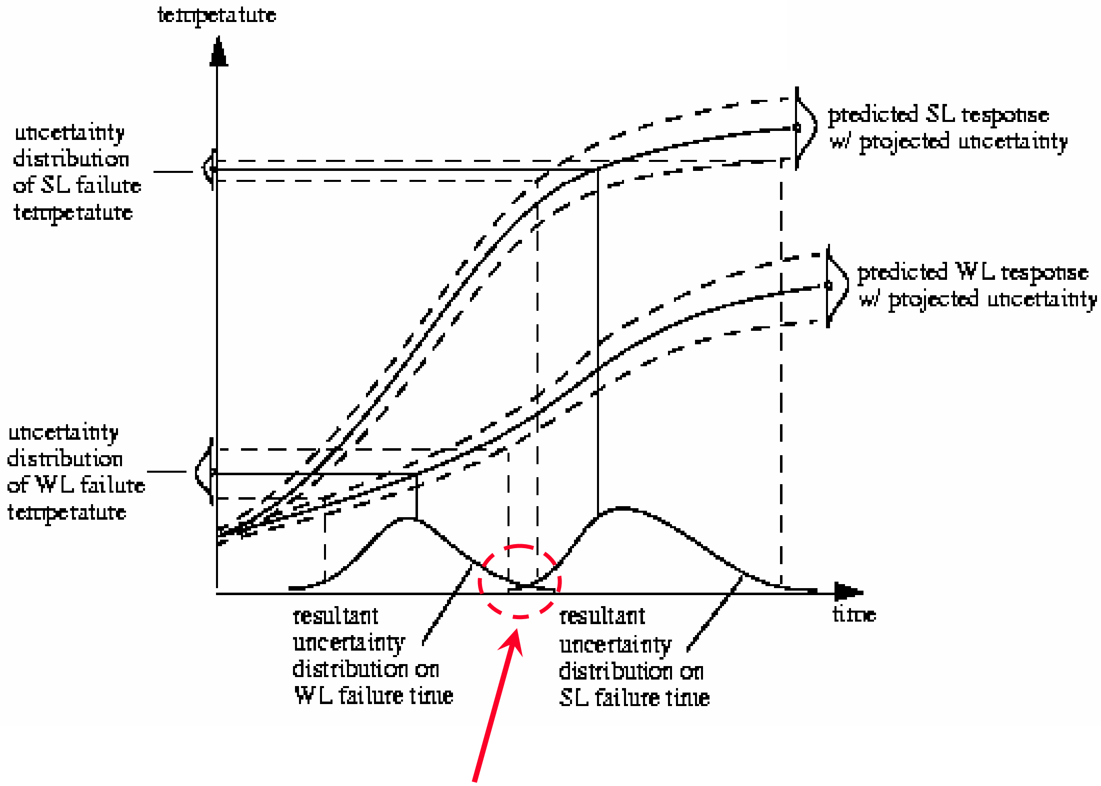
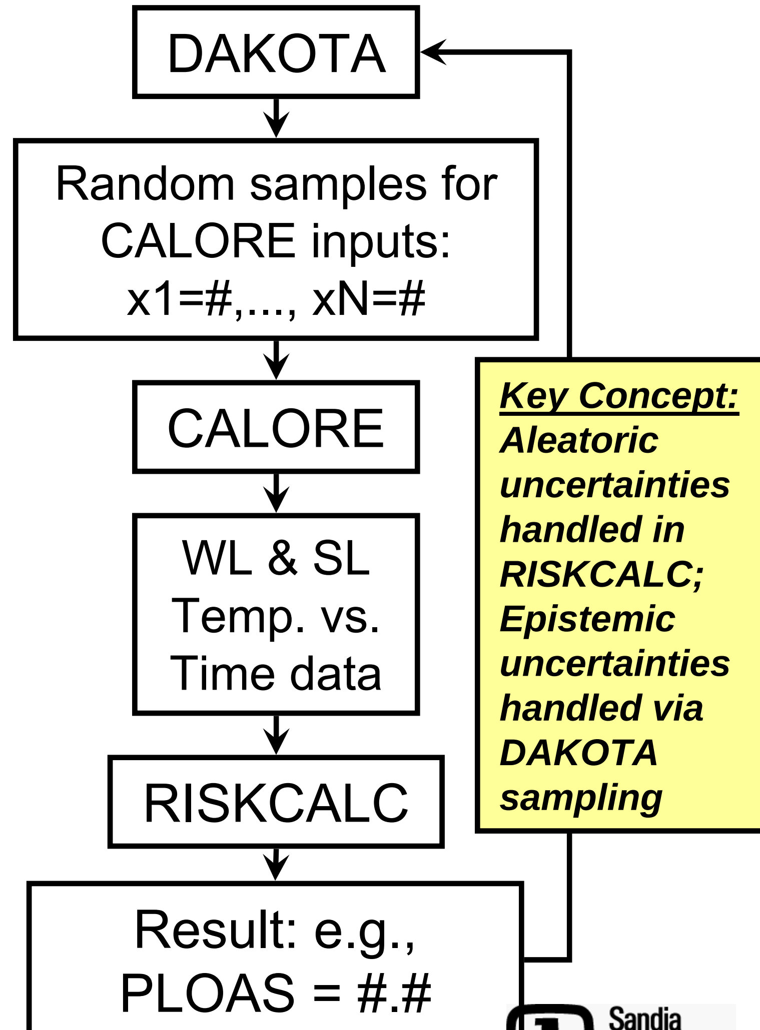


