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1411, Optimization and Uncertainty Estimation, Manager Scott Mitchell

Department Review, May 16, 2006

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Highlights this performance year

- **ASC V&V Program**
  - Epistemic Uncertainty Modeling
    - First example of weapons application
  - Bayesian approaches to validation
  - Verification Milestone for LHS
- **PRIDE LDRD**
  - Parameter Study Analysis/Surrogate Modeling
  - Bayesian approach in multi-fidelity GP analysis
  - Robust Design
- **DAKOTA Capabilities**
  - Implemented Dempster-Shafer Theory of Evidence
  - Implemented Gaussian Process model within Trust-Region Optimization
  - Continued support for JEGA, LHS, sampling-based SA, and quasi-MC methods

ASC V&V Epistemic UQ Application

- SNL has focused much effort on methods to quantify epistemic uncertainty
- One method that has emerged as a strong candidate is Dempster-Shafer Theory of Evidence
- To date, most of the results presented on Dempster-Shafer have been on analytic test problems
- We wanted to test the efficacy and usability of Dempster-Shafer on a real application
  - **Examine computational needs**
  - **Get more insight about how to interpret the results and what they buy us over traditional probabilistic analysis**
  - **Investigate potential uses for V&V applications**
- This is the first application of evidence theory to a weapons application
- I am the PI on this, funded through Marty Pilch
- Work in collaboration with Angel Urbina, Bill Oberkampf, and Jon Helton

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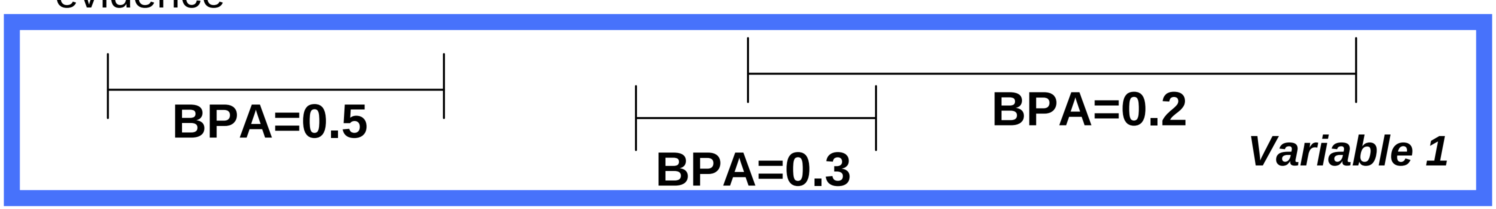
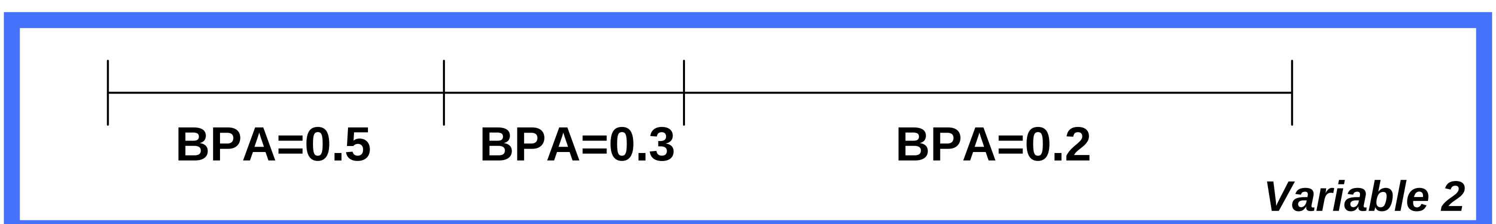
ASC V&V
Epistemic Uncertainty Quantification

