# Uncertainty Quantification Algorithms and Software Enabling V&V

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*Optimization and Uncertainty Quantification*

**July 22, 2008**

**Verification & Validation for Nuclear Systems Analysis Workshop**
***Idaho Falls, ID***

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.

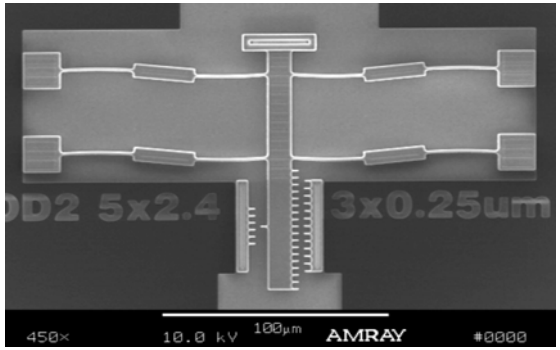
# Outline

***Advanced algorithms enable robust, efficient uncertainty quantification for validating models with experimental data and making credible predictions.***

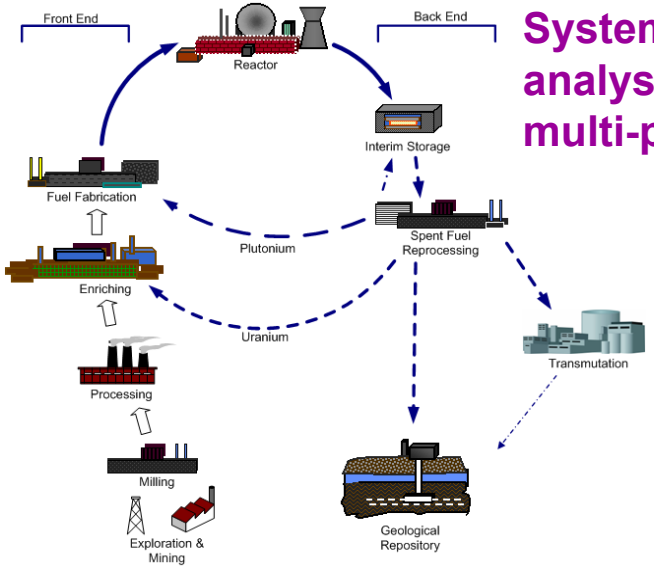
- **Uncertainty quantification for credible simulation**
- **UQ algorithms research in DAKOTA**
  - **Aleatory UQ methods: beyond Monte Carlo**
  - **Challenges in epistemic UQ methods**
- **Sandia's QASPR program: computational model-based system qualification**

*Slide credits: Mike Eldred, Laura Swiler, Barron Bichon, Joe Castro, Genetha Gray, Bill Oberkampf, Matt Kerschen, others*

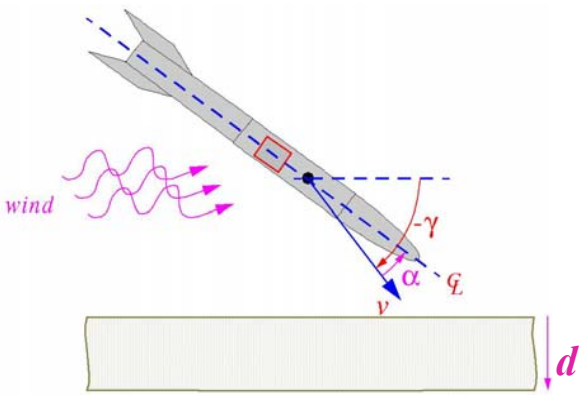
# Insight from Computational Simulation




Micro-electro-mechanical systems (MEMS): quasi-static nonlinear elasticity, process modeling

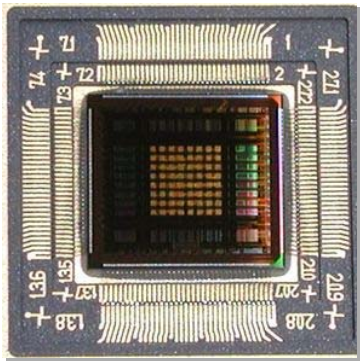


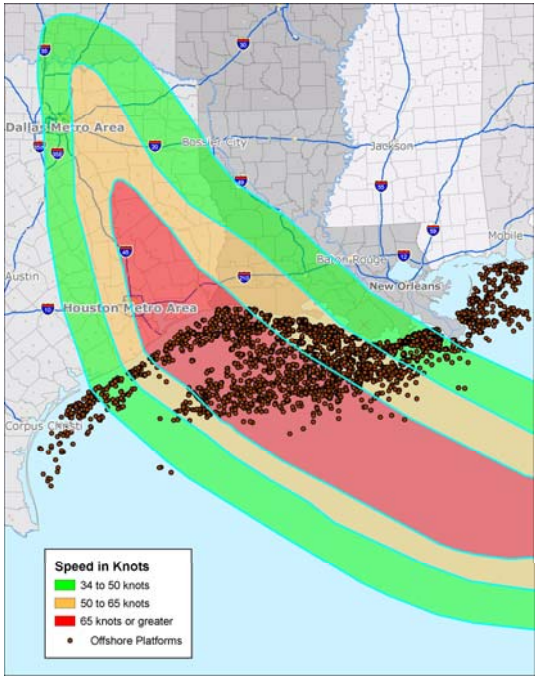

Systems of systems analysis: multi-scale, multi-phenomenon




Earth penetrator: nonlinear PDEs with contact, transient analysis, material modeling

Electrical circuits: networks, PDEs, differential algebraic equations (DAEs), E&M






Hurricane Katrina: weather, logistics, economics, human behavior

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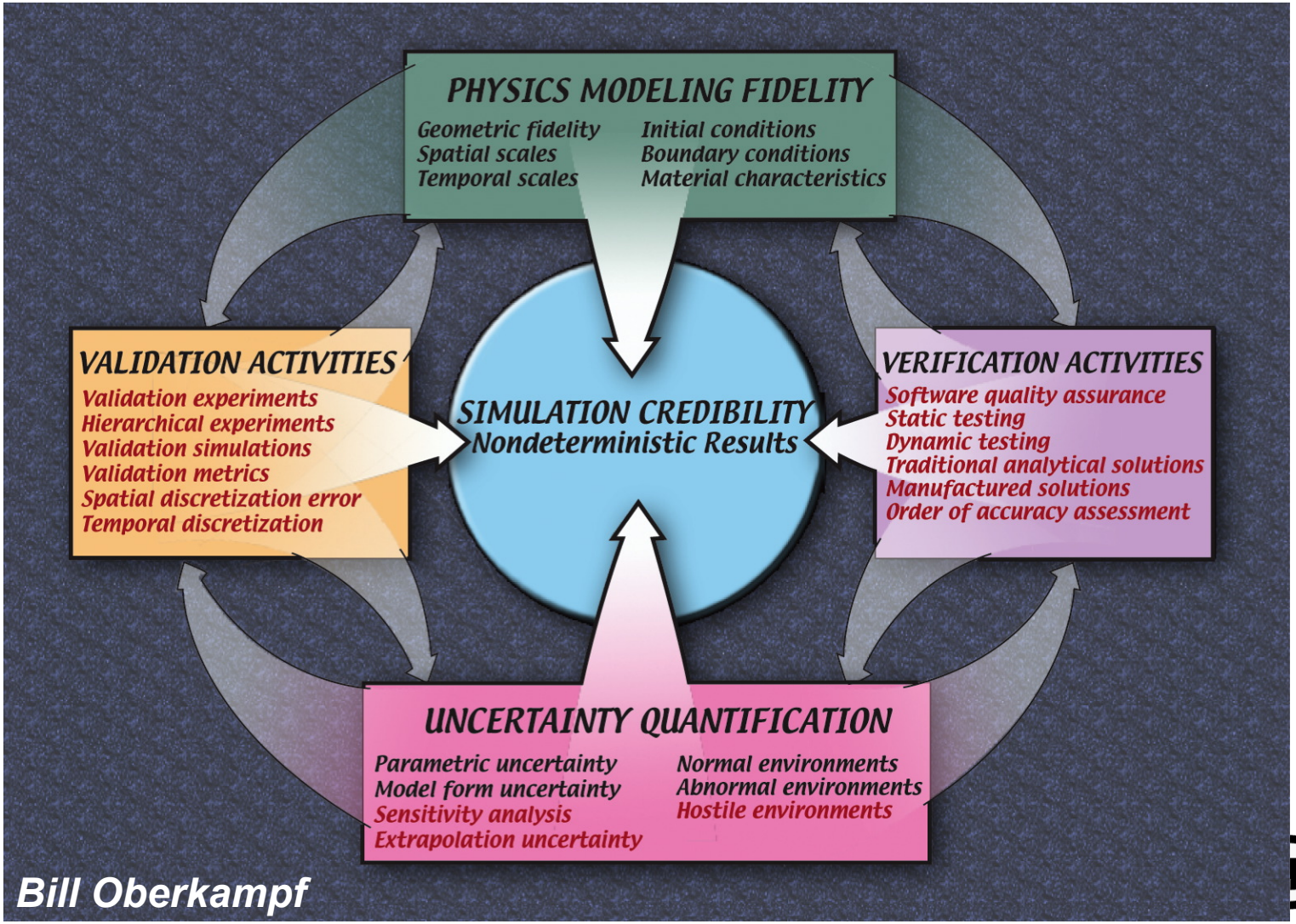
# UQ in Credible Simulation

**Ultimate purpose (arguably): insight, prediction, and risk-informed decision-making → *need credibility for intended application***




*Bill Oberkampf*

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# Uncertainties to Quantify

***A partial list of uncertainties affecting computational model results***

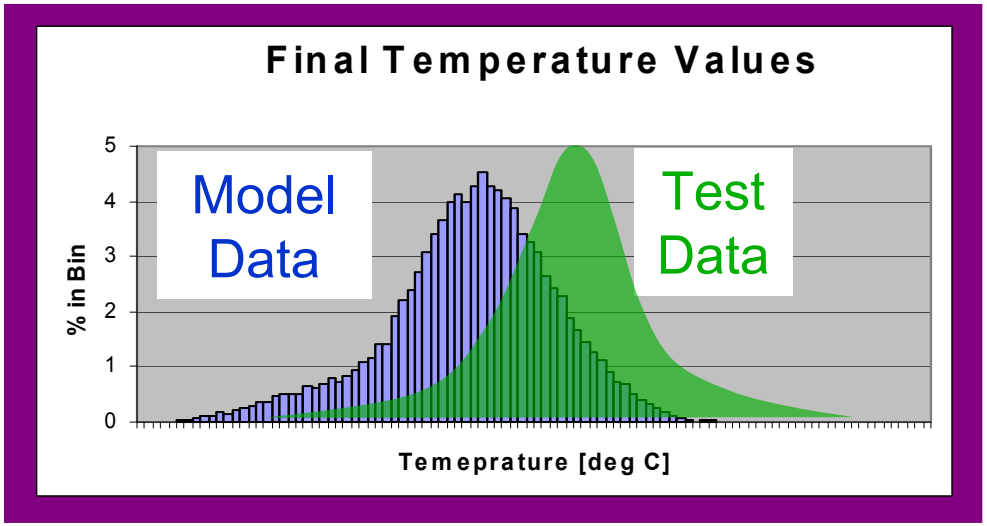
- **typical parametric uncertainty, incl. random fields/processes**
  - **physics/science parameters**
    ***(e.g., cross sections, reaction rates; seismic spectra)***
  - **statistical variation, inherent randomness**
  - **operating environment, interference**
    ***(e.g., debris, corrosion, oxidation, and erosion)***
  - **initial, boundary conditions; forcing**
  - **geometry / structure / connectivity *(e.g., fuel rod packing)***
  - **material properties**
  - **manufacturing quality**
- **model form / accuracy *(e.g., equation of state)***
- **program: requirements, technical readiness levels**
  ***(also economics, regulations, schedules)***
- **human reliability, subjective judgment, linguistic imprecision**

- **numerical accuracy: mesh, solver, approximation error**
- **experimental error: measurement error, bias**

# Uncertainty Quantification

- **A single optimal design or nominal performance prediction is often insufficient for**
  - **decision making / trade-off assessment**
  - **quantification of margins and uncertainties (QMU):** ***How close are my uncertainty-aware code predictions to required performance expectations or limits?***
  - **validation with experimental data ensembles**

- ***Need to make risk-informed decisions, based on an assessment of uncertainty***

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# Categories of Uncertainty

***Often useful algorithmic distinctions, but not always a clear division***

- **Aleatory** ***(think probability density function)***
  - **Inherent variability (e.g., in a population)**
  - **Irreducible uncertainty – can't reduce it by further knowledge**

