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9211, Optimization and Uncertainty Estimation, Manager Scott Mitchell

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Highlights this performance year

PRIDE LDRD

- Parameter Study Analysis/Surrogate Modeling
- Bayesian approach in two major areas: regression analysis and multi-fidelity GP analysis
- Robust Design

- **ASC V&V Program**
  - Bayesian approach to calibration
- **DAKOTA Capabilities**
  - Quasi-Monte Carlo Sampling Methods, CVT
  - Variance-Based Decomposition (sensitivity analysis)
  - Continued support for JEGA and LHS
  - Starting Dempster-Shafer Theory of Evidence

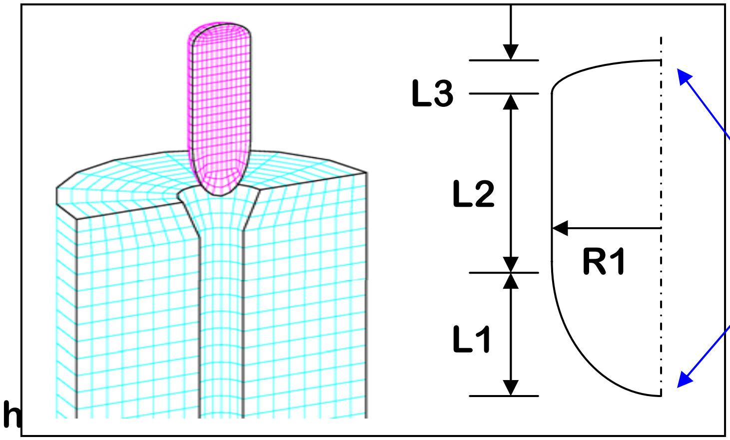
PRIDE LDRD

PRIDE: Penetrator Reliability Investigation and Design Exploration

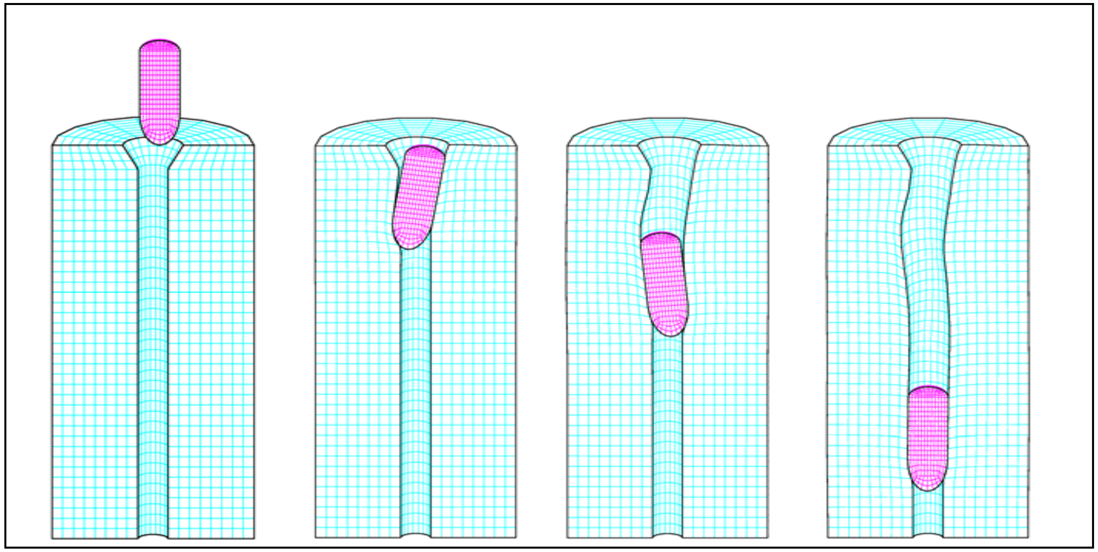
- How can we efficiently optimize an earth penetrator weapon design given the uncertainties in delivery conditions, target geology and model parameters?
- Develop and implement new optimization under uncertainty (OUU) methods using surrogate models in a multi-fidelity hierarchy with Bayesian statistics to enable credible and reliable penetrator design modeling.
- This year, my focus was on two areas:
  - **Robust design in the spirit of Taguchi**
  - **Bayesian approaches**

