SAND2013-5849C

An Approach to QMU for Computational Analyses Involving Limited Resources

Brian Rutherford

Department 0431, MS0829, Sandia National Laboratories, Albuquerque, NM, 87185, USA

Tel: (1-505-844-3120)
e-mail: bmruthe@sandia.gov

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

QMU Background -- Relevant Definitions

<u>Quantification of Margins and Uncertainties</u> (QMU) is a scientific methodology that identifies relevant nuclear-warhead parameters and quantifies, using available experimental and computational tools, the margin of that parameter relative to its failure point and the uncertainties associated with the parameter. … .

<u>Aleatory Uncertainty</u> arises from an inherent randomness in the properties or behavior of the system under study.

<u>Epistemic Uncertainty</u> derives from a lack of knowledge about the appropriate value to use for a quantity that is assumed to have a fixed value in the context of a particular analysis.

… . NNSA Policy Letter: NAP-XX, Draft 5/1/07 (Taken from Helton, SAND2009-3055)

Focus for QMU Analyses: Addressing Requirements

REQUIREMENT: We need to be ***YY***% certain (confident) that at least ***XX***% of the unit population will yield a response lower than the threshold *T*.

The values of ***XX*** and ***YY*** and the comparisons ‘at-least’ versus ‘at-most’ and ‘lower’ versus ‘upper’ are parameters of the requirement.

This can often be approached using tolerance bound methodology

Special Issue on Quantification of Margins and Uncertainties, Edited by J.C. Helton and M. Pilch, *Reliability Engineering and System Safety*; (2011) 96, 959-1256.