- **Epistemic** ***(think bounded intervals)***
  - **Subjective uncertainty**
  - **Related to what we don't know**
  - **Reducible: If you had more data or more information, you could make your uncertainty estimation more precise**

- **In practice, people try to transform or translate uncertainties to the aleatory type and perform sampling and/or parametric analysis**

# Uncertainty Quantification

***Forward propagation: quantify the effect that uncertain (nondeterministic) input variables have on model output***

**Input Variables *u***
**(physics parameters, geometry, initial and boundary conditions)**

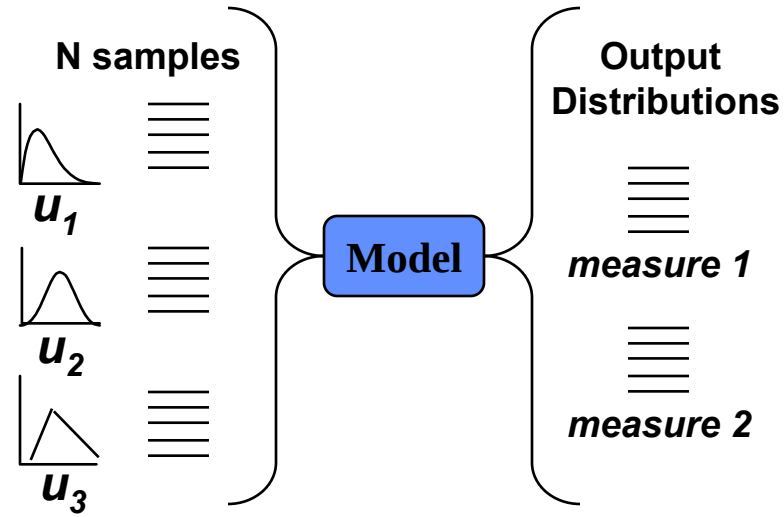
→ **Computational Model** →

**Variable Performance Measures *f(u)***

*(possibly given distributions)*

## Potential Goals:

- **based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)**
- **identify parameter correlations/local sensitivities, robust optima**
- **identify inputs whose variances contribute most to output variance (global sensitivity analysis)**
- **quantify uncertainty when using calibrated model to *predict***




***Typical method: Monte Carlo Sampling***

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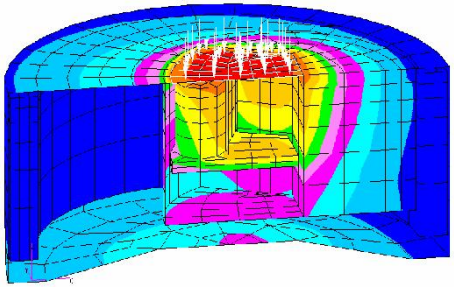
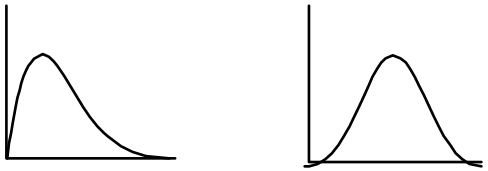
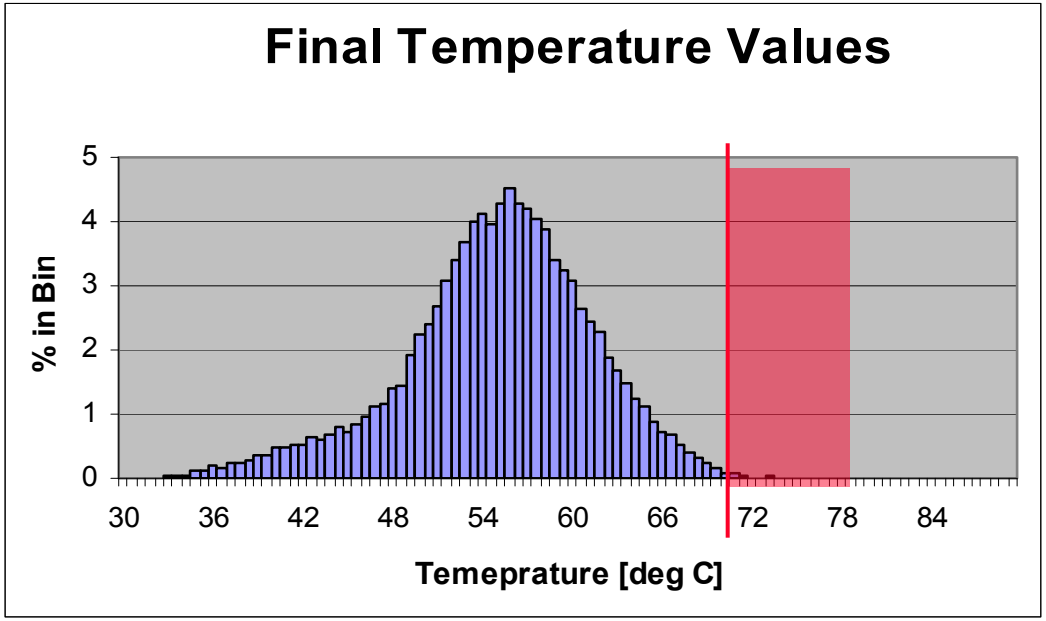
# Uncertainty Quantification Example

- **Device subject to heating** (experiment or computational simulation)
- Uncertainty in composition/ environment (thermal conductivity, density, boundary), parameterized by $u_1, \ldots, u_N$
- Response temperature $f(u)=T(u_1, \ldots, u_N)$ calculated by heat transfer code








***Given distributions of $u_1,\ldots,u_N$, UQ methods calculate statistical info on outputs:***

- Probability distribution of temperatures
- Correlations (trends) and sensitivity of temperature
- Mean($T$), StdDev($T$), Probability($T \geq T_{critical}$)

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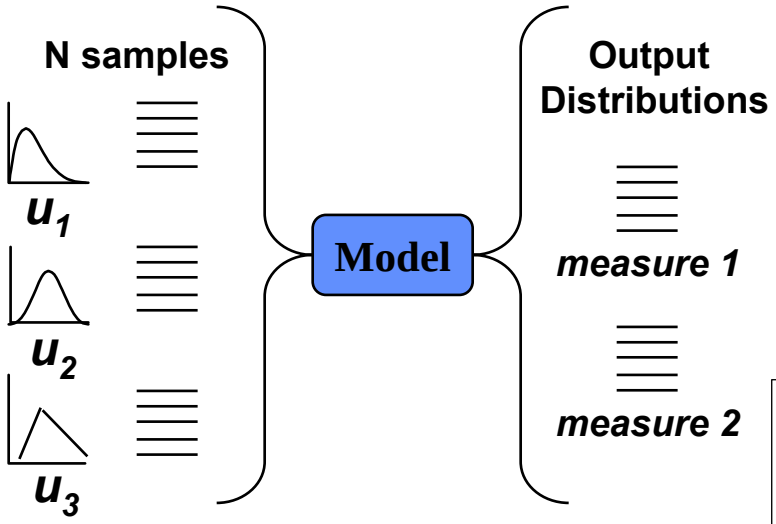
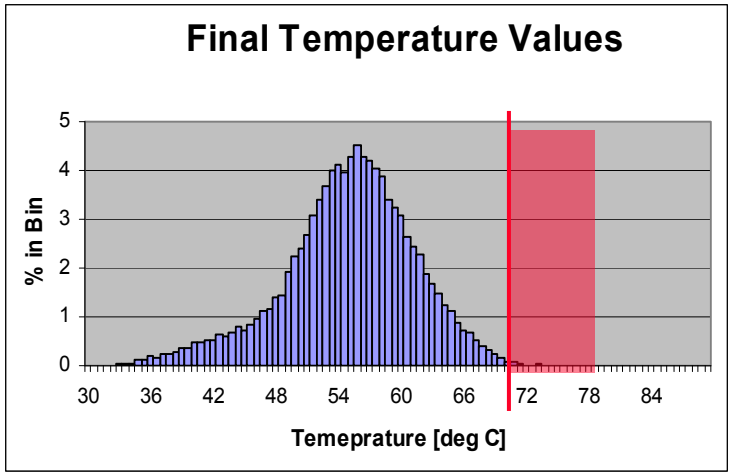
# UQ: Sampling Methods

***Given distributions of $u_1,\ldots,u_N$, UQ methods…***




***…calculate statistical info on outputs $T(u_1,\ldots,u_N)$***




- **Monte Carlo sampling**
- **Quasi-Monte Carlo**
- **Centroidal Voroni Tessalation (CVT)**
- **Latin Hypercube sampling**

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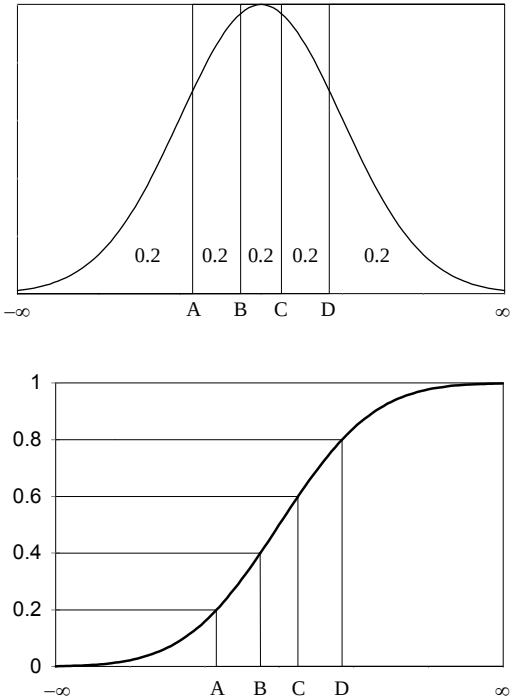
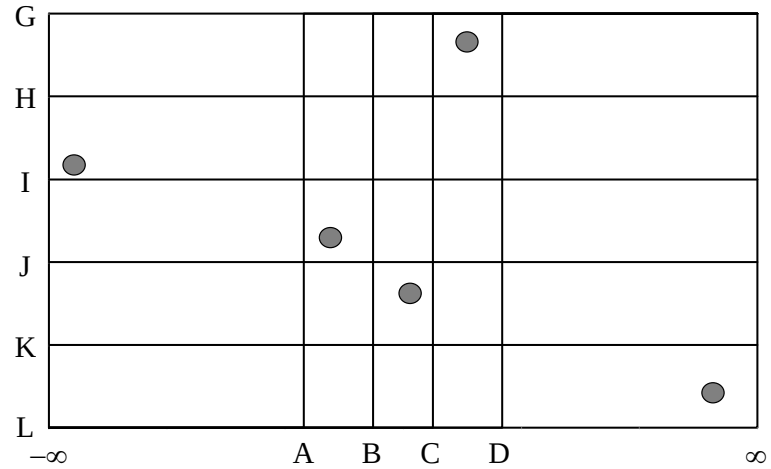
# Latin Hypercube Sampling (LHS)

- Specialized Monte Carlo (MC) sampling technique: workhorse method in DAKOTA / at Sandia
- *Stratified random sampling among equal probability bins* for all 1-D projections of an n-dimensional set of samples.
- McKay and Conover (early), restricted pairing by Iman




Intervals Used with a LHS of Size n = 5 in Terms of the pdf and CDF for a Normal Random Variable




A Two-Dimensional Representation of One Possible LHS of size 5 Utilizing X1 (normal) and X2 (uniform)