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

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Robust Design

- Renewed interest in the statistical community during the mid-1990s: Myers and Kim, Montgomery, Shoemaker and Wu, Welch et al., Box and Jones.
- Revision of Taguchi's work. Taguchi had the idea that products lack high quality because of inconsistency in performance, often the result of uncontrollable factors. *Choose a design that is robust to environmental or process variations.*
- Idea is that one has noise variables (uncontrollable) and control (design) variables. Instead of have separate design of experiments, treat both with a combined array.
- Generate a response model, treating control and noise variables as fixed effects (question: can we do this? In computer experiments, yes)
- Look at the slopes of the response model in the direction of the noise variables → want the slopes to be near zero for robustness

Robust Design

- x are the control variables, z are the noise variables, y is the response, $\varepsilon \sim N(0,\sigma^2)$, Δ are the dispersion effects created by the noise variables

$$y = x'\beta + z'\gamma + x'\Delta z + \varepsilon$$

- $E(z) = 0$
- $Var(z) = V$

$$\hat{u}_z(y(x)) = x'\hat{\beta}$$

$$\hat{\sigma}_z^2(y(x)) = (\hat{\gamma} + \hat{\Delta}'x)'V(\hat{\gamma} + \hat{\Delta}'x) + \hat{\sigma}_\varepsilon^2$$

$$(\hat{\gamma} + \hat{\Delta}'x) = {\partial \hat{y}}/{\partial z} = l(x)$$

•Can use this to obtain confidence intervals on the location (in x) of minimum process variance

Robust Design: Displacement Response

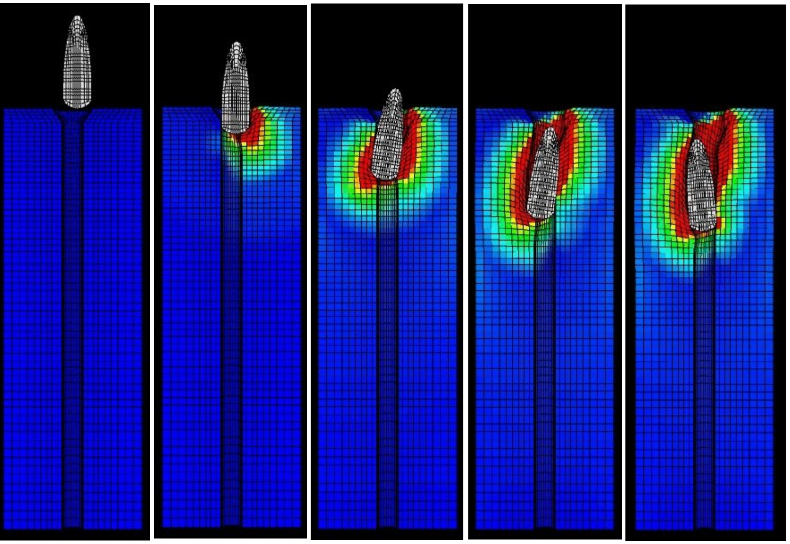
- DISPLACEMENT: **Will a long or short penetrator be better able to compensate for angle of attack, cavity radius, etc. to improve depth of penetration?**

- In the low fidelity model, we found no strongly significant interaction terms between the noise and the control variables in the regression model of the displacement response.

- Important point: If there are no interaction terms between the noise and control variables, the uncertainty in the noise variables will have a constant effect on the displacement and there is no opportunity for reducing the process variance by a choice of the design variables.