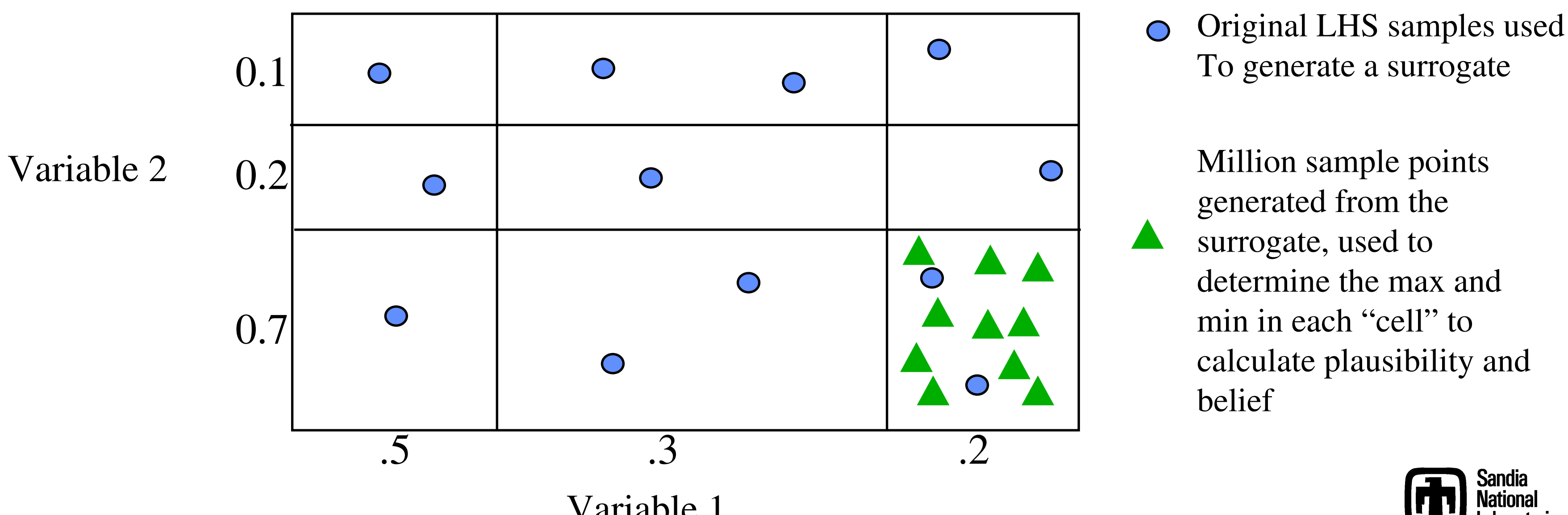
- Epistemic uncertainty refers to the situation where one does not know enough to specify a probability distribution on a variable
- Sometimes it is referred to as subjective, reducible, or lack of knowledge uncertainty
- For each uncertain input variable, one specifies “basic probability assignment” for each potential interval where this variable may exist.
- Intervals may be contiguous, overlapping, or have “gaps”
- In Dempster-Shafer theory, belief is a lower bound on the probability that is consistent with the evidence
- Plausibility is the upper bound on the probability that is consistent with the evidence





ASC V&V
Epistemic Uncertainty Quantification

- Look at various combinations of intervals. In each joint interval “box”, one needs to find the maximum and minimum value in that box (by sampling or optimization)
- Order these beliefs and plausibility to get CDFs
- Draws on the strengths of DAKOTA
  - **Requires surrogates**
  - **Requires sampling and/or optimization for calculation of plausibility and belief within each interval “cell”**
  - **Easily parallelized**



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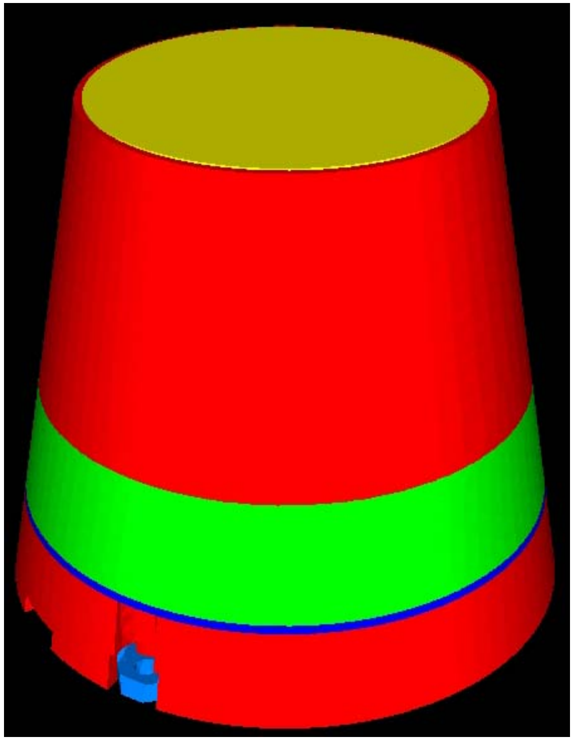
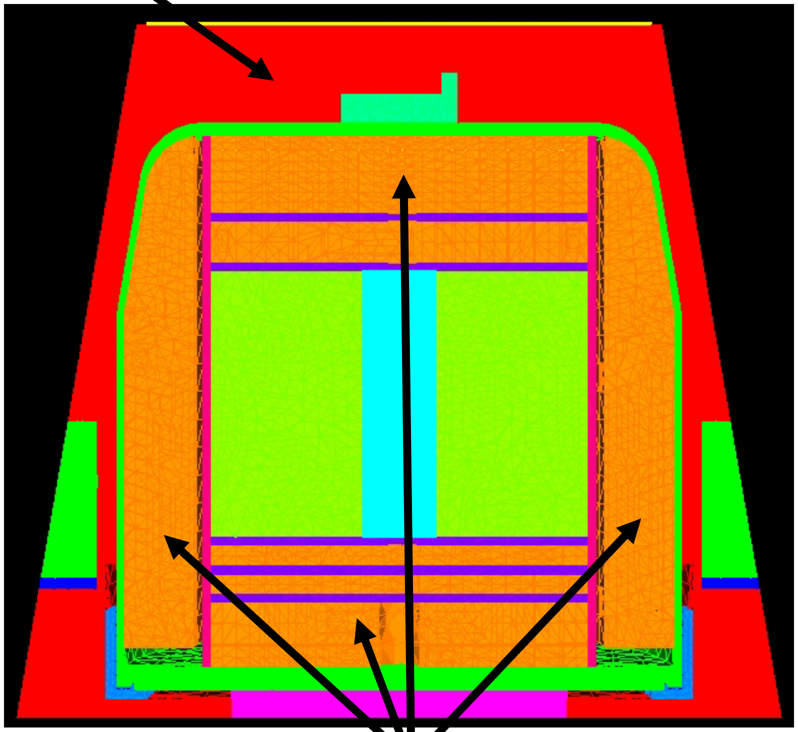
ASC V&V Thermal Battery Assembly