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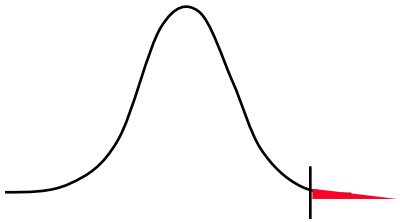
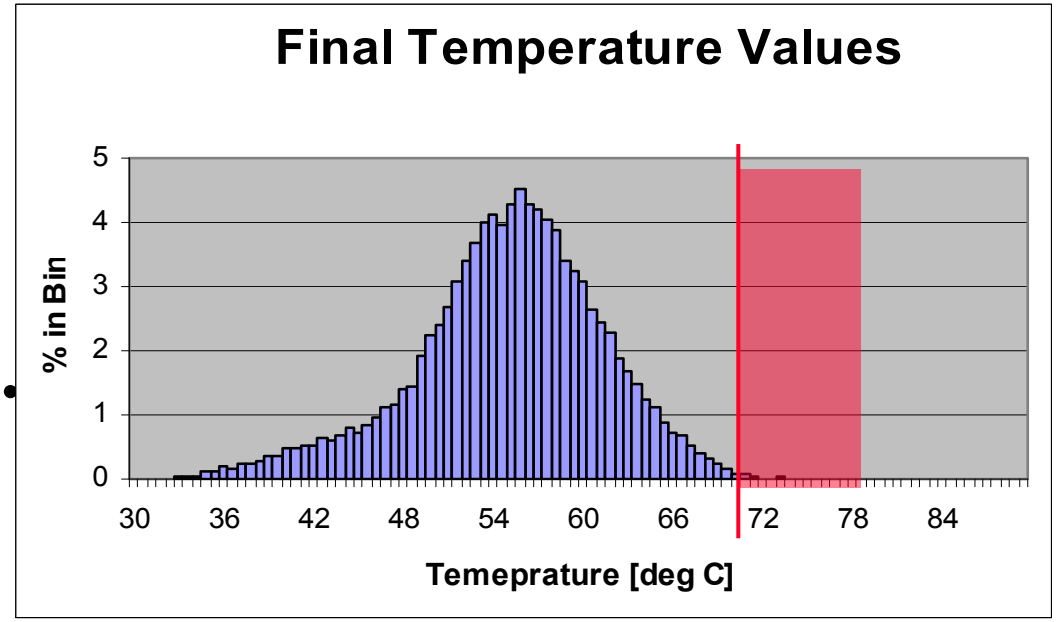
# Calculating Probability of Failure

- ***Given uncertainty in materials, geometry, and environment, determine likelihood of failure Probability($T \geq T_{critical}$)***






- **Could perform 10,000 Monte Carlo samples and count how many exceed the threshold…**
- **Or directly determine input variables which give rise to failure behaviors by solving an optimization problem.**

***By combining optimization, uncertainty analysis methods, and surrogate (meta-) modeling in a single framework, DAKOTA enables more efficient UQ.***

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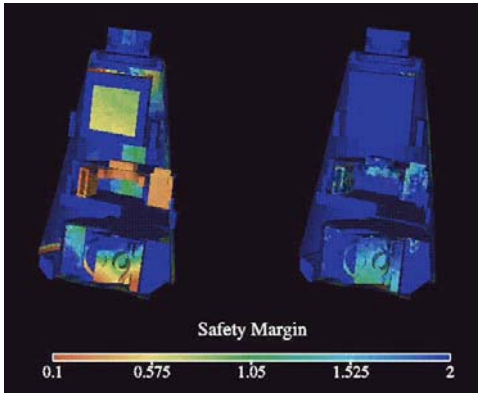
# DAKOTA Motivation

**Goal: perform iterative analysis on (potentially massively parallel) simulations to answer fundamental engineering questions:**

- **What is the best performing design?**
- **How safe/reliable/robust is it?**
- **How much confidence do I have in my answer?**




**Nominal** **Optimized**

**DAKOTA**
**optimization, sensitivity analysis, parameter estimation, uncertainty quantification**

**parameters**
(design, UC, state)

**response metrics**

**Computational Model (simulation)**
- **Black box:** any code: mechanics, circuits, high energy physics, biology, chemistry
- **Semi-intrusive:** Matlab, ModelCenter, Python SIERRA multi-physics, SALINAS, Xyce

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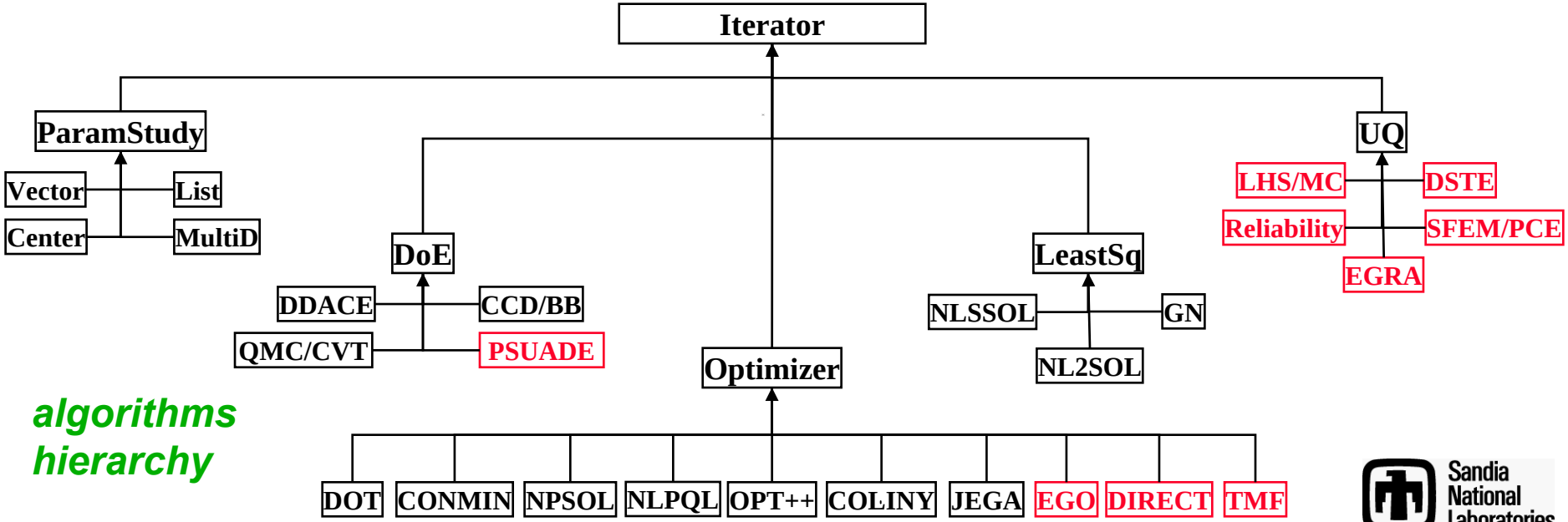
# DAKOTA C++/OO Framework Goals

- **Unified software infrastructure:** reuse tools and common interfaces; *integrate commercial, open-source, and research algorithms*
- **Enable algorithm R&D**, e.g., for non-smooth/discontinuous/multimodal responses, probabilistic analysis and design, mixed variables, unreliable gradients, costly simulation failures
- **Facilitate scalable parallelism:** ASCI-scale applications and architectures; *4 nested levels of parallelism possible*
- **Impact:** tool for DOE labs and external partners; broad application deployment; *free via GNU GPL* (>3000 download registrations)




***algorithms hierarchy***

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# Flexibility with Models & Strategies

***DAKOTA models map inputs to response metrics of interest:***

**variables/parameters**

- **design: continuous, discrete**
- **uncertain: (log)normal, (log)uniform, interval, triangular, histogram, beta/gamma, EV I, II, III**
- **state: continuous, discrete**

→

**user application**
(simulation)
system, fork, direct, grid

**optional approximation** (surrogate)

- **global (polynomial 1/2/3, neural net, kriging, MARS, RBF)**
- **local (Taylor); multipoint (TANA/3)**
- **hierarchical, multi-fidelity**

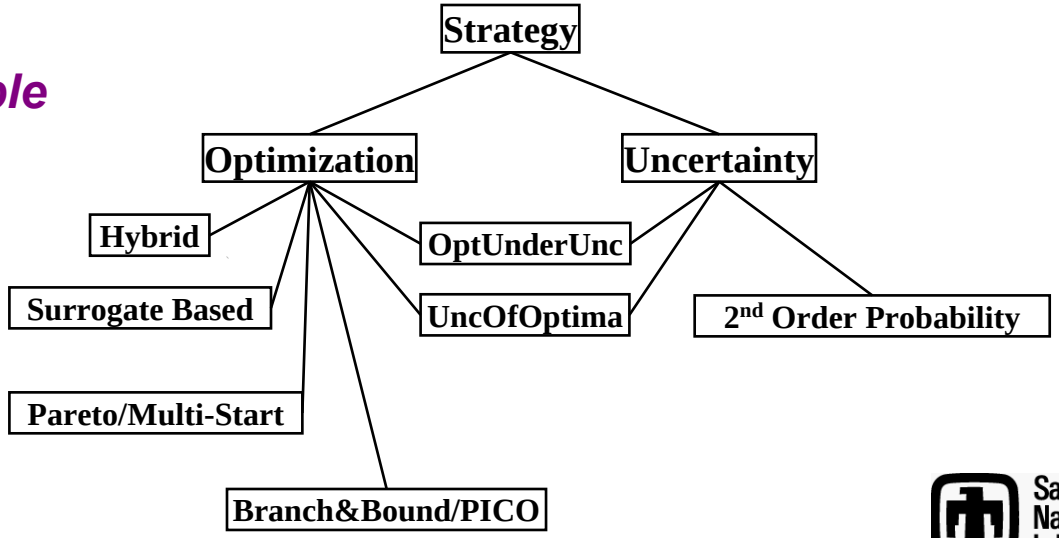
→

**responses**

- **functions: objectives, constraints, LSQ residuals, generic**
- **gradients: numerical, analytic**
- **Hessians: numerical, analytic, quasi**

***DAKOTA strategies enable flexible combination of multiple models and algorithms.***

- ***nested***
- ***layered***
- ***cascaded***
- ***concurrent***
- ***adaptive / interactive***

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# Alternatives to Sampling

***LHS sampling is robust, trusted, ubiquitous, but advanced methods may offer advantages:***

- **for a modest number of random variables, polynomial chaos expansions may converge considerably faster to statistics of interest**
- **if principal concern is with failure modes (tail probabilities), consider global reliability methods**

# Generalized Polynomial Chaos Expansions

***Approximate response stochasticity with Galerkin projection using multivariate orthogonal polynomial basis functions defined over standard random variables***

e.g. $R = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi})$ using

$$\begin{array}{lclcl}
\Psi_0(\boldsymbol{\xi}) & = & \psi_0(\xi_1)\ \psi_0(\xi_2) & = & 1 \\
\Psi_1(\boldsymbol{\xi}) & = & \psi_1(\xi_1)\ \psi_0(\xi_2) & = & \xi_1 \\
\Psi_2(\boldsymbol{\xi}) & = & \psi_0(\xi_1)\ \psi_1(\xi_2) & = & \xi_2 \\
\Psi_3(\boldsymbol{\xi}) & = & \psi_2(\xi_1)\ \psi_0(\xi_2) & = & \xi_1^2 - 1 \\
\Psi_4(\boldsymbol{\xi}) & = & \psi_1(\xi_1)\ \psi_1(\xi_2) & = & \xi_1 \xi_2 \\
\Psi_5(\boldsymbol{\xi}) & = & \psi_0(\xi_1)\ \psi_2(\xi_2) & = & \xi_2^2 - 1
\end{array}$$

***$R(\xi) \approx f(u)$***

- **Intrusive**
- **Nonintrusive: estimate response coefficients using sampling (expectation), quadrature/cubature (num integration), point collocation (regression)**

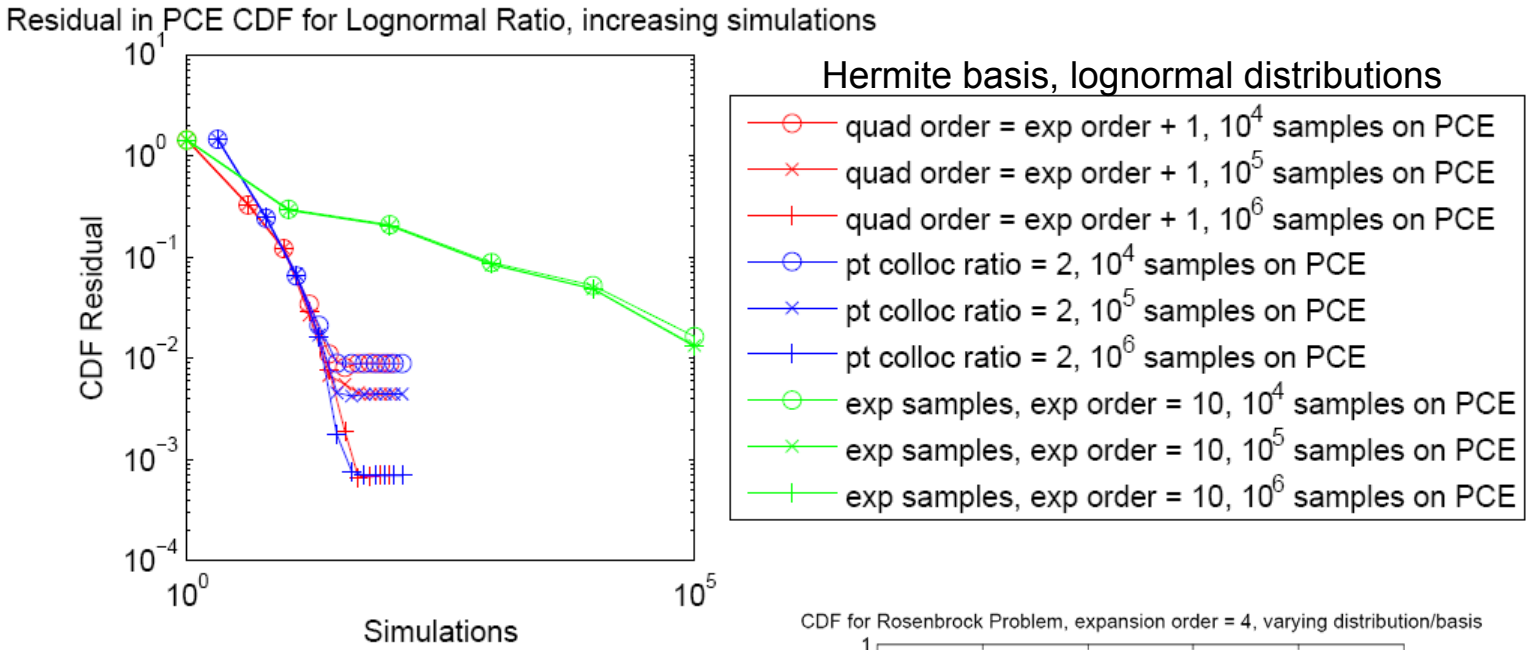
## Wiener-Askey Generalized PCE with adaptivity