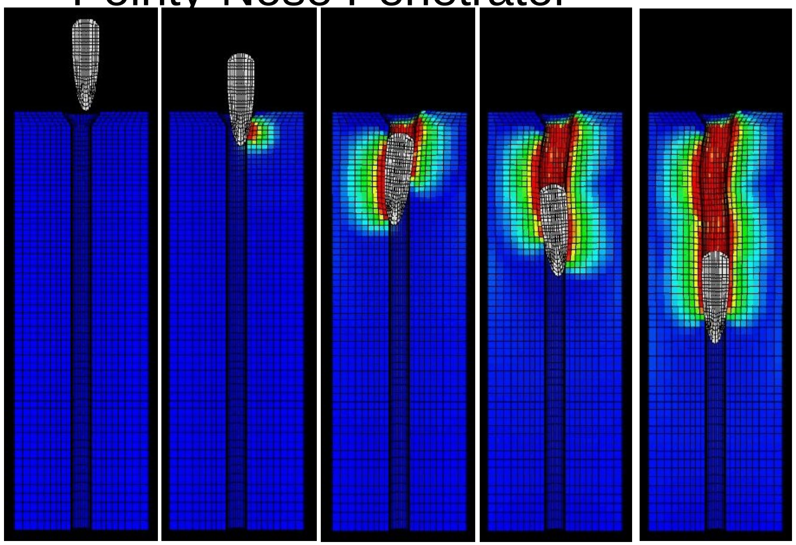
Robust Design: Acceleration Response

Blunt-Nose Penetrator



•Short penetrator nose tip with long penetrator aft end results in poor ground penetration.

Pointy-Nose Penetrator



•Long penetrator nose tip with short penetrator aft end results in good ground penetration.

•**Unexpected finding: observed large aft axial accelerations** – not shown.

Important point: Acceleration is very strongly influenced by the noise variables, especially OS and AoA. There are some significant interaction terms, namely L1*OS. We can design to reduce the acceleration variance, but we will not be able to "design out" the effects of the uncertainty.

Key: Red means high strain in earth material (largest ground deformation)

Bayesian Multi-Fidelity Approach

Assumptions

- Different levels of the same code are correlated in some way.
- The codes have a degree of smoothness in the sense that output values for similar inputs are reasonably close.
- Prior beliefs each level of code can be modeled using a Gaussian process.

Two papers

- Kennedy, M. C. and A. O'Hagan. "Predicting the output from a complex computer code when fast approximations are available." *Biometrika*, 87, pp. 1-13. 2000.
- Deng Huang, Theodore T. Allen, William I. Notz, and R. Allen Miller, "Sequential Kriging Optimization Using Multiple Fidelity Evaluations", submitted to *Structural and Multidisciplinary Optimization*.

Multi-Fidelity Bayesian Approach

For L levels of a system, suppose that, $L = 1, \ldots, m,$

$$f_L(\mathrm{x}) = f_{L-1}(\mathrm{x}) + \delta_L(\mathrm{x})$$

where $\delta_L(\mathrm{x})$ is independent of $f_1(\mathrm{x}), f_2(\mathrm{x}), \ldots, f_{L-1}(\mathrm{x})$.

- $\delta_L(\mathrm{x})$ models the "systematic error" of a lower-fidelity system, (L–1), as compared to the next higher-fidelity system, L.
- $f_{L-1}(\mathrm{x})$ and $\delta_L(\mathrm{x})$ are modeled as Gaussian processes
- A Gaussian process is a stochastic process such that two points are distributed as a multivariate normal, with a mean that is some type of basis function and a covariance structure
- $\delta_L(x) = b_L(x)^T \beta_L + Z_L(x) + \varepsilon_L$

$$\mathrm{cov}\left[\delta_{\mathrm{L}}(\mathbf{x}), \delta_{\mathrm{L}}(\mathbf{x}')\right] = \sigma^2_{Z,\mathrm{L}} \exp\left[\sum_{j=1}^{d} -\theta_{\mathrm{L},j}(x_j - x'_j)^2\right]$$