Probability of failure given by amount of tail overlap.

Thermal Response UQ Study: Approach

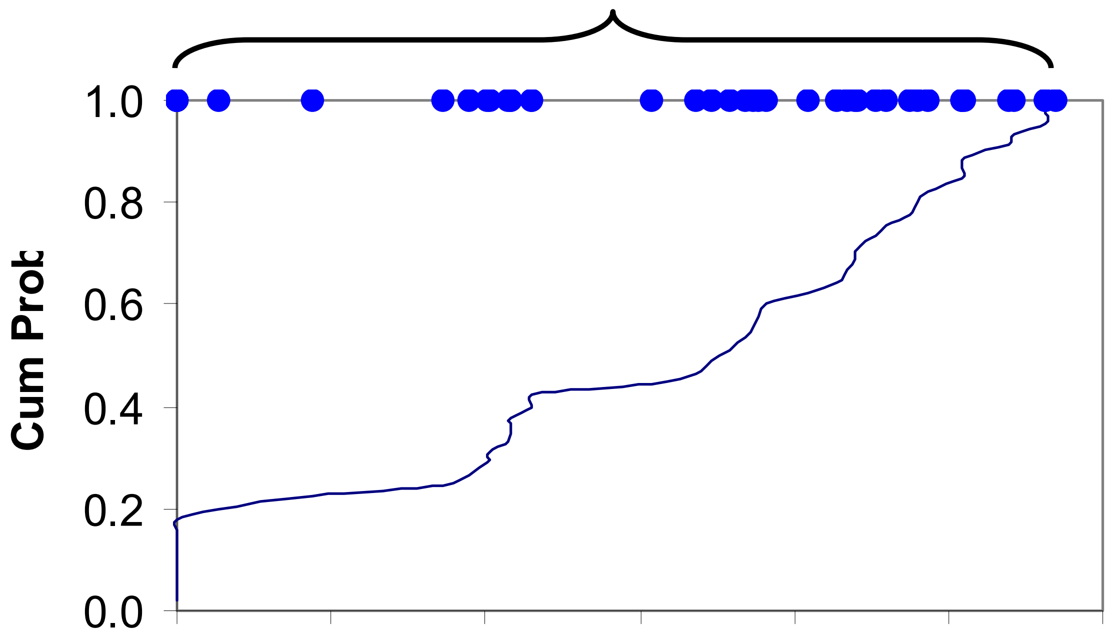
(PLOAS = Probability of Loss of Assured Safety)