Thermal Battery Assembly (TBA)



Thermal Battery Assembly Epistemic UQ

- Treated the elastic property of min-K as an epistemic variable with 3 intervals: [3.0, 3.2] (3.2,3.4], and (3.4, 3.5]
- Treated the foam density as a probabilistic variable

Min K	Foam
3.0 — 3.2 — 3.4 — 3.5 1/3 · 1/3 · 1/3	**Probabilistic** • **Used a kernel density estimator based on actual data**
3.0 — 3.2 — 3.4 — 3.5 0.2 · 0.6 · 0.2	**Probabilistic** • **Used a kernel density estimator based on actual data**

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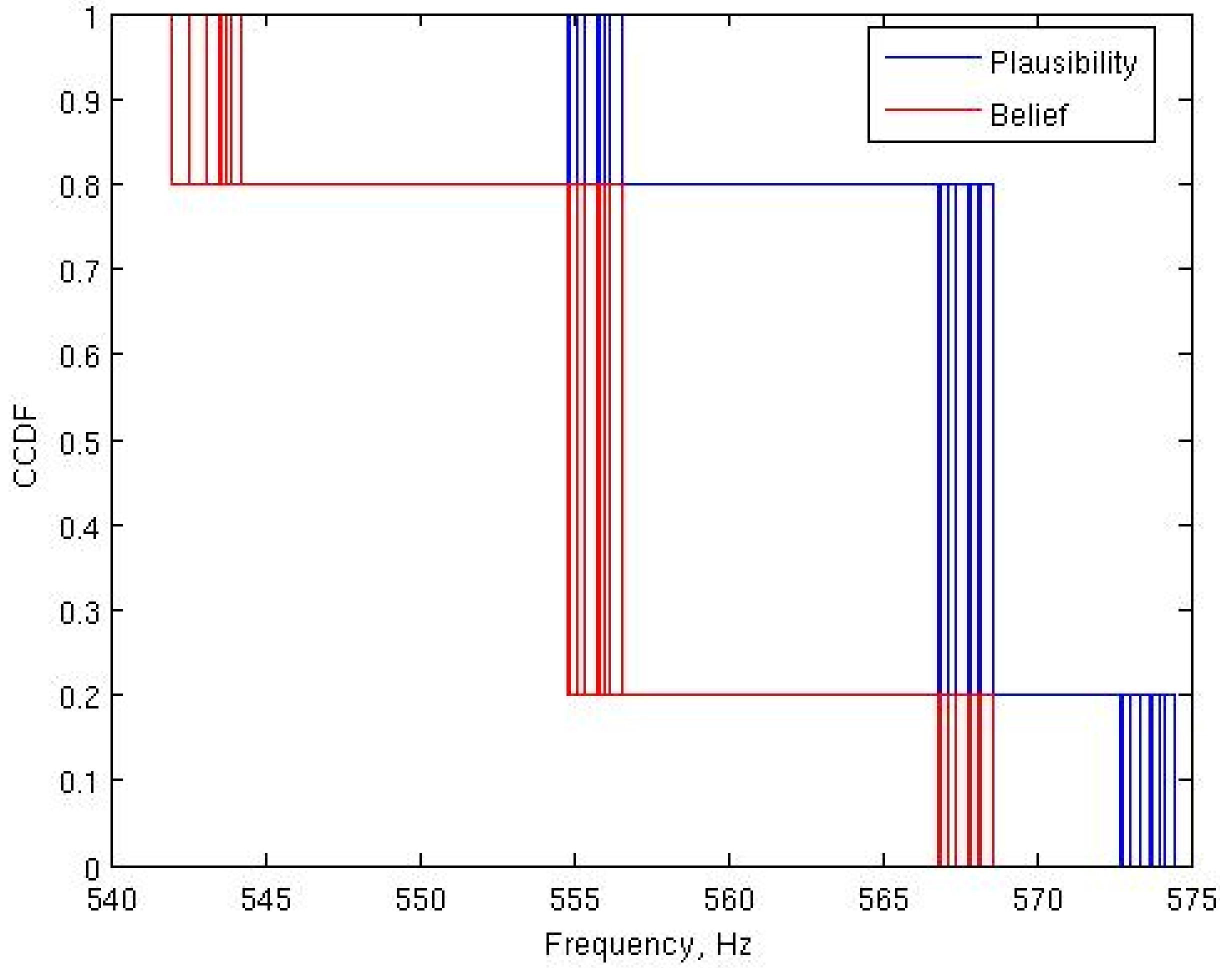
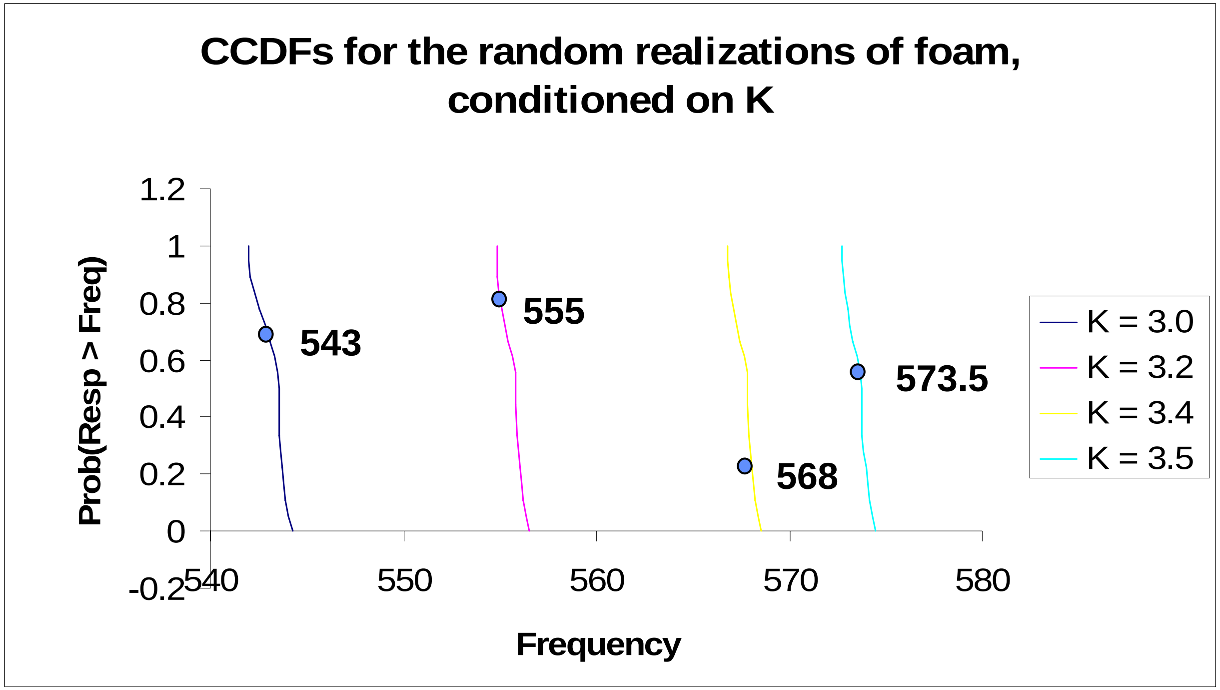
Thermal Battery Assembly
CCDFs for Belief and Plausibility