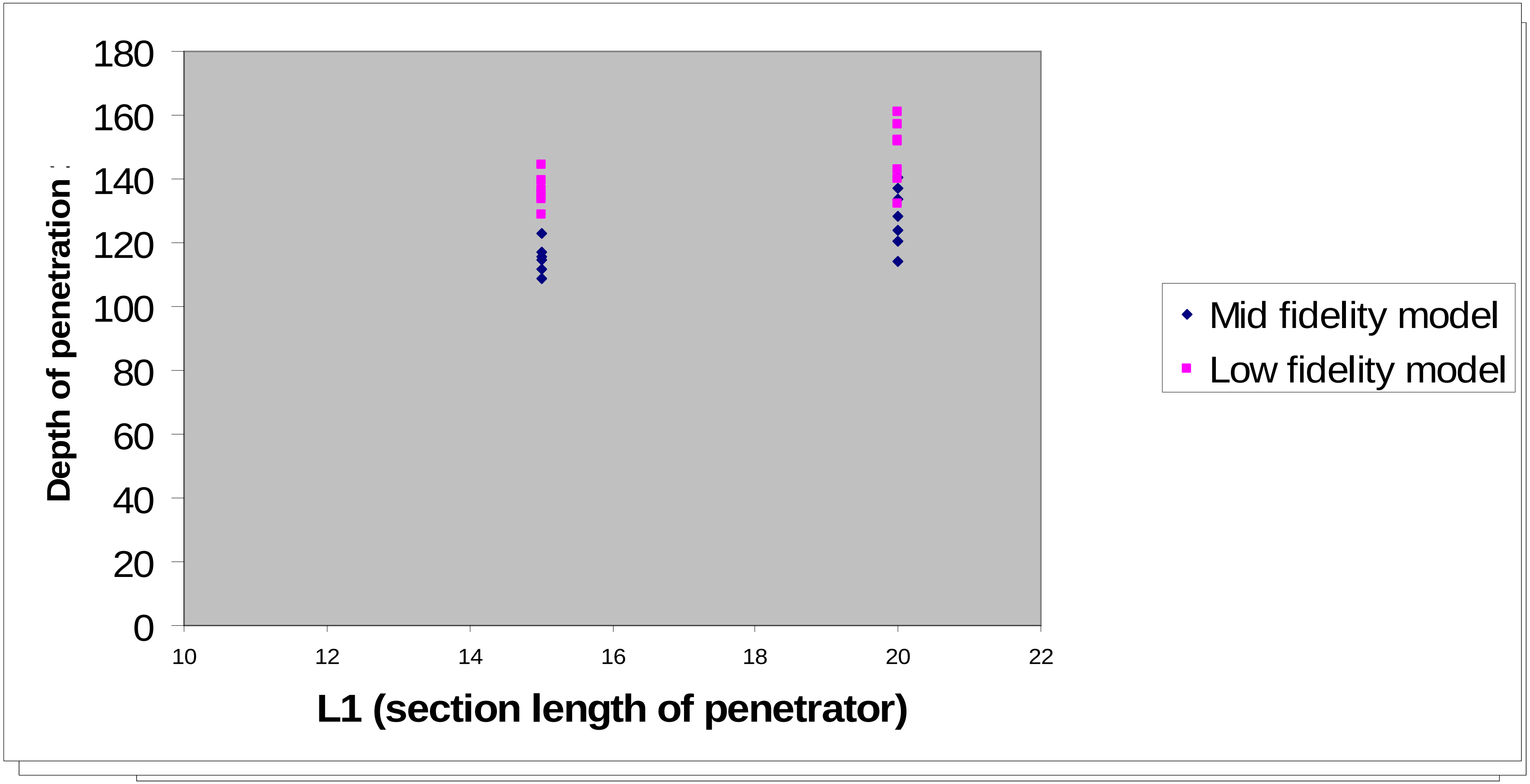
- $f_2(\mathrm{x}) = f_1(\mathrm{x}) + \delta_2(\mathrm{x})$

Bayesian Multi-Fidelity Approach

- I took the results of a 13 point orthogonal array penetrator study at Low-fidelity and the same 13 point OA study at Mid-fidelity. I used this data to construct the GP emulator for $f_1(x)$ and also to construct the GP emulator for $\delta_2(x)$, based on the difference in the low and mid level results.
- The emulators were constructed assuming a linear regression mean for the GP and maximum likelihood estimation of the hyperparameters governing the covariance matrix
- The emulators were then used to predict the value of the mid-level model at six new points: $\hat{f}_2(x) = \hat{f}_1(x) + \hat{\delta}_2(x)$
- Independently, I ran the mid-lc penx model at these six points to verify the results.