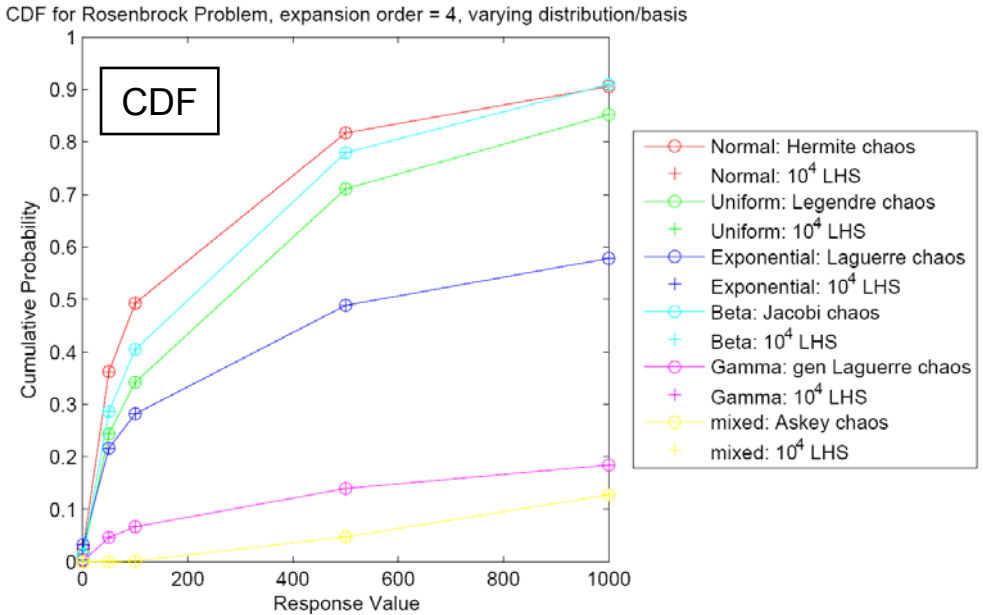
- Tailor basis: optimal basis selection leads to exponential convergence rates

| Distribution | Density function | Polynomial | Weight function | Support range |
|---|---|---|---|---|
| Normal | $\frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}}$ | Hermite $He_n(x)$ | $e^{\frac{-x^2}{2}}$ | $[-\infty, \infty]$ |
| Uniform | $\frac{1}{2}$ | Legendre $P_n(x)$ | $1$ | $[-1, 1]$ |
| Beta | $\frac{(1-x)^\alpha (1+x)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}$ | Jacobi $P_n^{(\alpha,\beta)}(x)$ | $(1-x)^\alpha (1+x)^\beta$ | $[-1, 1]$ |
| Exponential | $e^{-x}$ | Laguerre $L_n(x)$ | $e^{-x}$ | $[0, \infty]$ |
| Gamma | $\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$ | Generalized Laguerre $L_n^{(\alpha)}(x)$ | $x^\alpha e^{-x}$ | $[0, \infty]$ |

- Tailor expansion order/integration order: adaptivity based on PC error estimates
  - Isotropic/anisotropic tensor-product quadrature & sparse grid Smolyak cubature

# PCE: Fast Convergence



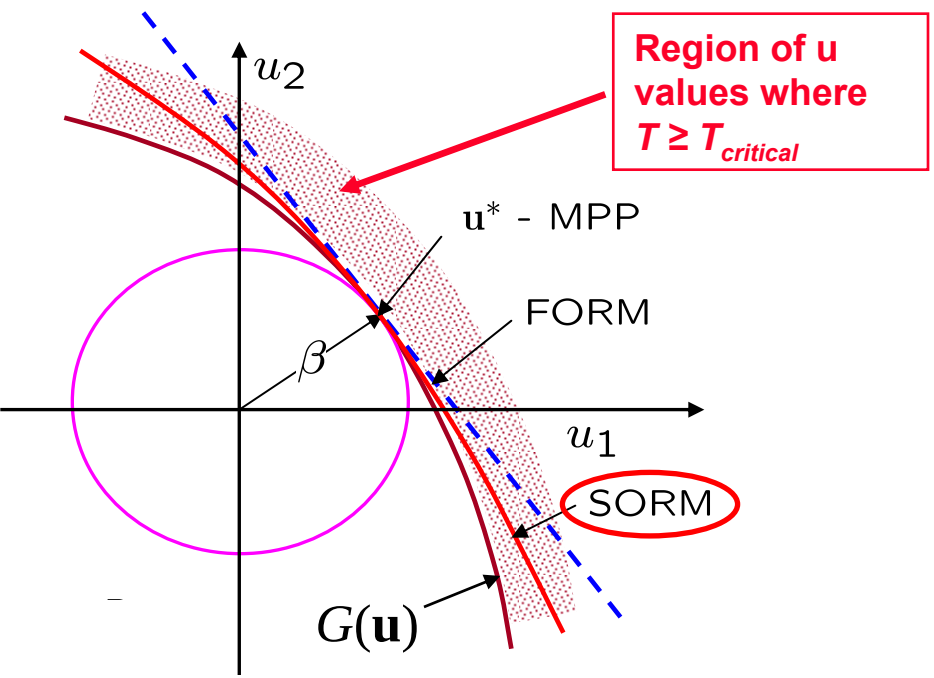



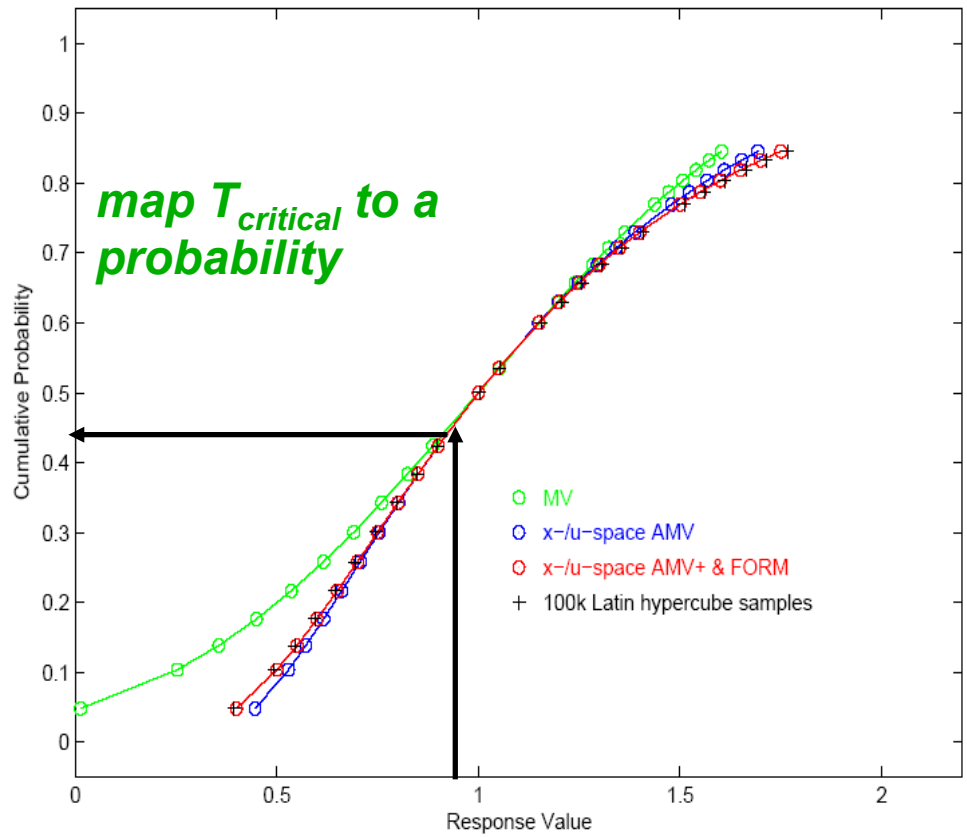
# Analytic Reliability: MPP Search

***Perform optimization*** **in uncertain variable space to determine Most Probable Point (of response or failure occurring) for *G(u) = T(u)*.**

## Reliability Index Approach (RIA)

$$\text{minimize} \quad \mathbf{u}^T\mathbf{u}$$
$$\text{subject to} \quad G(\mathbf{u}) = \bar{z}$$



# Reliability: Algorithmic Variations

***Many variations possible to improve efficiency, including in DAKOTA…***

- **<u>Limit state linearizations</u>: use a local surrogate for the limit state *G(u)* during optimization in u-space (or x-space):**

$$\text{u-space AMV:} \quad G(\mathbf{u}) = G(\mu_\mathbf{u}) + \nabla_u G(\mu_\mathbf{u})^T(\mathbf{u} - \mu_\mathbf{u})$$

$$\text{u-space AMV+:} \quad G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T(\mathbf{u} - \mathbf{u}^*)$$

$$\boxed{\text{u-space AMV}^2\text{+:} \quad G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T(\mathbf{u} - \mathbf{u}^*) + \tfrac{1}{2}(\mathbf{u} - \mathbf{u}^*)^T \nabla_u^2 G(\mathbf{u}^*)(\mathbf{u} - \mathbf{u}^*)}$$

*(could use analytic, finite difference, or quasi-Newton (BFGS, SR1) Hessians in approximation/optimization – results here mostly use SR1 quasi-Hessians.)*

- **<u>Integrations (in u-space to determine probabilities)</u>: may need higher order for nonlinear limit states**

$$1^{\text{st}}\text{-order:} \left\{ \begin{array}{lcl} p(g \le z) & = & \Phi(-\beta_{cdf}) \\ p(g > z) & = & \Phi(-\beta_{ccdf}) \end{array} \right. \qquad 2^{\text{nd}}\text{-order:} \left\{ p = \Phi(-\beta) \underbrace{\prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta\kappa_i}}}_{\text{curvature correction}} \right.$$

- **MPP search algorithm:** Sequential Quadratic Prog. (SQP) vs. Nonlinear Interior Point (NIP)
- **Warm starting (for linearizations, initial iterate for MPP searches):** speeds convergence when increments made in: approximation, statistics requested, design variables

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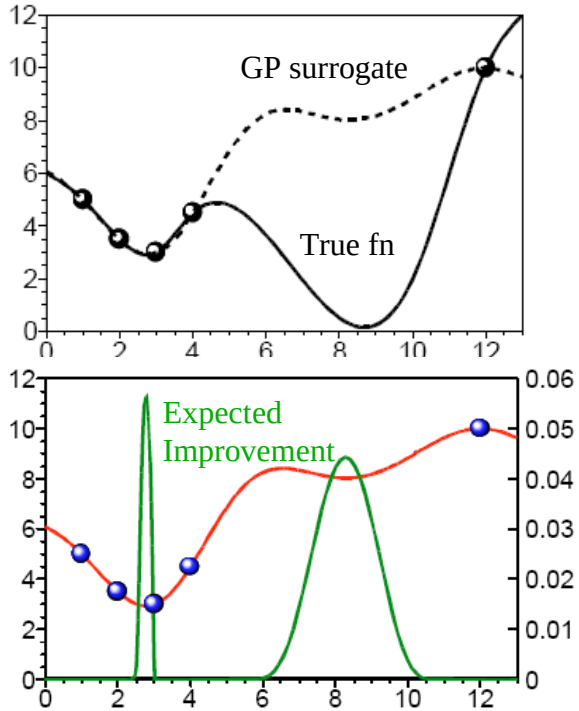
# Efficient Global Reliability Analysis