Different Representation of the Epistemic Uncertainty



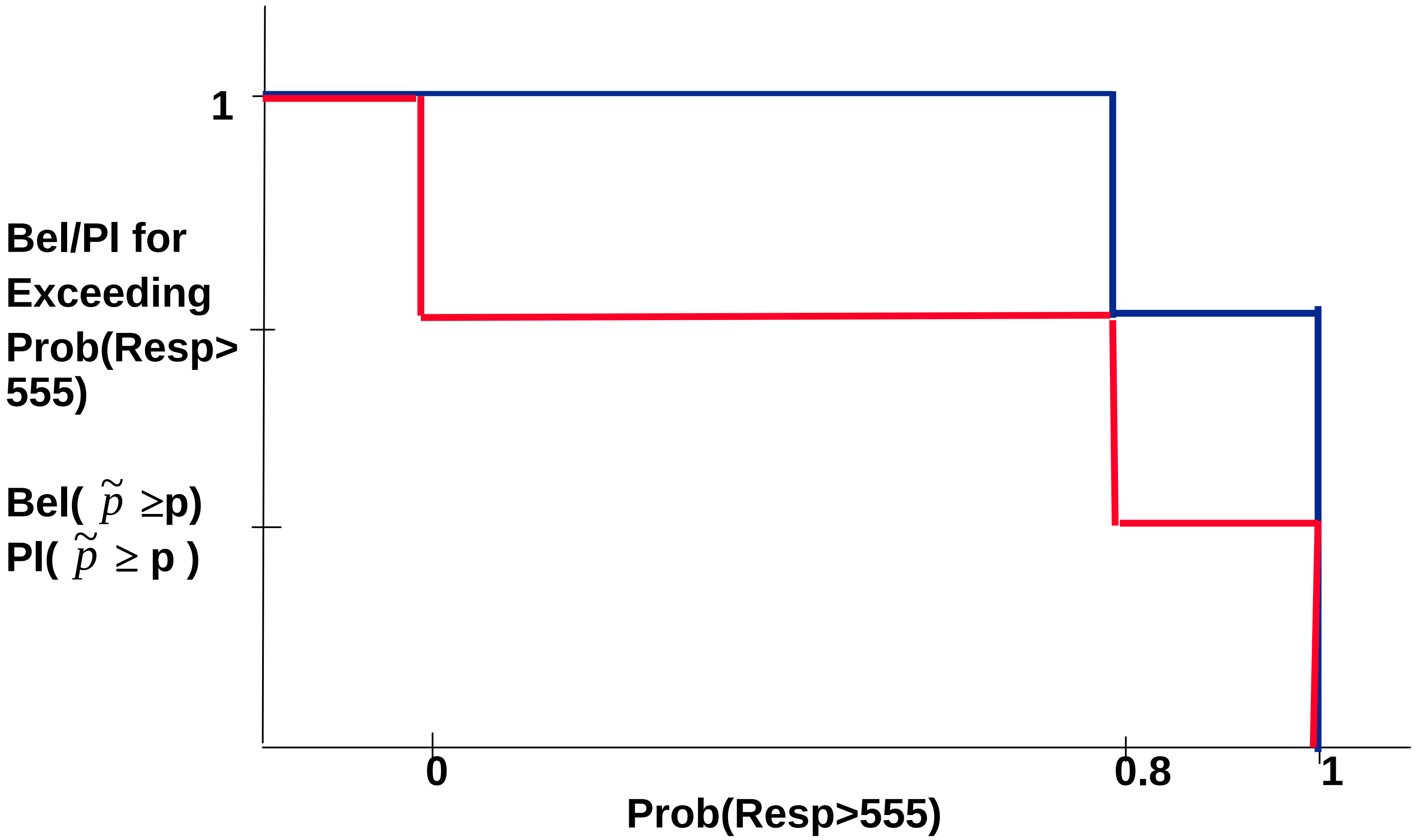
P(Freq > 555|K=3.2) = 1 if Freq < 554.8

0 if freq > 556.5

177.4 – 0.49F + 29.73 K

•Idea is to look at the range of the exceedence probability (CCDF value) given the epistemic structure on K