Design Variables			Uncertain Variables				
L1	L2	L3	OS	AoA	TS	IV	CR
17	7	13	0.50	0.010	2700	12500	5.0
25	10	10	0.75	0.013	2800	12500	4.6
15	10	15	0.90	0.020	2700	12000	4.8
20	5	15	0.20	0.005	2800	14000	4.7
15	10	15	0.20	0.005	2800	14000	4.8
20	5	15	0.90	0.02	2700	12000	4.7

Mid-fidelity estimation



Comments on the Bayesian Autoregressive Process

- Gaussian process models are good surface fitting emulators, especially when we are trying to capture local behavior about a delta term between simulations of varying fidelity
- This approach is more accurate than assuming a constant bias term between low and high fidelity models
- This approaches offers potential savings in trust region optimization, for example, where we can use a low fidelity surrogate plus a delta term to approximate a high fidelity model
- Important point: GPs capture uncertainty in the estimation process as well. We have shown only the point predictions at the new points of interest, but variance terms are also available.

Next Steps in the Bayesian Multi-fidelity Approach

- Incorporate a two-level fidelity approach in a trust region method, with automatic calculation of the variance parameters
- Use an expected improvement function with global optimization methods to generate adaptive samples
- The uncertainty estimation gives us a way to determine the points chosen next in optimization: For example, construct an expected improvement function which captures the tradeoff between
  - **improving the objective and reducing the variance,**
  - **the reduction in the posterior variance estimate when a surrogate of a given level is used,**
  - **the cost of the different levels.**
- One of my contributions has been to model the GP mean with a regression term, not as a constant. My experience has been that the difference between high and low fidelity models often has a significant linear trend. I also model the delta term mean in the calibration work with a regression model.

ASC V&V Program: Bayesian Calibration

- The Gaussian process approach for model calibration is similar to the high/low fidelity model presented above, only this time the delta term models the difference between experimental data and code runs:

  Experimental data = z_i = Code Output + $\delta(x_i)$ + e_i

- I have started using this formulation in V&V "challenge problems" being developed by Marty Pilch's group
- Purpose of these challenge problems are to present the reader with a "real world" V&V problem and ask him/her to take experimental data, model data, and evaluate the ability of the model to predict what the results are for a new set of inputs (extrapolate)
- Variety of uncertain variables, also measurement error and measurement bias, and model approximation error (due to incomplete physics)
- I have looked at the thermal challenge problem in detail: Heat conduction in a cylinder
- If extrapolation region is far from existing data, GP reverts to a constant variance process: not as useful

DAKOTA UQ Summary

- **We need to improve the UQ capabilities within DAKOTA to address user needs:**
  - Multi-fidelity approaches
  - Epistemic uncertainty representation
  - More sophisticated methods such as surrogate representations of UQ
  - Help users meet their ASC V&V Milestones

- **FY05 Areas of interest:**
  - Sensitivity Metrics
  - Bayesian Methods
  - 2nd-order Probability
  - Reliability Methods
  - Evidence Theory

Team members:

Laura Swiler, PI

Mike Eldred

- **Future Development Focus**
  - Incremental LHS
  - Importance Sampling
  - Bayesian Methods
  - Evidence Theory