- **EGRA (B.J. Bichon) performs reliability analysis with EGO (Gaussian Process surrogate and NCSU DIRECT optimizer) coupled with Multimodal adaptive importance sampling for probability calculation.**

- **Created to address nonlinear and/or multi-modal limit states in MPP searches.**




From Jones, Schonlau, Welch, 1998

# Efficient Global Reliability Analysis

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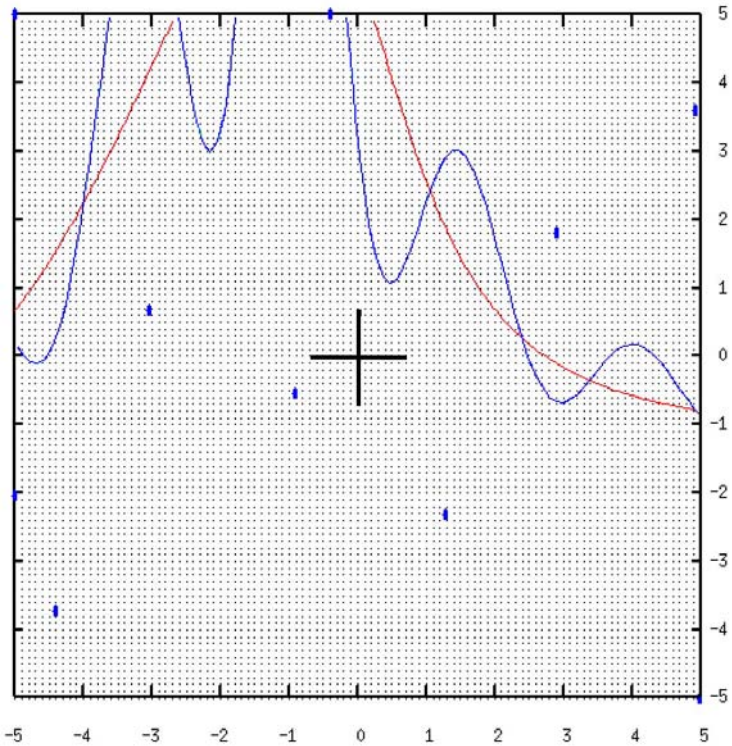
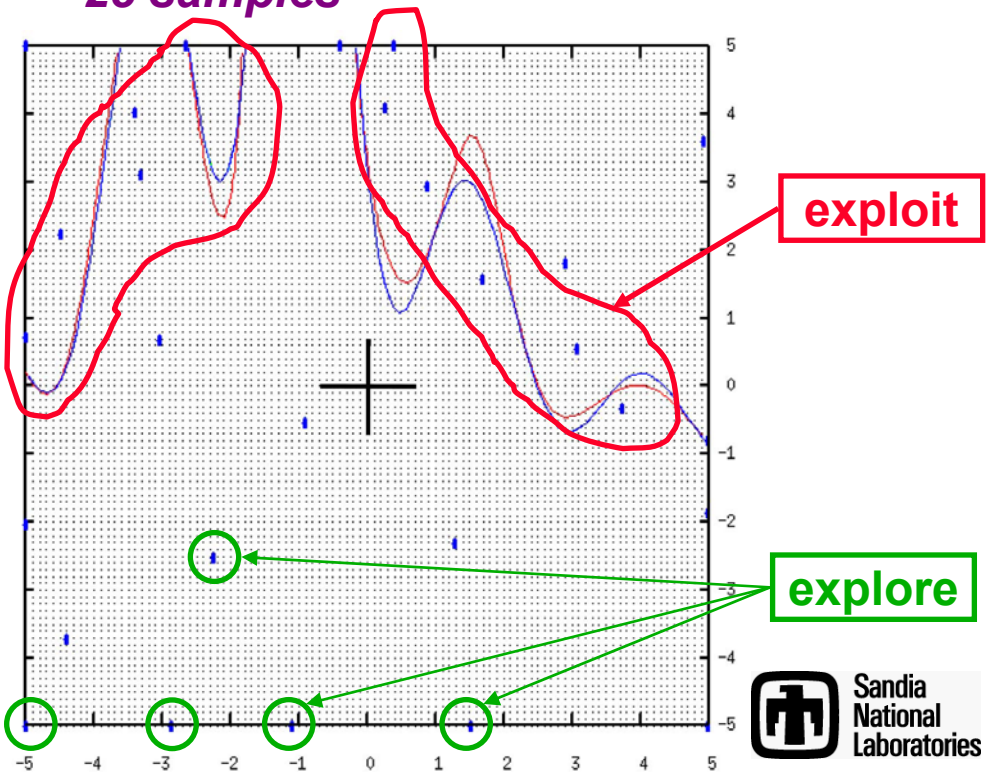
***Gaussian process model of reliability limit state with***

***10 samples***




***28 samples***

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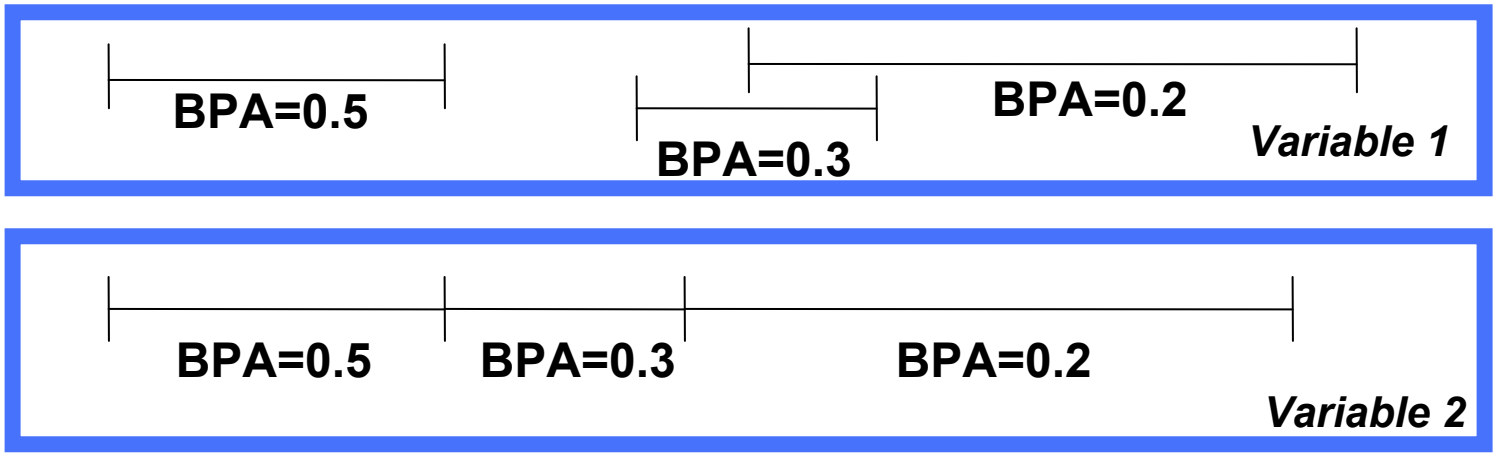
# Challenge: Epistemic UQ

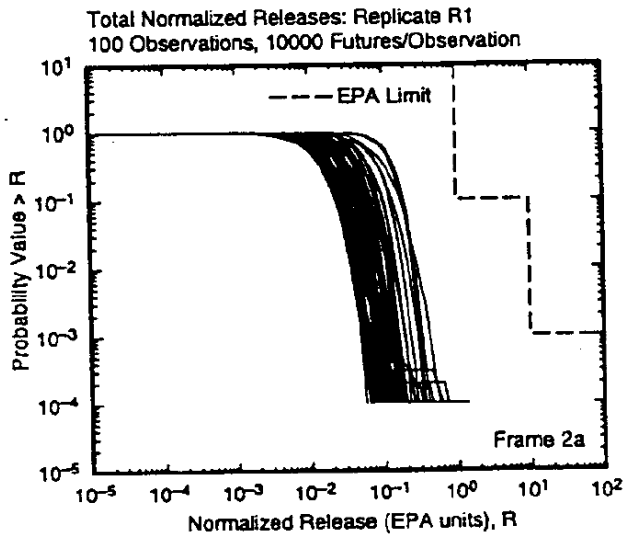
- **Epistemic uncertainty:** insufficient information to specify a probability distribution
- Subjective, reducible, or lack-of-knowledge uncertainty (given more resources to gather information, could reduce the uncertainty)
- For example:
  - "*I expect this parameter to have a lognormal distribution, but only know bounds on its mean and standard deviation,*" or
  - *Dempster-Shafer belief structures:* "basic probability assignment" for each interval where the uncertain variable may exist; contiguous, overlapping, or gapped



# Propagating Epistemic UQ

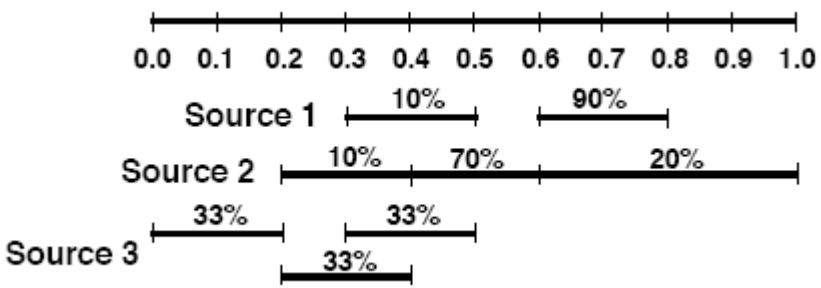
## Second-order probability

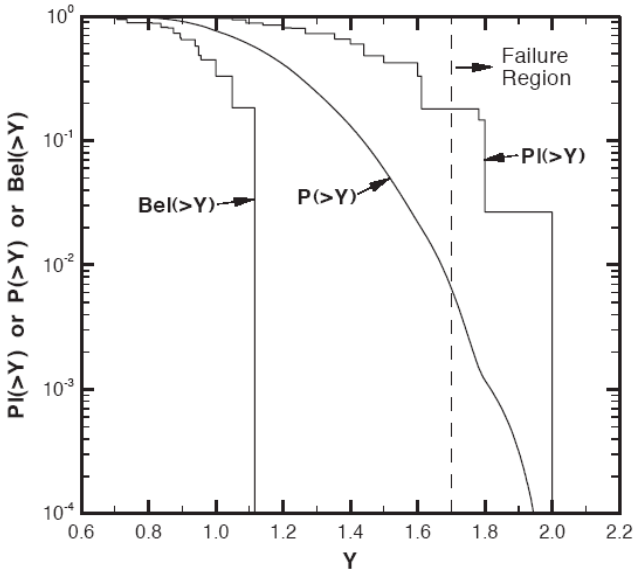
- Two levels: distributions/intervals on distribution parameters
- New Outer level can be epistemic (e.g., interval)
- Inner level can be aleatory (probability distrs)
- Strong regulatory history (NRC, WIPP).