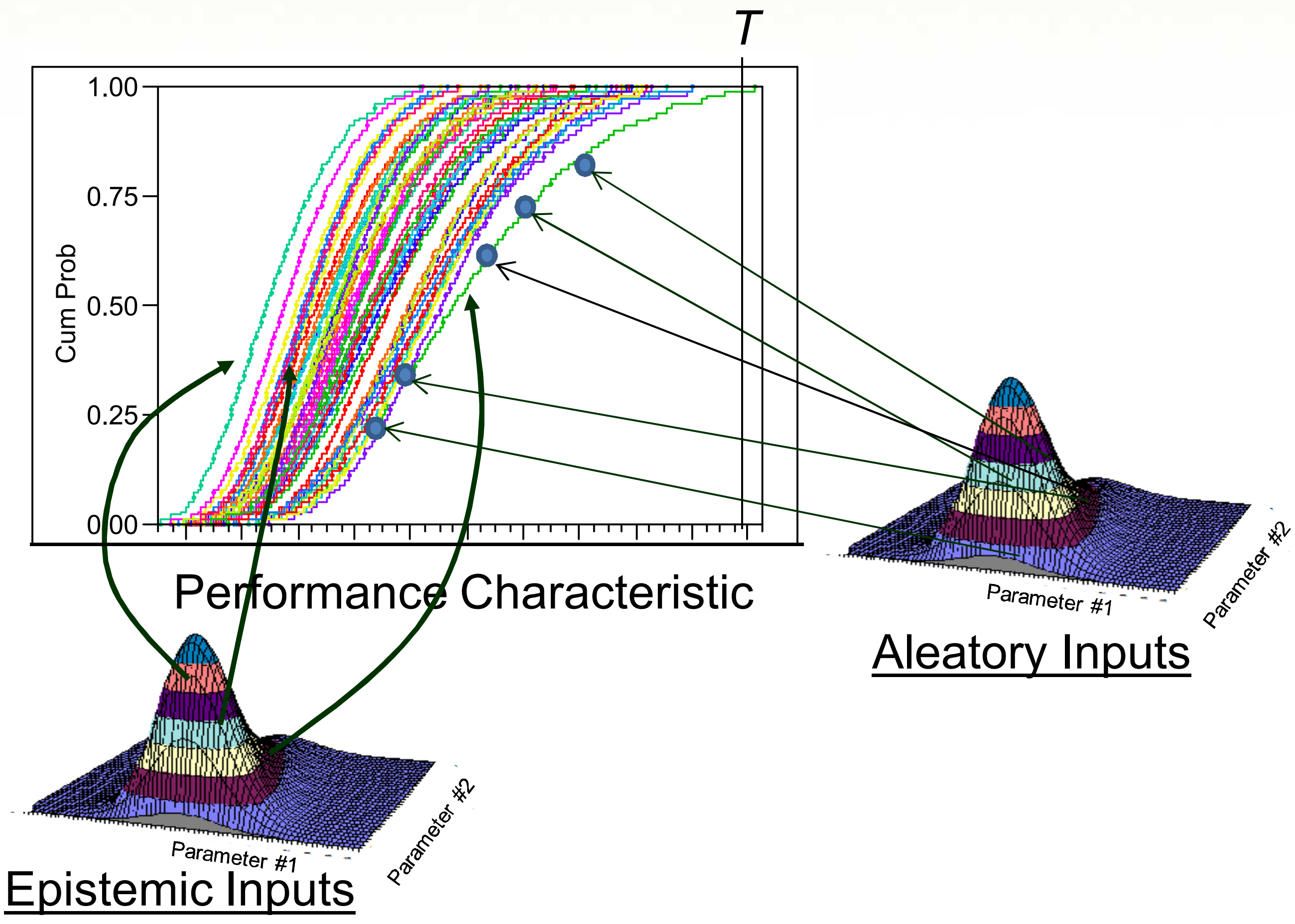
Probability-of-Frequency Approach

Basic Idea for Computational Simulation Response Data

Also referred to as the

"Second-Order Sampling Method" –

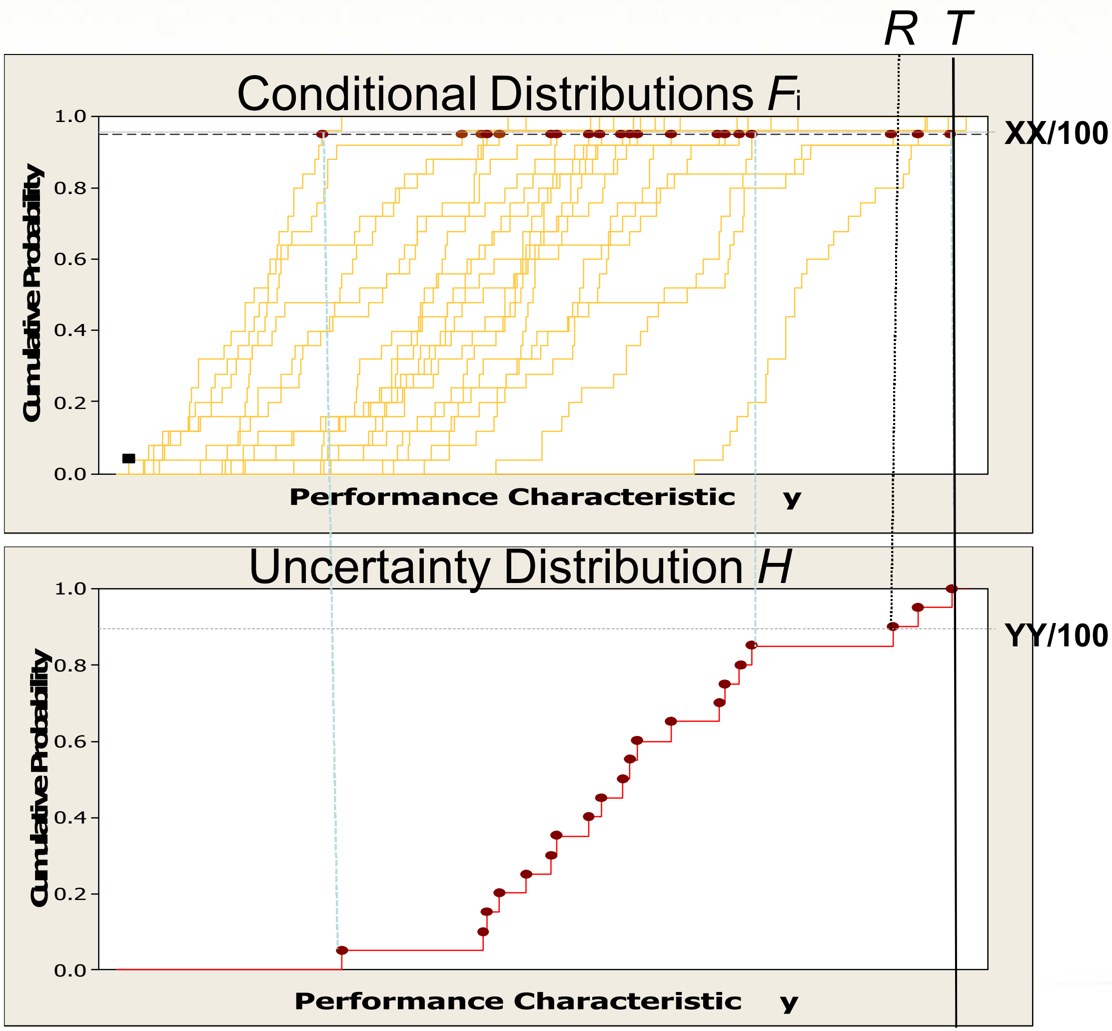
referring to the process for sampling



Helton, JC. Quantification of Margins and Uncertainty: Conceptual and Computational Basis. *Reliability Engineering and System Safety*; (2011) 96, 976-1013.

Probability-of-Frequency Approach

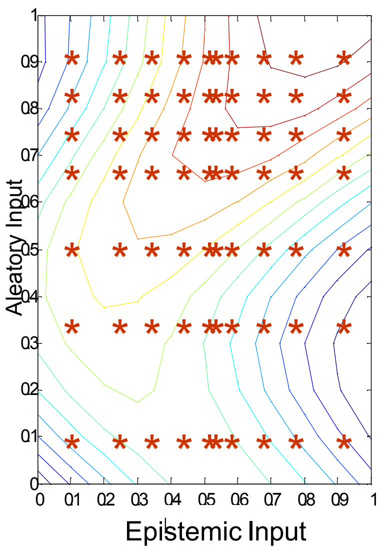