Calculation of Belief and Plaus for K=3.2, q=555



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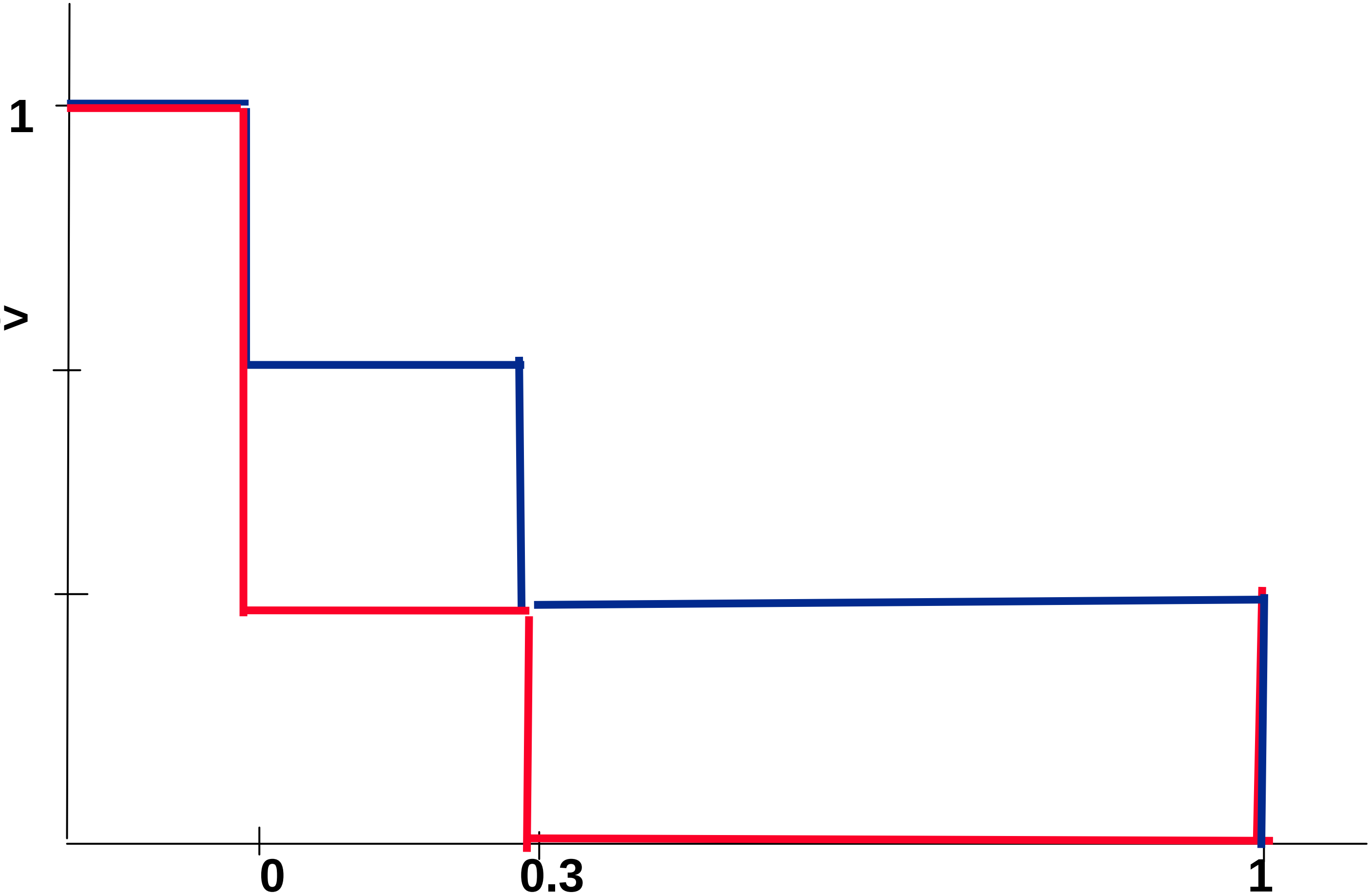
Calculation of Belief and Plaus for K=3.4,F=568

Bel/Pl for Exceeding Prob(Resp> 568)

Bel($\tilde{p} \geq$p)
Pl($\tilde{p} \geq$ p)



Prob(Resp>568)

ASC V&V Epistemic UQ
Thermal Battery Application

- The alternate form of presenting the epistemic results presents the belief / plausibility of exceeding the CCDF probability
- Each graph is conditional on ONE particular frequency
- As you move along the response values, the belief/plausibility of exceeding the CCDF values decrease
- If the effect of the foam variability were larger, we would see more granularity in the belief and plausibility curves
- The differences in min-k variation > the differences in the foam variation: this analysis provided valuable sensitivity information
- Presentation and interpretation of epistemic uncertainty results is challenging
- This type of analysis can be used for decision support
- IMPACT: First application of a weapon system application of evidence theory, identified computational issues with Dempster-Shafer implementation, identified interpretation issues with presentation of results

PRIDE LDRD

Penetrator Reliability Investigation and Design Exploration

- How can we efficiently optimize an earth penetrator weapon design given the uncertainties in delivery conditions, target geology and model parameters?
- Develop and implement new optimization under uncertainty (OUU) methods using surrogate models in a multi-fidelity hierarchy to enable credible and reliable penetrator design modeling.
- Surrogate is a Gaussian Process
  - **Idea of spatial covariance**
  - **Bayesian updating is done on parameters that govern the covariance**
  - **One big advantage is that a GP allows quantification of uncertainty in prediction**
- This year, my focus is on implementation of a Bayesian multifidelity Gaussian process in DAKOTA
- I am the technical lead on PRIDE
- IMPACT: Develop methods that can be applied to other design problems (i.e., MEMS)