## Dempster-Shafer theory of evidence

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

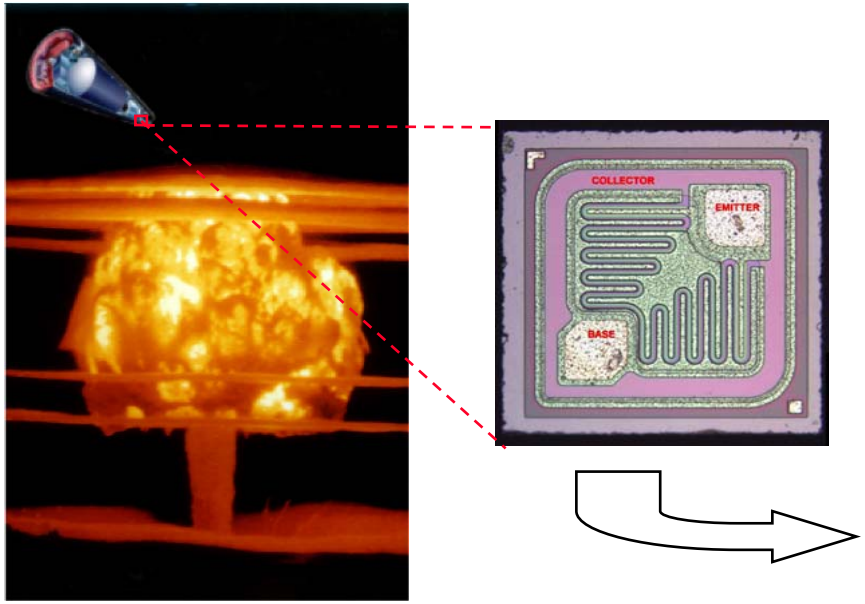


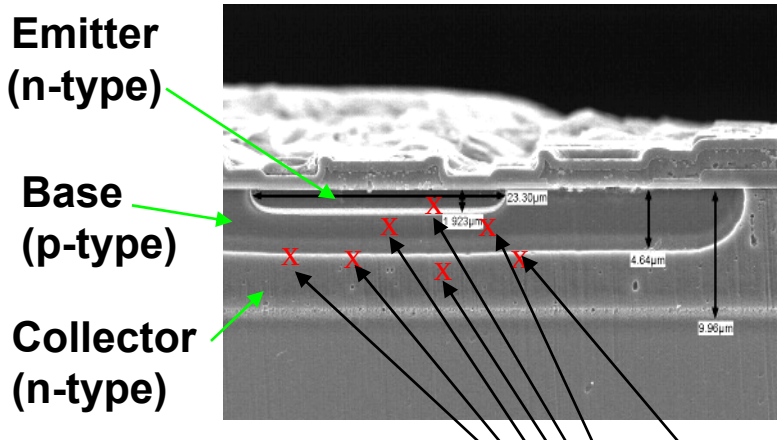
# DAKOTA UQ Algorithms Summary
# Goal: bridge robustness/efficiency gap

| | Production | New | Under dev. | Planned | Collabs. |
|---|---|---|---|---|---|
| Sampling | LHS/MC, QMC/CVT | IS/AIS/MMAIS, Incremental LHS | | Bootstrap, Jackknife | Gunzburger |
| Reliability | 1st/2nd-order local: MVFOSM/SOSM, x/u AMV/AMV$^2$/ AMV+/AMV$^2$+, x/u TANA, FORM/SORM | Global: EGRA | | | Renaud, Mahadevan |
| Polynomial chaos/ Stochastic collocation | | Wiener-Askey gPC: sampling, quad/cubature, pt collocation SC: quadrature | SC: cubature gPC/SC: arbitrary input PDFs | Adaptivity, Wiener-Haar | Ghanem |
| Other probabilistic | | | | Dimension reduction | Youn |
| Epistemic | Second-order probability | Dempster-Shafer evidence theory | | Bayesian, Imprecise probability | Higdon, Williams, Ferson |
| Metrics | Importance factors, Partial correlations | Main effects, Variance-based decomposition | Stepwise regression | | Storlie |

# Neutron Radiation Exposure Degrades Electronics

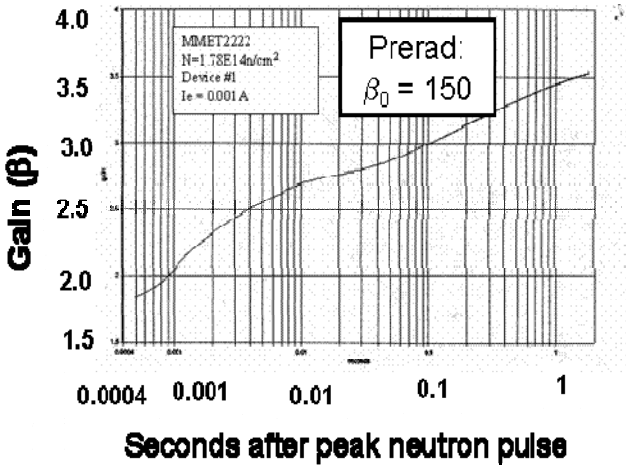



neutrons create damage




damage degrades gain

- **Military requirement: certify to hostile environment**

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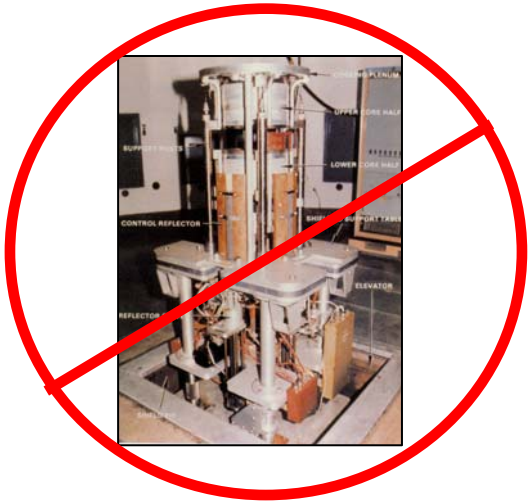
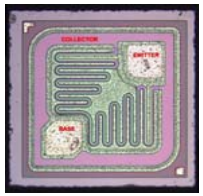
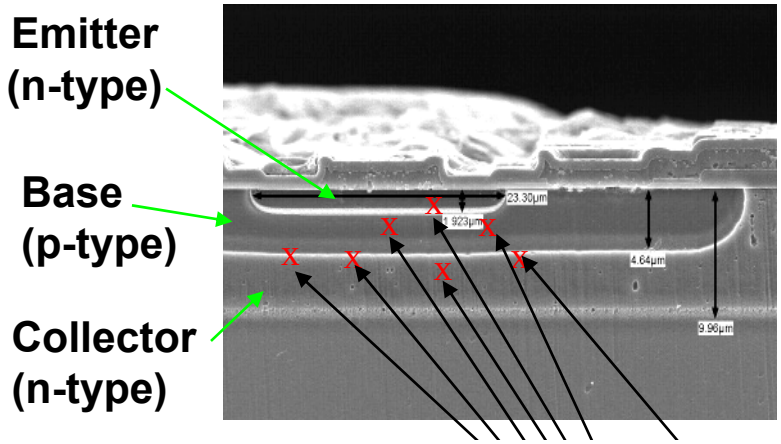
# Neutron Radiation Exposure Degrades Electronics





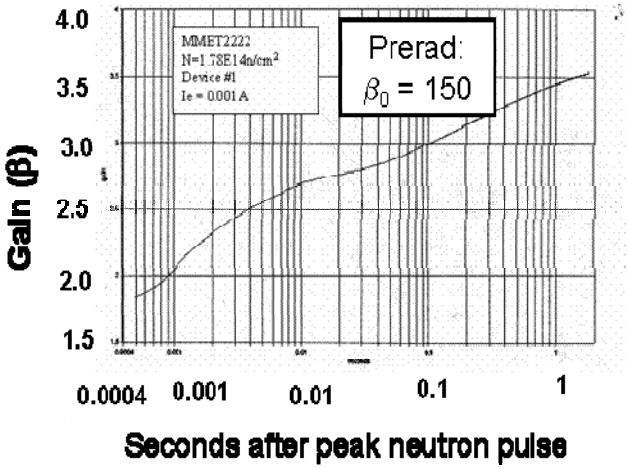
pass/fail testing

neutrons create damage




damage degrades gain

- Military requirement: certify to hostile environment
- SPR dismantled end of FY06 to improve security posture

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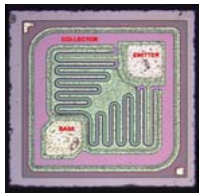
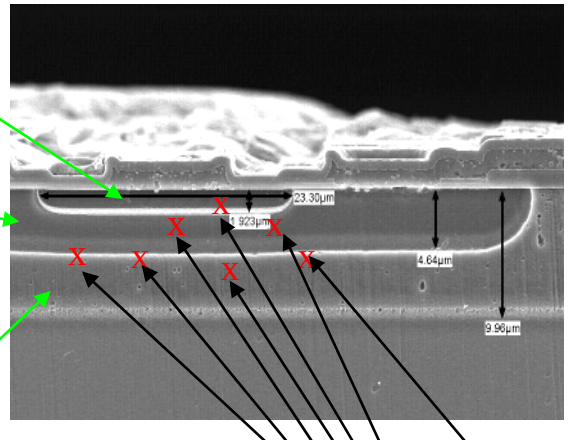
# Neutron Radiation Exposure Degrades Electronics

QASPR
QUALIFICATION ALTERNATIVES TO SPR



quantified uncertainty

neutrons create damage

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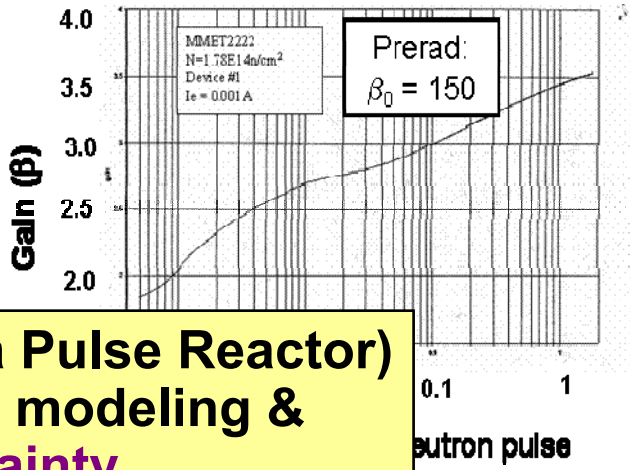


**QASPR (Qualification Alternatives to Sandia Pulse Reactor) methodology will certify qualification via modeling & simulation with quantified uncertainty**

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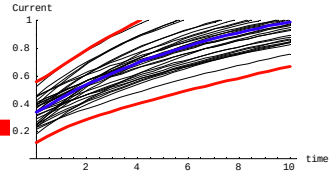
# QASPR: Science-Based Engineering Methodology For Qualification