- **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 <= 10^{-6}

Margin = $10^{-6}/PLOAS_{max}$

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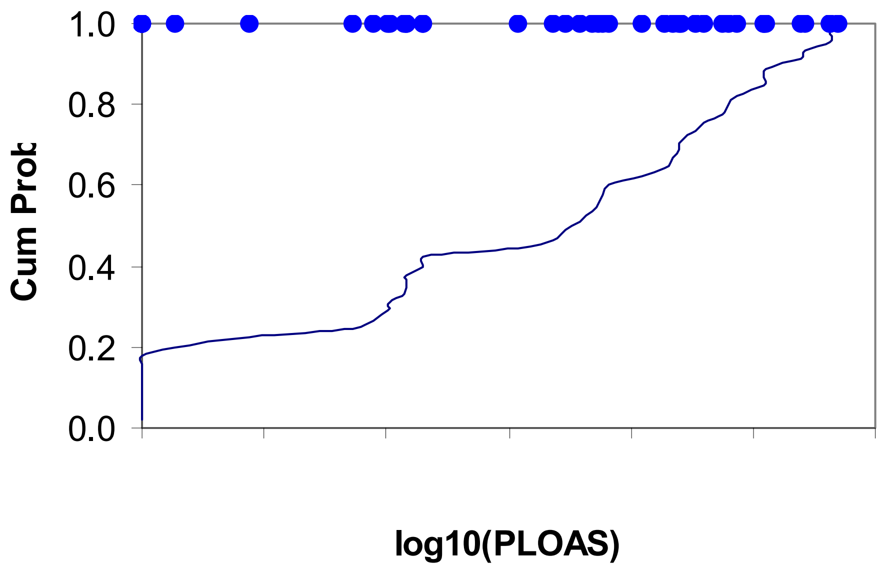
Thermal Response UQ Study Predicts Probability of Loss of Assured Safety

- 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
- References

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.
  - Don't just assume all uncertain parameters are Normally distributed, or uniformly distributed.
  - 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.

Points of Contact

- **Programmatic:**
  - **Marty Pilch: SNL ASC V&V Program Manager**
    - **Email: mpilch@sandia.gov**

- **Technical:**
  - **Tony Giunta: UQ & sensitivity analysis methods, V&V topics, DAKOTA applications**
    - **Email: aagiunt@sandia.gov**
  - ***Many other SNL Verification, Validation, and UQ experts!***

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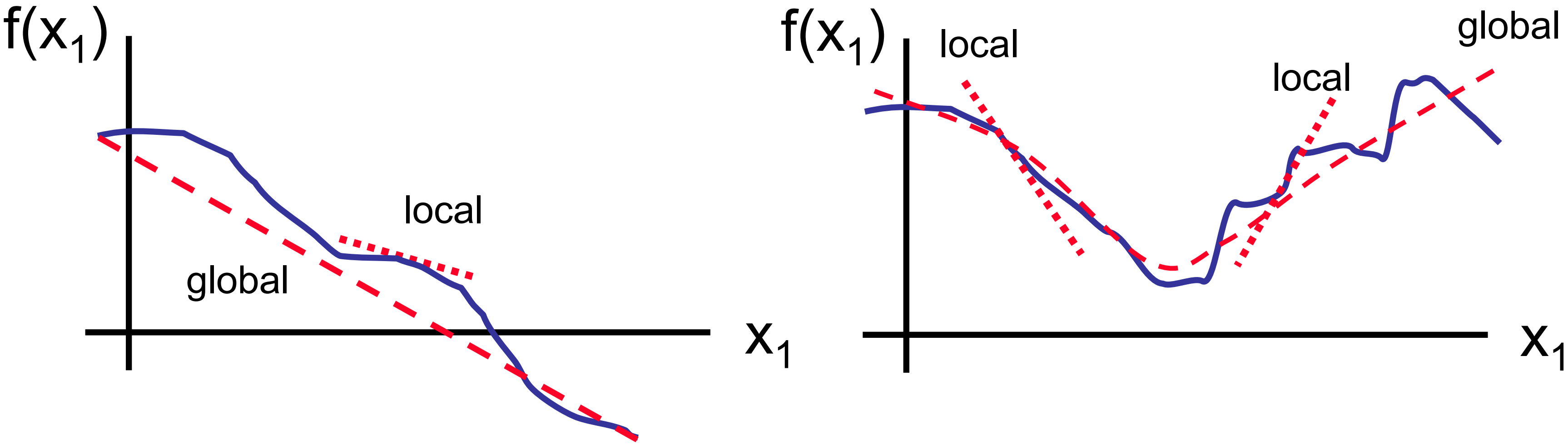
Extra Vugraphs