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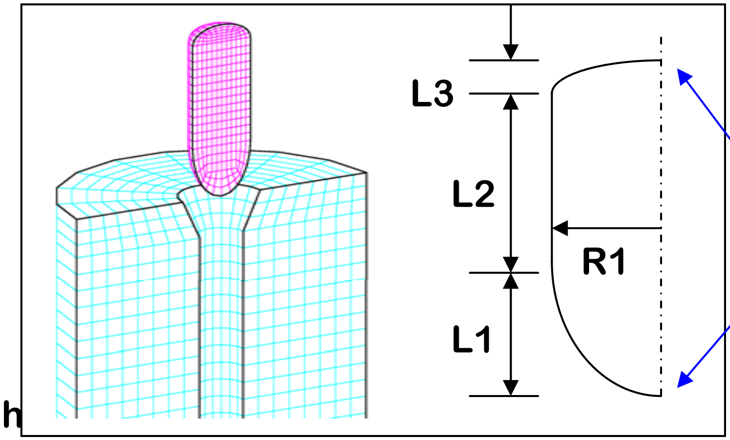
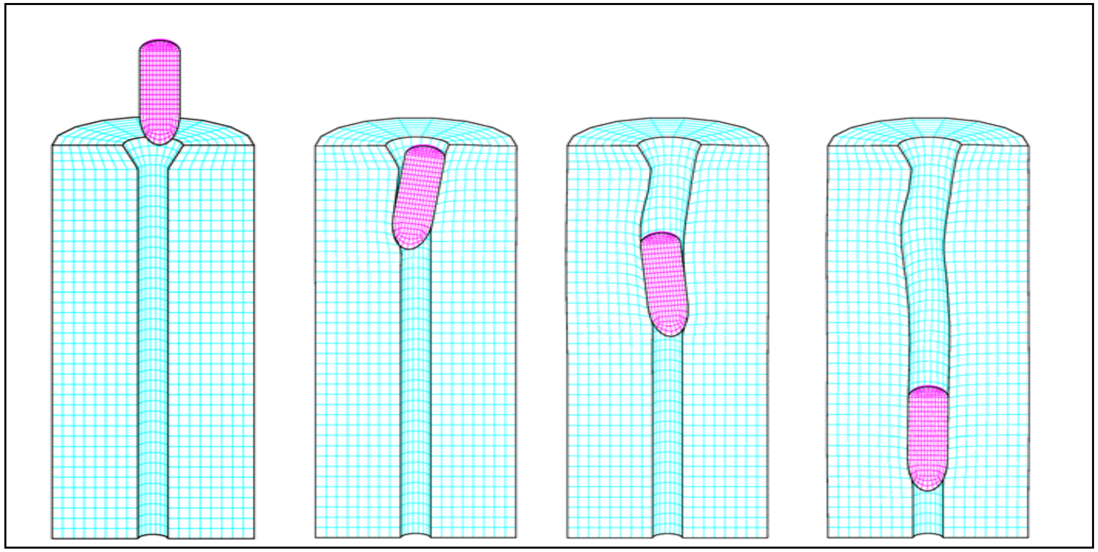
Low-Fidelity Penetrator Model

Right: Parameterized FEM.
Low-fidelity model, 4000 Elements



Below: Low-fidelity simulation, using Presto, showing progress through penetration shaft created by shape charge.



- Optimization Problem: Maximize depth of penetration while minimizing accelerations.
- Design Variables:
  L1, L2, L3
- Constraints:
  Upper & lower bounds on Weight, R1
- Uncertainties:
  AoA=Angle of attack
  IV =Impact velocity
  OS=Offset
  CR=Cavity radius
  TS=Target strength

Gaussian Process Status

- GaussProcApproximation class has been added as a derived Approximation class type in the DAKOTA hierarchy
- This lets us use the surrogate framework
- Trust region surrogate framework with the GP approximation is working
- Optimization of the maximum likelihood function to obtain covariance parameters is working, using Opt++
- Worked with Patty Hough to define the optimization of the covariance parameters. Currently, we perform this optimization once per trust region
- Performance of GP is comparable to neural nets, kriging
- Next step is implementing a two-level Bayesian autoregressive model:
  - $f_H(x) = f_L(x) + \delta(x)$
- Also will implement the maximization of an "expected improvement" function, where the objective is a weighting of the performance measure plus an estimate of prediction variance obtained by the GP prediction
- The goal is to look in parts of the space which have few samples and thus high prediction variance

DAKOTA UQ Summary

- **We need to improve the UQ capabilities within DAKOTA to address user needs:**
  - Multi-fidelity approaches
    - **Multi-level Gaussian Process model within Trust-Region Optimization**
  - Epistemic uncertainty representation
    - **Implementation of Dempster-Shafer Evidence Theory**
  - More sophisticated methods such as surrogate representations of UQ
  - Help users meet their ASC V&V Milestones
- **Future Development Focus**
  - Incremental LHS
  - Importance Sampling
  - Efficient Sensitivity Analysis Methods

  } Reduce function evaluations

  - Bayesian Methods
  - Evidence Theory

  } Epistemic uncertainty

UQ Needs for the next 5 years

- MOTIVATION:
  - **Improving the credibility of predictive simulations**

- ASC
  - **Must be able to use simulation tools to quantify margins under uncertainty (QMU)**
  - **Must be willing to state confidence in predictions given by a simulation**