**Risk Informed Decisions**




**Qualification Evidence**

DAKOTA

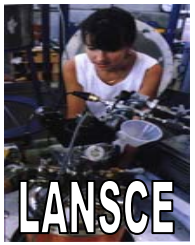
*uncertainty quantification*

UQ

EC

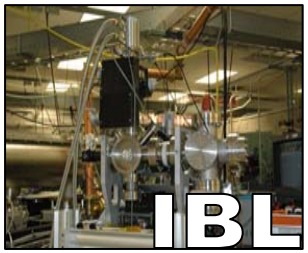
M&S

**validation**



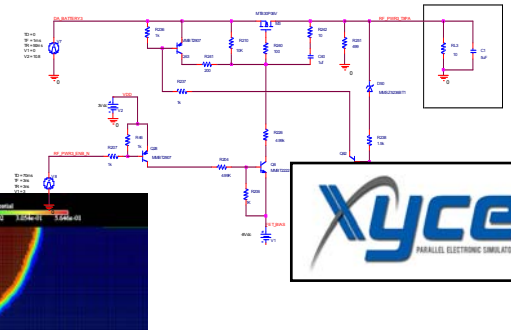

*select experiments in alternate facilities*

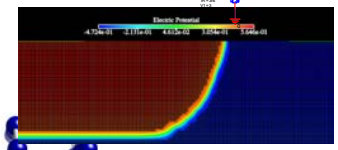
γ,n – 100 ms long pulse

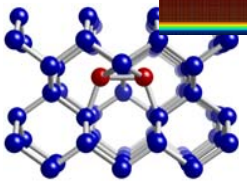



ion – 100 μs short pulse

*high performance, multi-fidelity, predictive computational modeling*







CHARON

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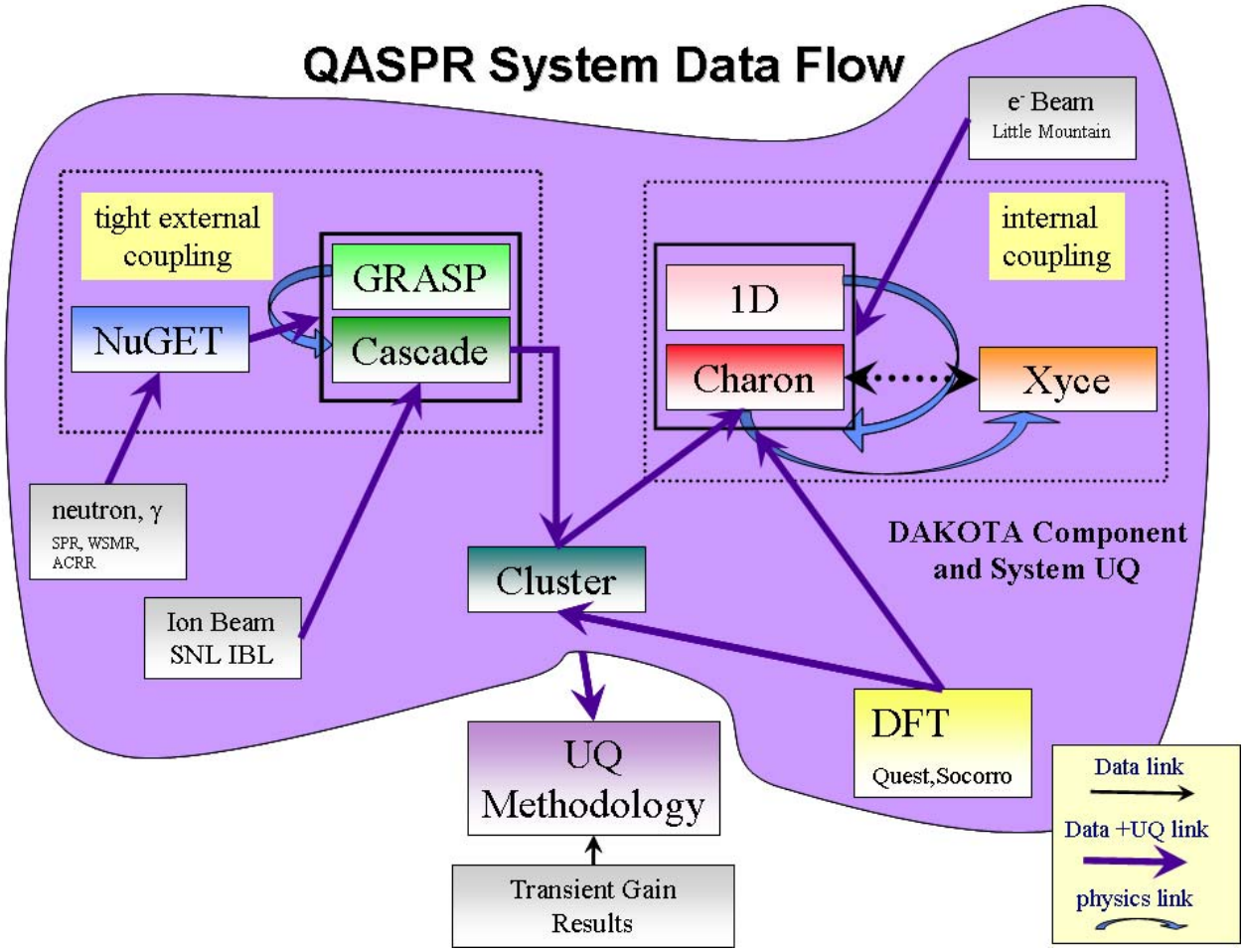
# V&V for QASPR Components




- Developing formal V&V plans
- Each computational code subject to code and solution verification
- UQ used to validate device model response against data ensembles
- Ultimately systems (circuit) V&V for qualification

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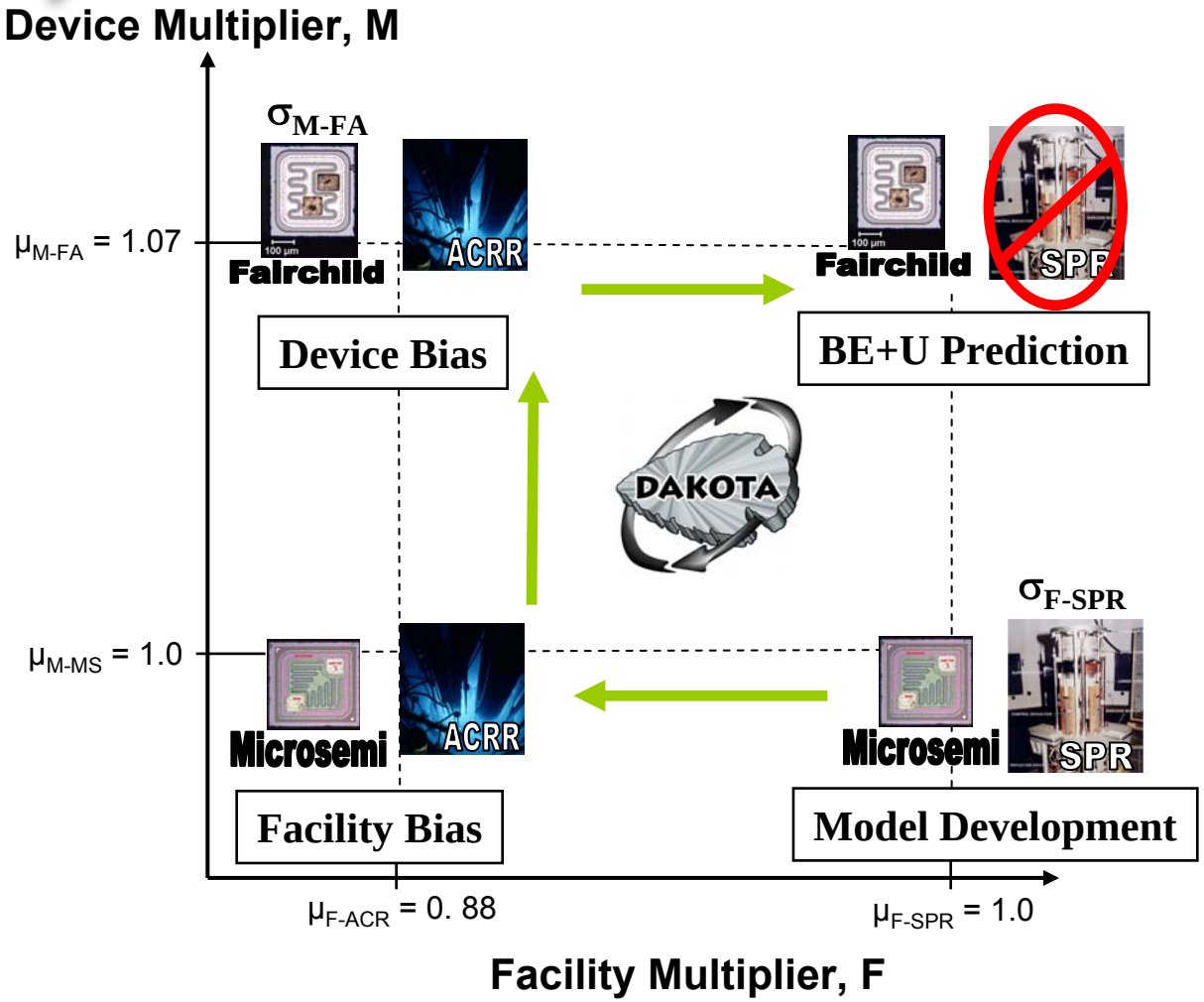
# Device Prototype: UQ Extrapolation to SPR




- Calibrated to other facilities, CHARON fills SPR gap
- Uncertainty & bias characterized by 2 degrees of freedom
  - facility multiplier
  - device multiplier
- Uncertainty quantified with D.O.E + statistical approach

**End UQ Methodology Goal: Best Estimate + Uncertainty Prediction for SPR**

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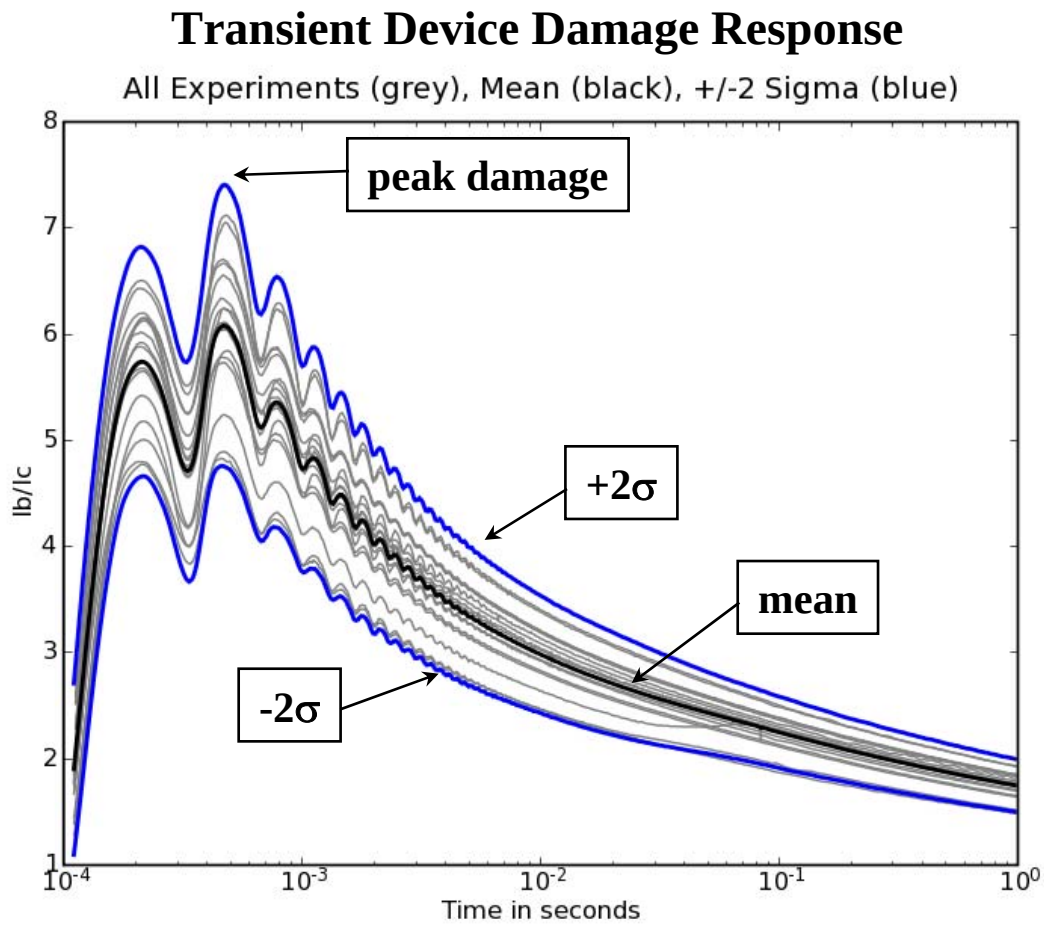
# Model Validation: Blind Prediction

- Fairchild response data within SPR hidden
- First *prototype* of the QASPR methodology (and real validation of the QASPR system)
- Prediction + Uncertainty (+/-2σ device and facility uncertainty)




**UQ algorithms have a critical role in system validation**

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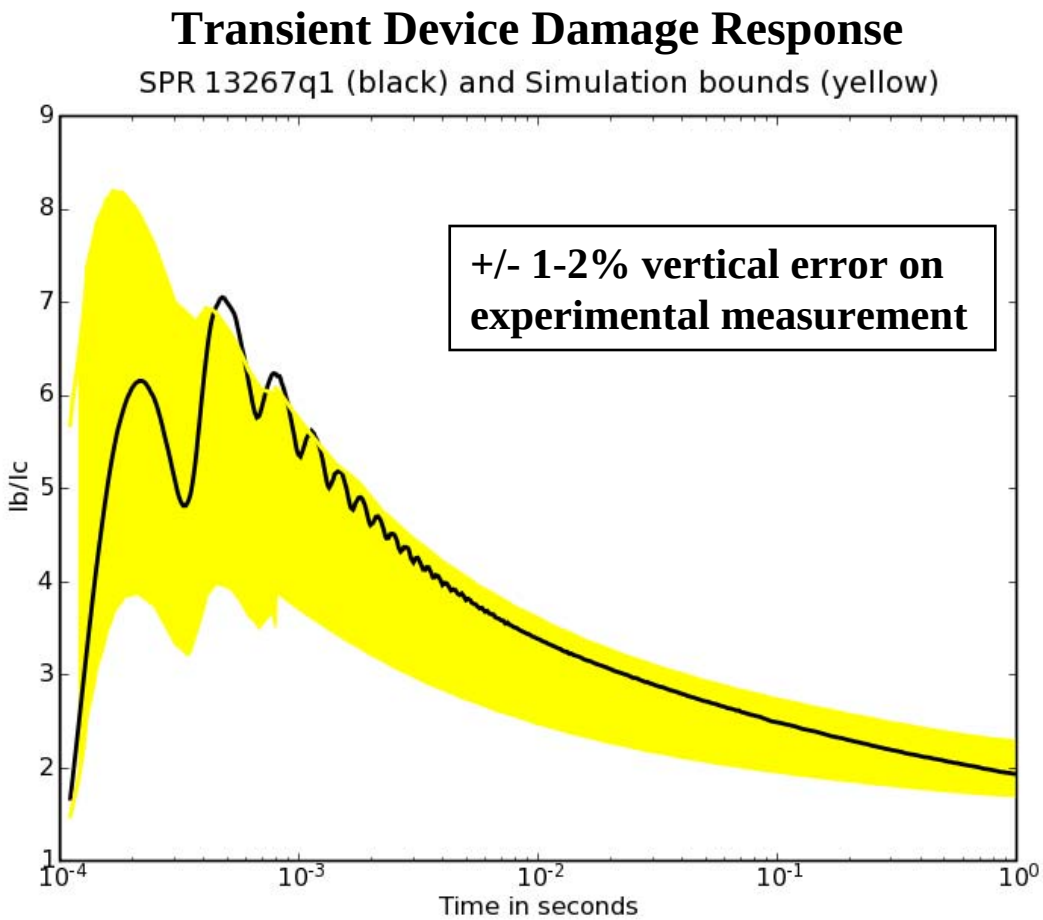