Conditional and Uncertainty Distributions



Sandia National Laboratories

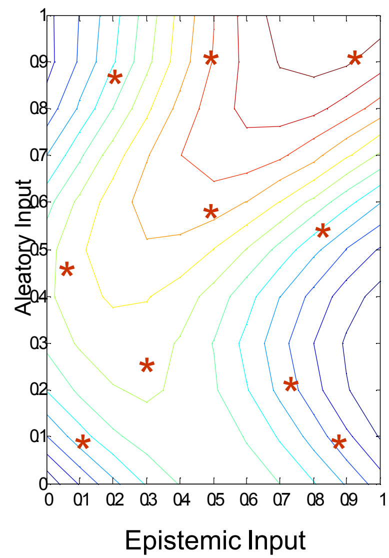
How can we Choose Simulation Points for an Efficient Analysis – Response Surfaces

Sampling Process



Second Order Sampling Process is actually applied to the sampling algorithm

Response Surface

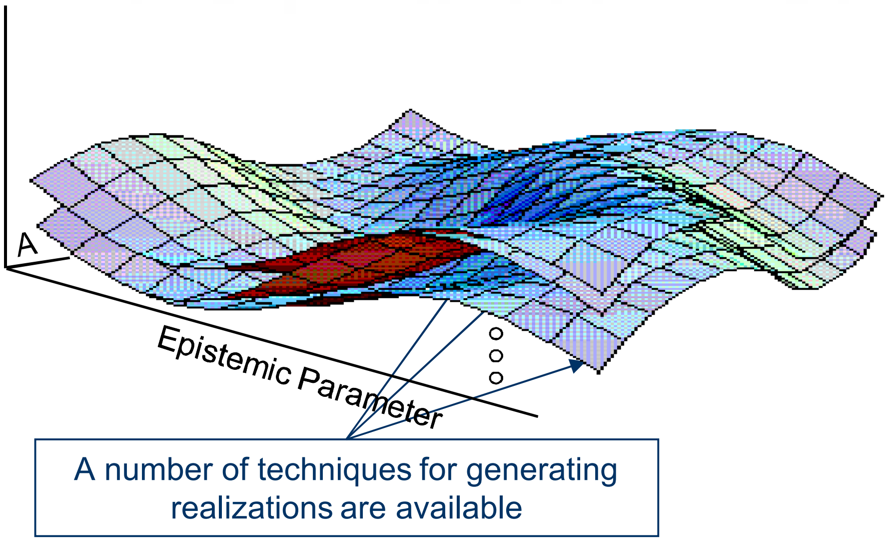


Second Order Sampling Process is utilized after a surrogate model is constructed

Problem is the uncertainty in the response surface is not accounted for.