Examples of Sensitivity Analysis Local vs. Global Sensitivity

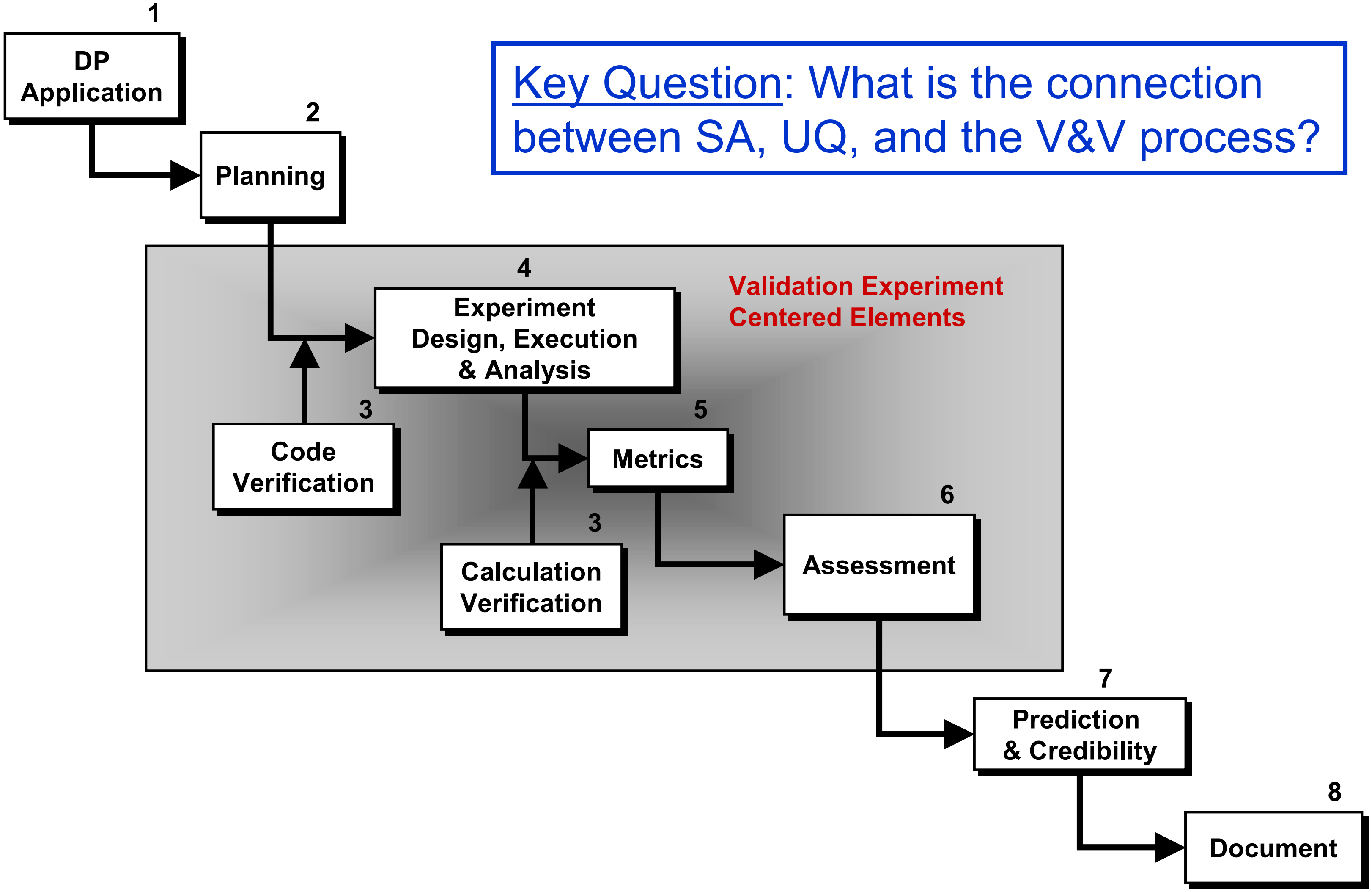


- Sensitivity analysis examines variations in $f(x_1)$ due to perturbations in x_1
  - Local sensitivities are typically partial derivatives.
    - Given a specific x_1, what is the slope at that point?
  - Global sensitivities are typically found via least squares.
    - What is the trend of the function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