- Driving Applications
  - **Stockpile Life Extension programs**
  - **Reliable Replacement Warhead RRW**
  - **MEMS**
  - **Nanotechnology**
  - **Homeland security**

- Some of these applications have huge uncertainties. Many existing methods only handle small uncertainties (e.g., 5 or 10% of mean value)

UQ Needs for the next 5 years

- Quantify "extrapolative" confidence
  - **Requires the use of response surface methods which handle uncertainty**
- Sampling for stochastic processes
  - **Sampling of random fields (in space and/or time, possibly non-stationary and non-Gaussian), not just random variables.**
- Intrinsic / Analytic UQ capability
  - **Expand the role of expansion methods such as Polynomial chaos**
  - **Many issues remain about the set of points on which to construct the basis for different distribution types, the type of integration method, etc.**
- Efficient (e.g. surrogate) methods for higher order moments and tail statistics
  - **Better quantification of surrogate accuracy**
- Adaptive Experimental Design
  - **Importance Sampling, Adaptive OAs**
- Efficient sensitivity analysis
- Epistemic UQ
  - **Capability to combine aleatory and epistemic uncertainty in one analysis**
- UQ treatment in multi-fidelity and/or hierarchical models
  - **Efficiency issue**
  - **More important, dealing with uncertainty at different time or length scales across simulations**

Service

- Mentoring
  - **John McFarland (Mahadevan's student in Vanderbilt's Reliability program)**
    - **Summer 05 and 06: Bayesian Belief Networks in calibration, prediction**
  - **Kay Vugrin (new staff member, Math).**
    - **Summer/Fall 05: Parameter estimation, covariance of estimators.**
  - **Raisa Slepoy (UNM, Statistics).**
    - **Summer 05: Sampling/response surface interactions**
  - **John Eddy (GAs/agents in multiobjective design).**
    - **2004-05: Member of dissertation committee. Successful defense Dec. 2005.**
    - **Now a member of Dept. 6642.**
  - **Brian Adams**
    - **New dept. member interested in nondeterministic methods, parameter est.**
  - **Dan Briand**
    - **Statistics, UNM. Prognostics; non-uniform time series analysis**
  - **Gio Kao (UIUC Computer Science)**
    - **Efficient heuristics for pruning large combinatorial problems, Pareto optimization**

- Reviewed 7 Papers for AIAA, IEEE, the European Journal of OR, etc.
- Interviewed 4 candidates for 1415 and 6642

Leadership

- **SAMSI: NSF Statistical and Applied Mathematical Sciences Institute**
  – 06-07 Program on Assessment and Utilization of Complex Computer Models
  – Engineering Model Subgroup
  – I am the technical lead from Sandia
  – Topics include model calibration, validation, extrapolation, model hierarchies, DACE
- **Leadership roles in ASC V&V community and UQ**
  – Technical lead on PRIDE
  – Active participant in V&V working group, Challenge Problem Workshop
  – Member of the LANL-SNL Epistemic Uncertainty Working Group
  – Helping to define V&V Center of Excellence, UQ role for next 5 years

Publications

- *Validation of the Thermal Challenge Problem using Bayesian Belief Networks.* J. McFarland and L. P. Swiler. SAND2005-5980.
- *Bayesian Approaches to Engineering Design Problems.* L. P. Swiler. SAND 2005-3294.
- *Conference Region Estimation Techniques for Nonlinear Regression: Three Case Studies.* K. W. Vugrin, L. P. Swiler, R. M. Roberts, N. Stuckey-Mack, and S.P. Sullivan.
- *Error Estimation Approaches for Progressive Response Surfaces.* V.J. Romero, R. Slepoy, L.P. Swiler, A.A. Giunta, and T. Krishnamurthy. Proceedings of the Society of Experimental Mechanics IMAC Conference, January 2006. SAND 2005-7760C.
- *Gaussian Process in Response Surface Modeling.* L.P. Swiler. Proceedings of the Society of Experimental Mechanics IMAC Conference, January 2006. SAND 2005-6892C.
- *Response Surface (Meta-Model) Methods and Applications*. B. M. Rutherford, L.P. Swiler, T. L. Paez, and A. Urbina. Proceedings of the Society of Experimental Mechanics IMAC Conference, January 2006.
- *Evaluation of Sampling Methods in Constructing Response Surface Approximations* 1st AIAA Non-Deterministic Approaches Conference (part of 47th AIAA/ASME/ASCE/AHS/ASC SDM conf) SAND2005-5283C.
- DAKOTA/LHS Verification for ASC Level 2 Milestone Review Jan. 2006.

- **PATENT AWARD: Patent 7013395, Method and Tool for Network Vulnerability Analysis**