An Approach to Accommodating Limited - Simulation Uncertainty – Response Modeling

- Used in the Geosciences in 2 and 3 dimensions – Called Stochastic Simulation
- Can be treated as a discrete probability measure (equal probability associated with each "realization")
- Provides an approach for propagating response uncertainty into uncertainty in an arbitrary performance characteristic



Deutsch CV, Journel AG. *GSLIB: Geostatistical Software Library and Users Guide Second Edition*. New York: Oxford University Press; 1998.

Gotway CA, Rutherford BM. In Armstrong M, Dowd P eds. Geostatistical simulations: proceedings of the geostatistical simulation workshop, Fontainbleau, France, 27-28 May 1993. Dordrecht: Kluwer Academic Publishers 1994.

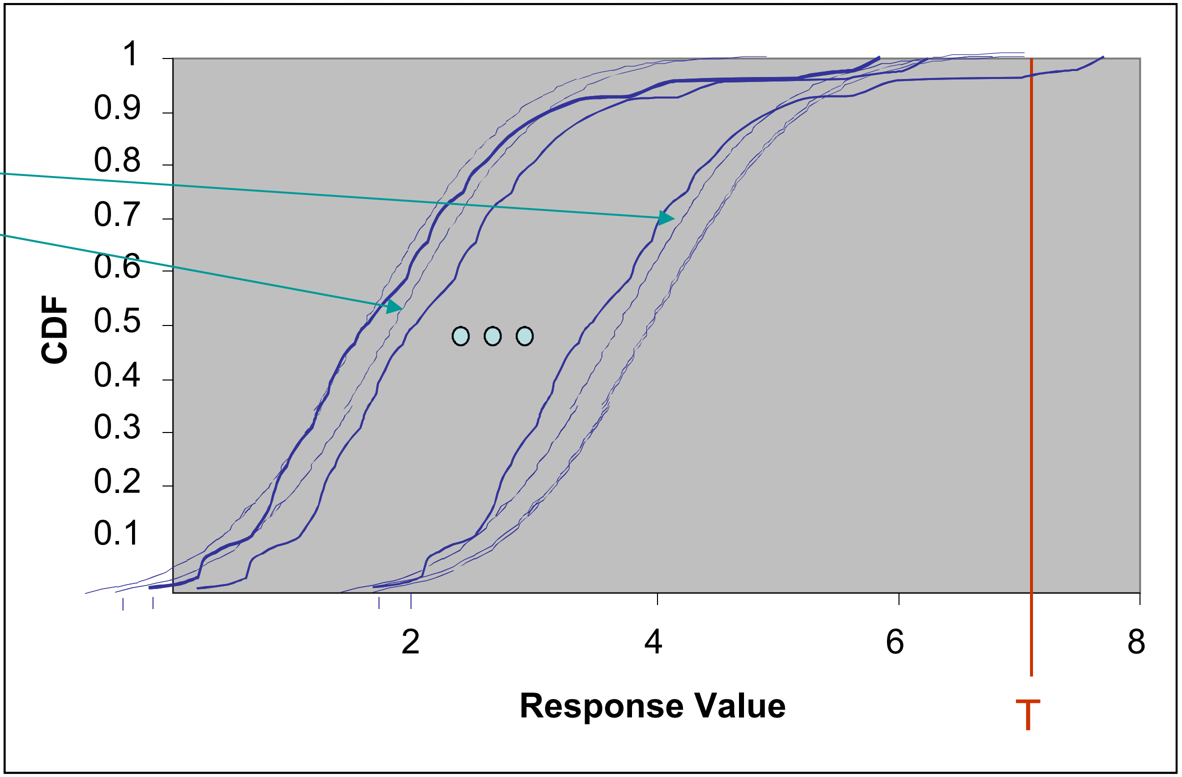
Rutherford B. A response-modeling alternative to surrogate models for support in computational analyses. *Reliability Engineering and System Safety* 2007;91:1322-30.