Quick Review of V&V Principles

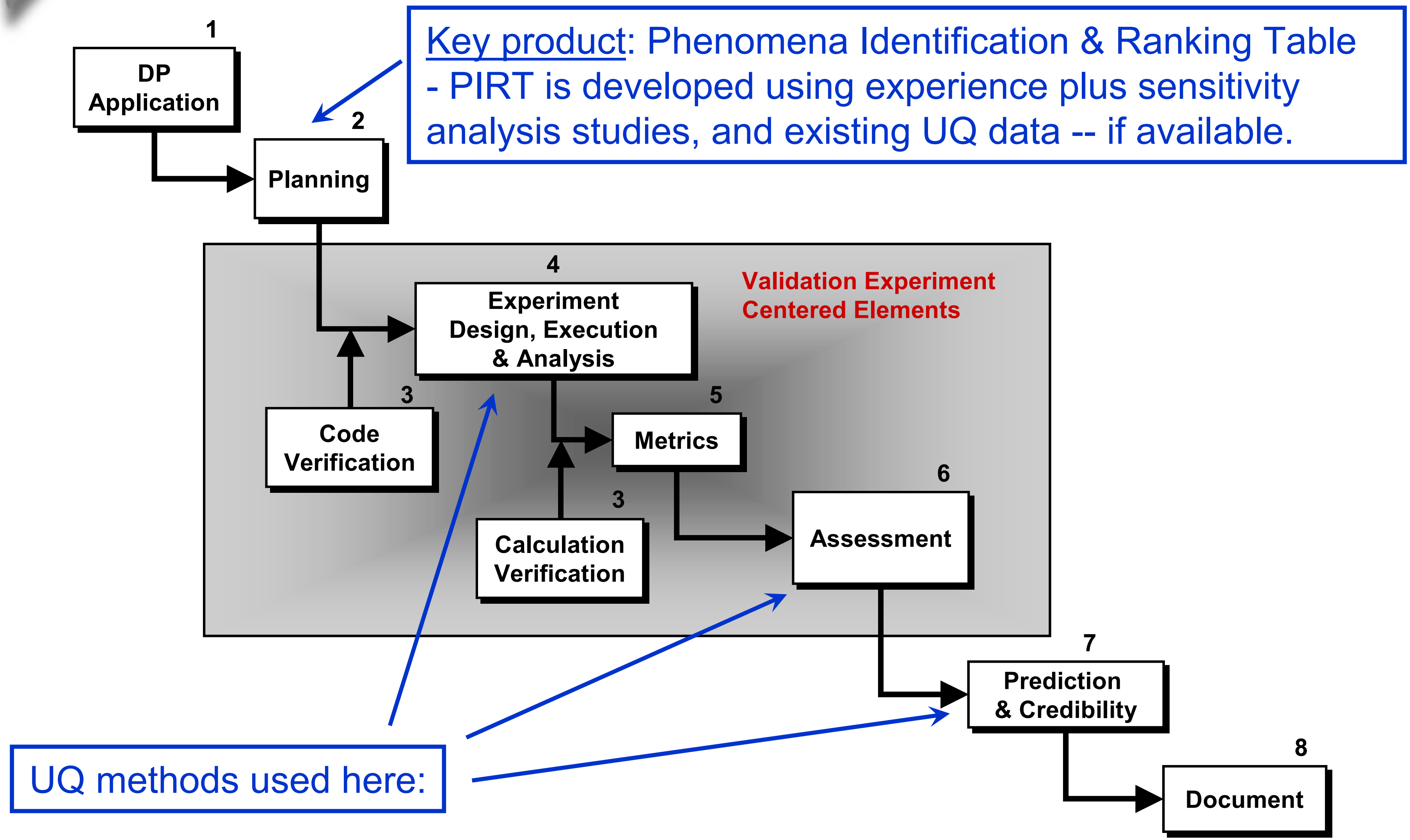
- **What is the V&V Process?**
- **How do sensitivity analysis and UQ impact the V&V process?**

Overview of the V&V Process



Key Question: What is the connection between SA, UQ, and 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 Level	Code/Model Adequacy	Status
Conductive Heat Transfer			
Material A	High	High	Good
Material B	Medium	Low	Fair (yellow)
Convective Heat Transfer			
Material A	Medium	High	Good
Material B	Medium	Unknown	Poor
Radiative Heat Transfer			
Material A	Low	High	Good
Material B	High	Low	Poor

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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**

Focus of this briefing.

- **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.***

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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

Goal:

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

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

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

- **Deflection = (PL^3)/(3EI), stress = My/I (y = distance from neutral axis)**
- **Deflection ~ 7.2 cm for P = 100 N**
- **Yield Load = 170 N, Deflection at Yield Load ~ 12.3 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

$\mu_x * (\partial\delta/\partial x)$

$\mu_P * (\partial\delta/\partial P) = 0.0724$

$\mu_L * (\partial\delta/\partial L) = 0.217$

$\mu_E * (\partial\delta/\partial E) = -0.0724$

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	.

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)?**