New Sampling Capabilities

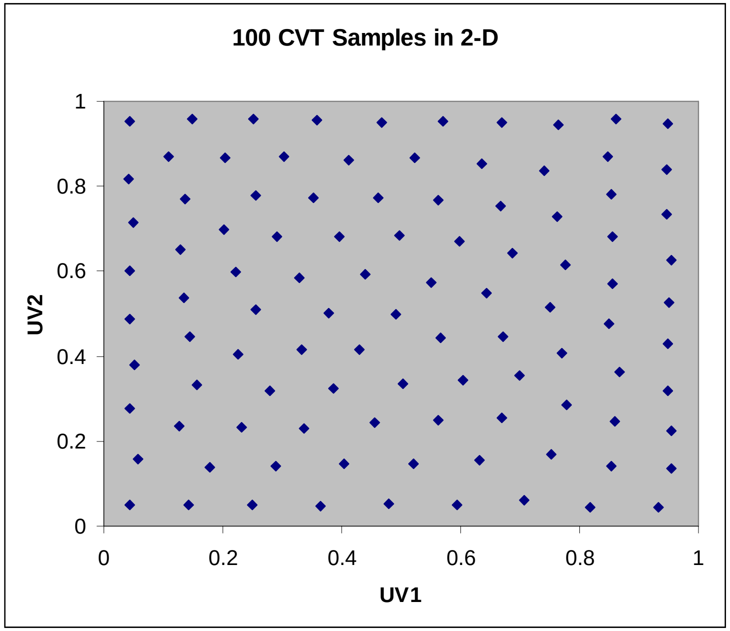
Motivations:

- Surrogates: Data fit, spanning ROM
- UQ

Types:

- **Pseudo Monte Carlo:** Latin Hypercube Sampling (LHS) is a stratified, structured sampling method that picks random samples from equal probability bins for all 1-D projections.
- **Quasi Monte Carlo:** deterministic sequences constructed to uniformly cover a unit hypercube with low discrepancy.
  E.g., Halton, Hammersley, Sobol
- **Centroidal Voronoi Tesselation (CVT):** generates nearly uniform spacing over arbitrarily shaped parameter spaces; originally developed for "meshless" mechanics methods.

New



Associated Tools:

- Volumetric quality, Latinization
- Correlations, Variance-based decomposition
  - Global Sensitivity Analysis: decompose output variance into sum of input variances, requires replicated samples

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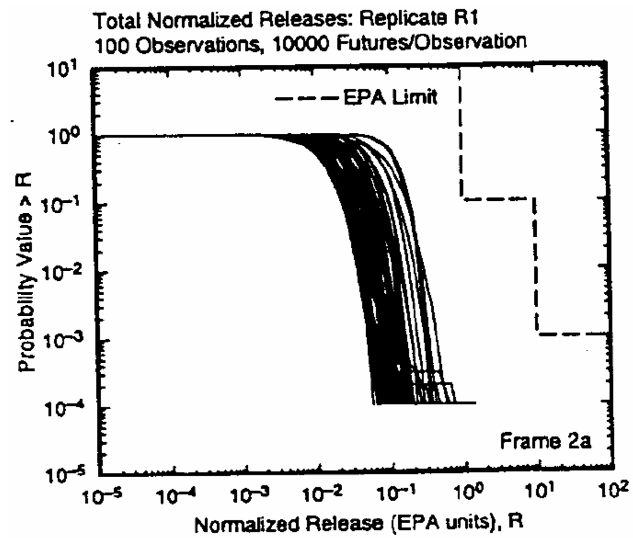
Epistemic UQ

Second-order probability

New

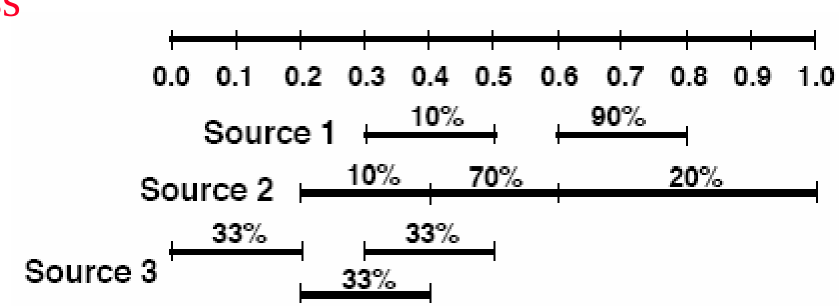
- Two levels: distributions/intervals on distribution parameters
- Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).