Probability of Frequency Approach

Using Response Modeling

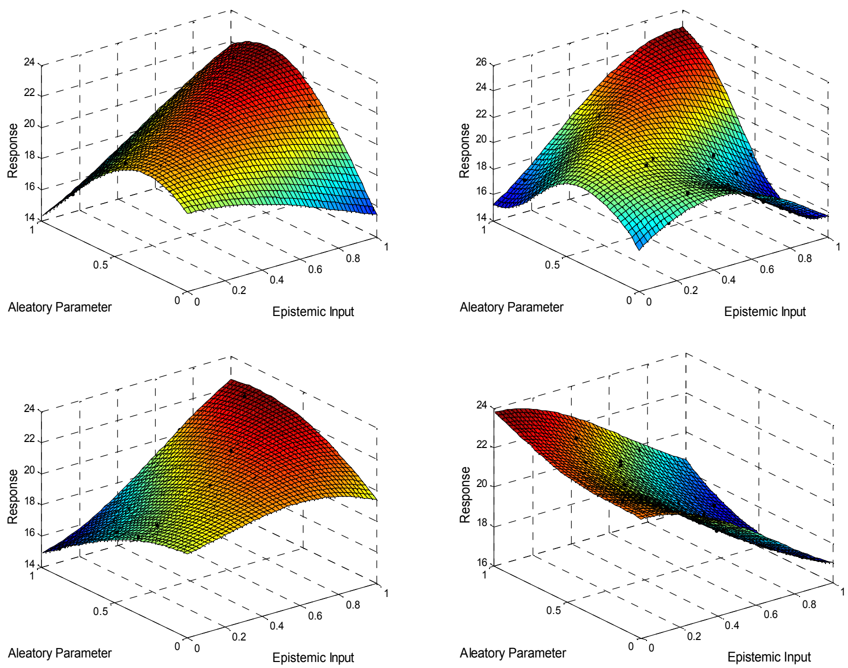
Each set of epistemic parameters would result in several (n_r) CDFs

The additional Uncertainty reflects our uncertainty in the Response Surface

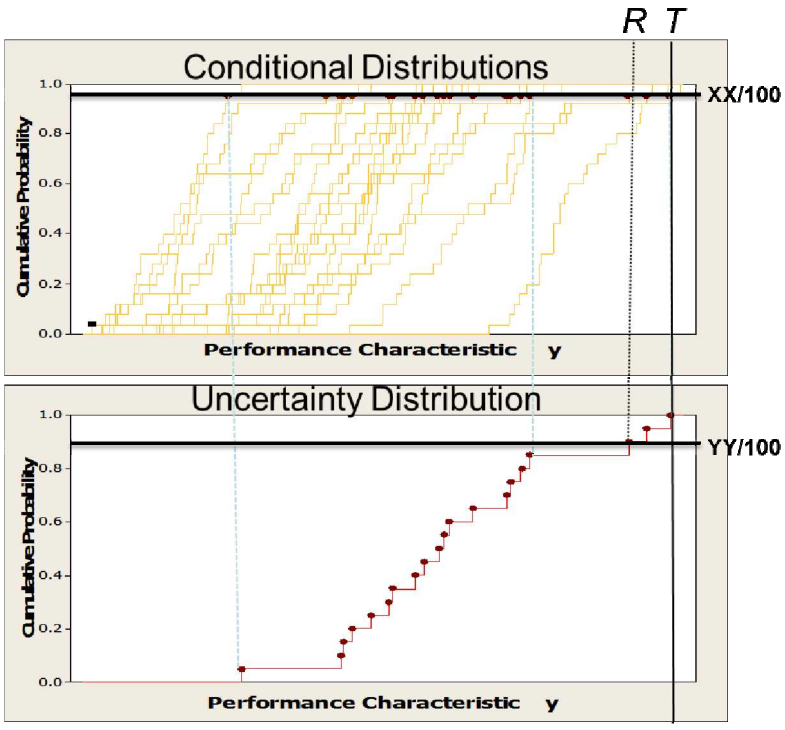


Test Problem(s)

Test over a Number of Randomly Generated "True" Surfaces



What We Would Hope to Accomplish



Want to be consistently close to the correct confidence (ie. the true *R* value)

Results – for 9 and 16 Point Simulations – Average Results over 300 Problems

9 Simulations		Mean	Std. Dev.	Abs. Diff.
Response Modeling		85%	.16%	.25 units
Response Surface		81%	19%	.27 units
Sampling		78%	.28%	.48 units

16 Simulations		Mean	Std. Dev.	Abs. Diff.
Response Modeling		86%	.14%	.14 units
Response Surface		80%	19%	.14 units
Sampling		79%	.25%	.35 units

Summary

- For experimental data, tolerance bounds often provide a straightforward solution to “the requirements“.
- The probability-of-frequency construct can be used for this same purpose for computational simulation data where there is additional epistemic uncertainty.
- When a limited number of simulations can be run there is additional uncertainty resulting from estimating the response through sampling or fitting a response surface. Response modeling can capture much of this additional uncertainty.