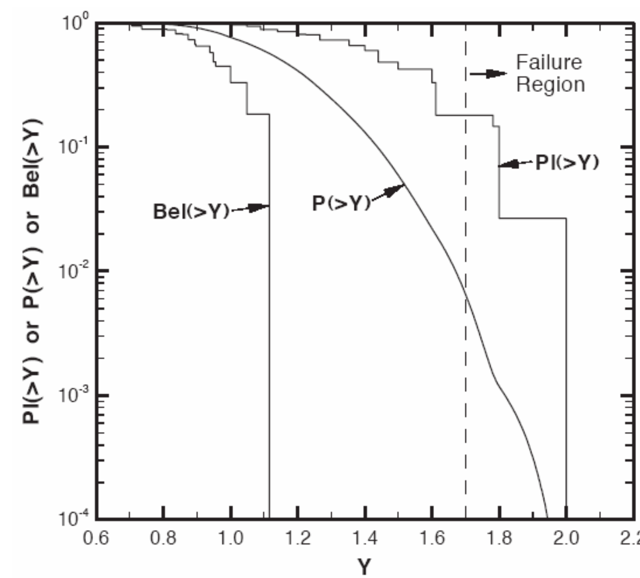


Dempster-Shafer theory of evidence

In progress

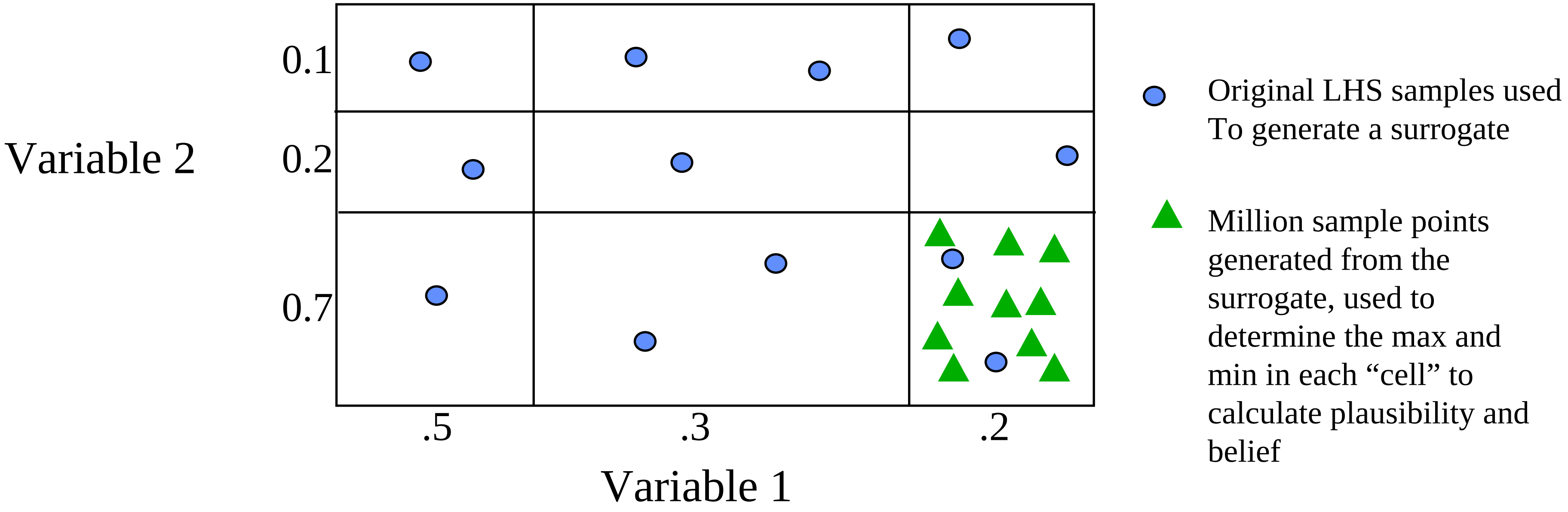
- Basic probability assignment (interval-based)
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals





Epistemic UQ

- Draws on the strengths of DAKOTA
  - **Easily parallelized**
  - **Requires surrogates**
  - **Requires sampling and/or optimization for calculation of plausibility and belief within each interval “cell”**



Service

- NSF Panel: Reviewed Engineering Research Center proposals for research centers focused on some aspect of critical infrastructures, risk, and reliability. (5-year, $17M NSF award)
- Taking on leadership roles in PRIDE LDRD, and ASC V&V community
  - **Attended two V&V conferences: Foundations ’04 and Tri-lab**
  - **Technical lead on PRIDE**
  - **Active participant in V&V working group**
- Developing collaboration with Sallie Keller-McNulty’s group at LANL (Bayesian Statistics)
  - **Meeting with David Higdon and Charlie Nakleh**
  - **Nozer Singpurwalla’s Bayesian class**
  - **Scott Ferson’s Imprecise probability course**
- Asked to participate in prognostics/military initiatives
  - **Keynote speech at the Prognostics and Health Management (PHM) Center of Excellence advisory board meeting in Dec. 04**
  - **Presentation on DAKOTA and surrogate modeling to the Navy’s Modeling and Simulation group (NAVSEA and ONR) in April**

Service

- Mentoring
  - **Barron Bichon (Mahadevan's student in Vanderbilt's Reliability program)**
    - **Summer 05: RBDO**
  - **Kay Vugrin (new staff member, Math).**
    - **Spring/Summer 05: Parameter estimation, covariance of estimators.**
  - **Raisa Slepoy (UNM, Statistics).**
    - **Summer 04: Sensitivity analysis for JSF SEM model**
    - **Summer 05: Sampling/response surface interactions**
  - **John Eddy(GAs/agents in design).**
    - **2004-05: Member of dissertation committee.**
  - **John McFarland (Mahadevan's student in Vanderbilt's Reliability program)**
    - **Summer 05: Bayesian Belief Networks in calibration, prediction**
  - **Other Interactions**
    - **Gio Kao – C.S. Urbana-Champaign; Pareto optimization**
    - **Dan Briand – Statistics, UNM. Prognostics; non-uniform time series analysis**

- Reviewed 7 Papers for AIAA, IEEE, the European Journal of OR, etc.
- Interviewed 8 candidates for 9211, 9133, 9143, and 15243

Publications

- *Penetrator Reliability Investigation and Design Exploration: Low Fidelity Penetrator Design Studies.* L. P. Swiler, T.G. Trucano, R. Heaphy, M. Chiesa, R. Settgast, P. D. Hough, and M. Martinez-Canales. SAND 2005-XXXX
- *Bayesian Approaches to Engineering Design Problems.* L. P. Swiler. SAND 2005-3294.
- *Error Estimation Approaches for Progressive Response Surfaces.* V.J. Romero, R. Slepoy, L.P. Swiler, and A.A. Giunta. Proceedings of the AIAA/ASME/ASCE/AHS/ASC 35th Structures, Structural Dynamics, and Materials Conference, April 2005. SAND2005-2047C.
- *Calibration, Validation, and Sensitivity Analysis: What's What."* T.G. Trucano, L.P. Swiler, T. Igusa, W.L. Oberkampf, M. Pilch. Accepted for publication in "Reliability Engineering and System Safety" journal. SAND 2004-6083J.
- *Calibration under Uncertainty.* L.P. Swiler and T.G. Trucano. SAND 2005-1498 .
- *Bayesian Methods in CS&E Models*. SAND 2005-0463 C. Presented at SIAM Computational Science and Engineering (CS&E) conference, Orlando FL, 2005.
- *Treatment of Model Uncertainty in Model Calibration.* L.P. Swiler and T.G. Trucano, in ASCE 9th Joint Speciality Conference on Probabilistic Mechanics and Structural Reliability Proceedings, PMC 2004. SAND2004-2317 C
- *Progressive Response Surfaces.* V.J. Romero, T. Krishnamurthy, and L.P. Swiler, in ASCE 9th Joint Speciality Conference on Probabilistic Mechanics and Structural Reliability Proceedings, PMC 2004.
- *A User's Guide to Sandia's Latin Hypercube Sampling Software: LHS UNIX Library/Standalone Version.* L.P. Swiler and G.D. Wyss. SAND 2004-2439.