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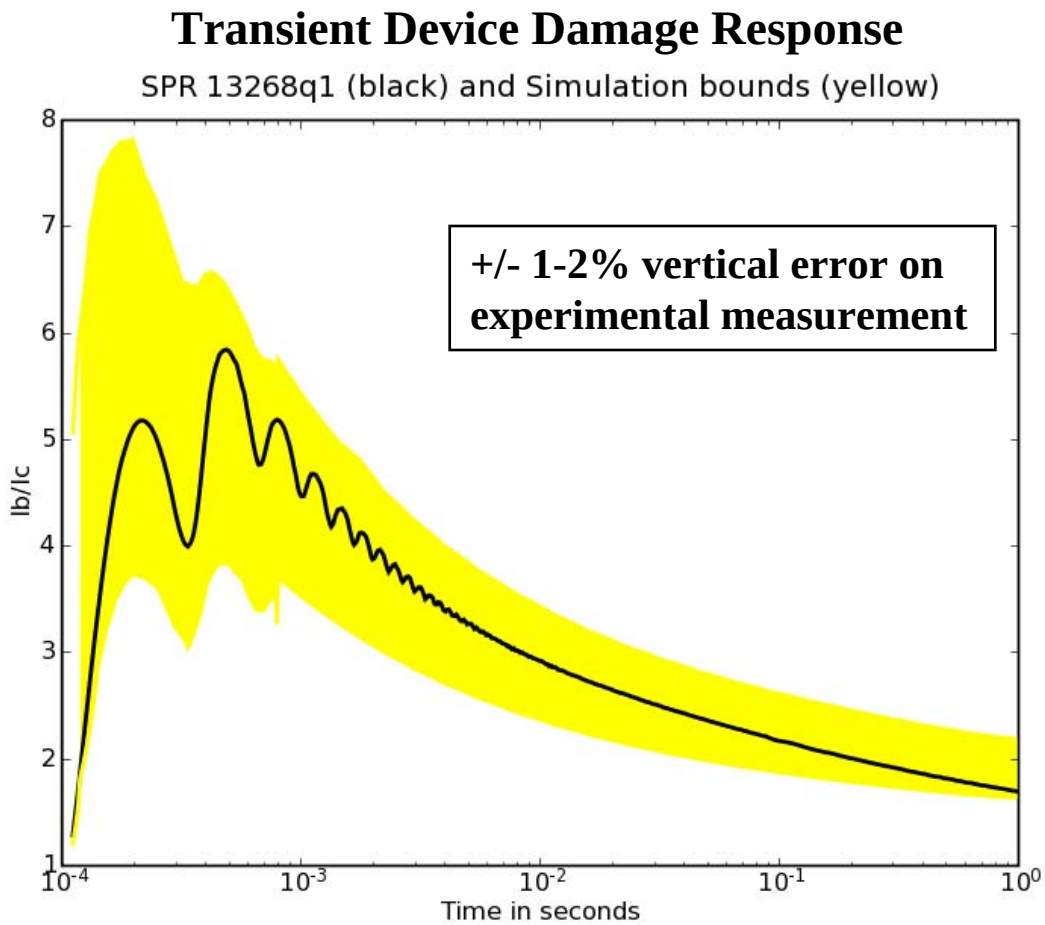


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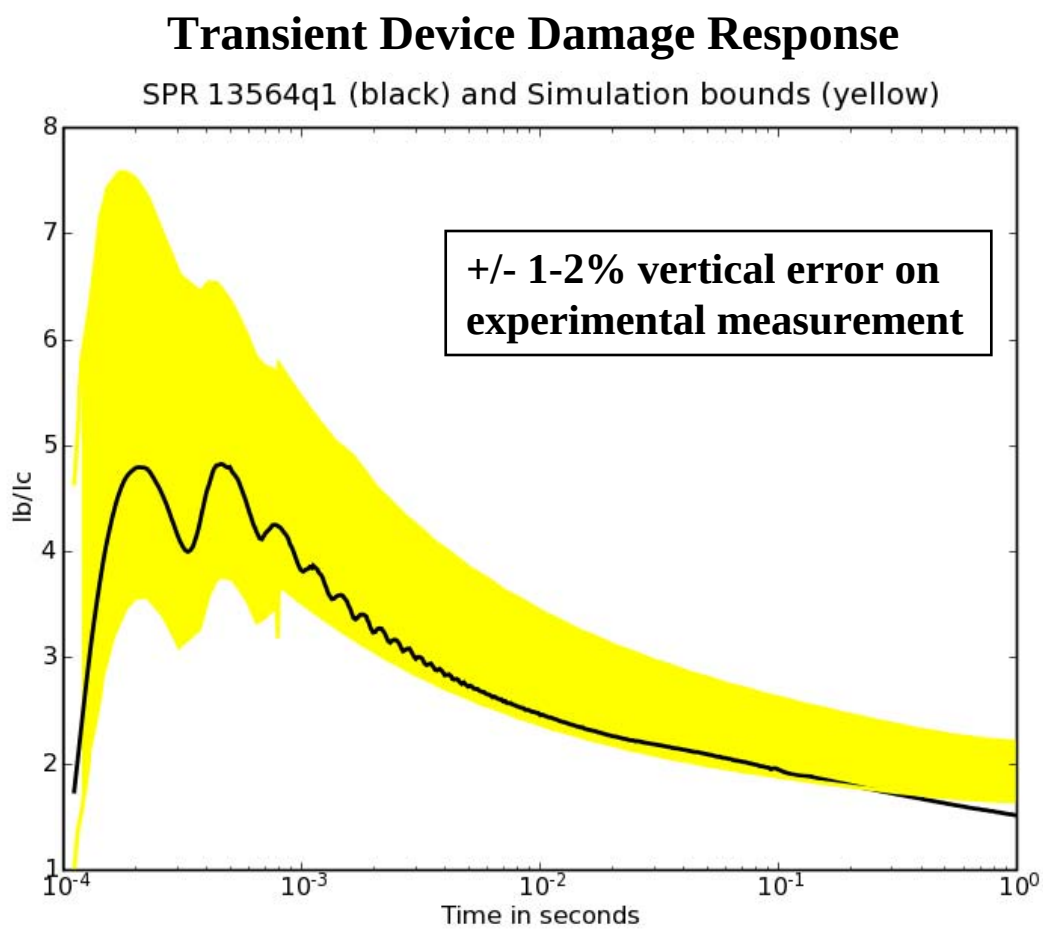


**UQ algorithms have a critical role in system validation**

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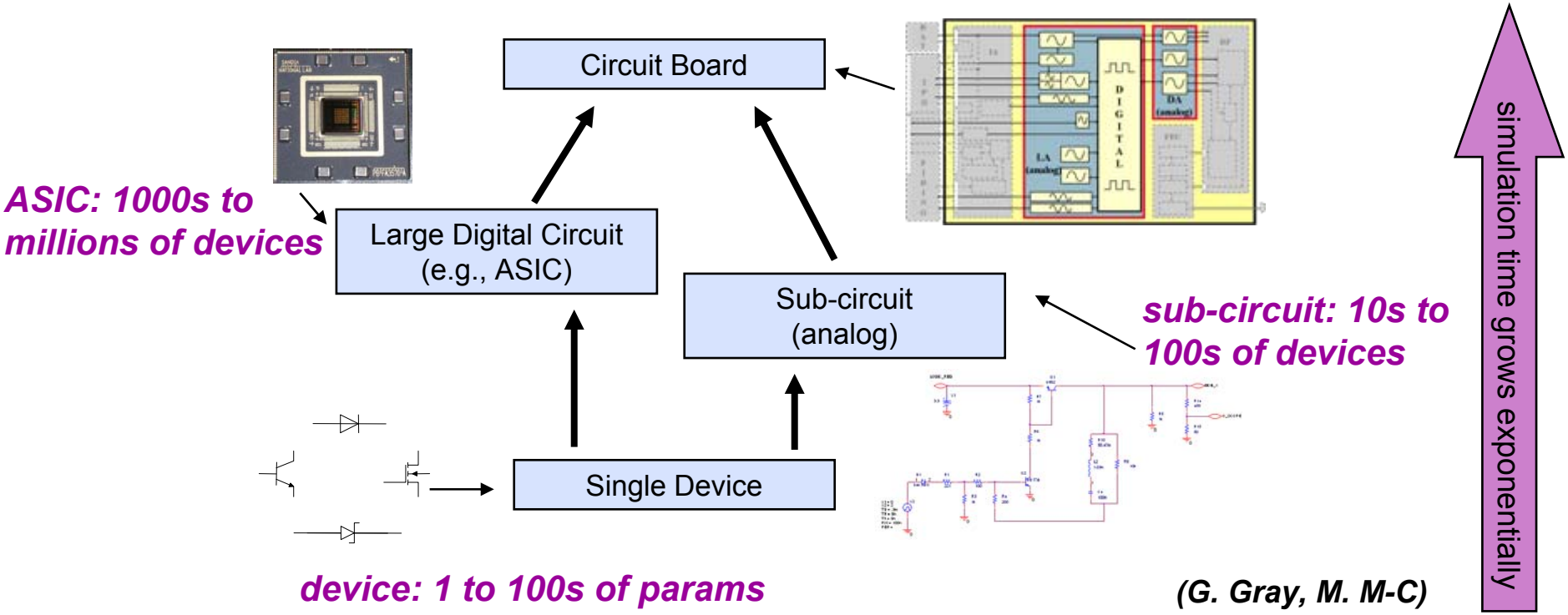
# Electrical Modeling Complexity

*complex device models + replicates in circuits*




*device: 1 to 100s of params*

*(G. Gray, M. M-C)*

- **simple devices:** 1 parameter, typically physical and measurable
- e.g., resistor @ 100Ω +/- 1%
- resistors, capacitors, inductors, voltage sources

- **complex devices:** many parameters, some physical, others "extracted" (calibrated)
- multiple modes of operation
- e.g., zener diode: 30 parameters, 3 bias states; many transistor models (forward, reverse, breakdown modes)

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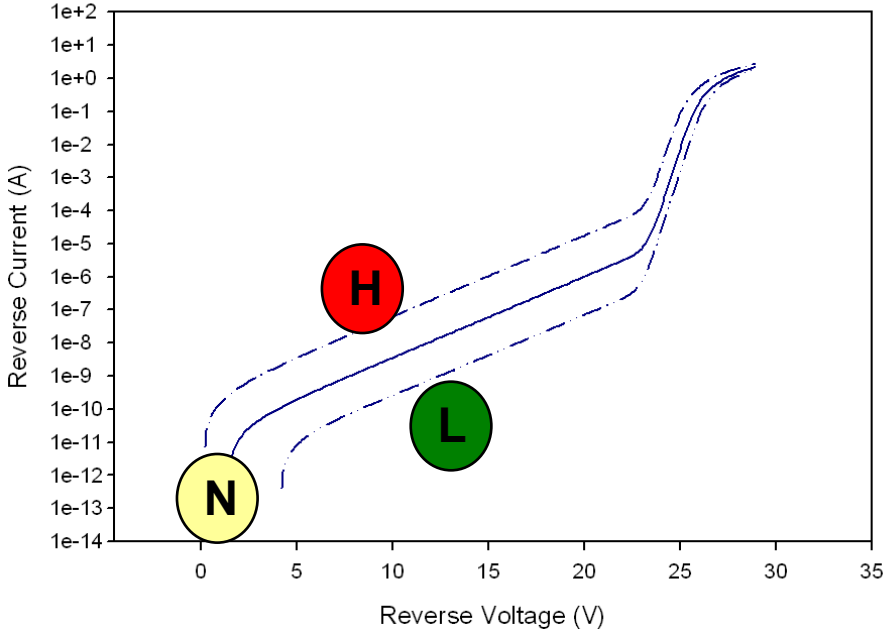
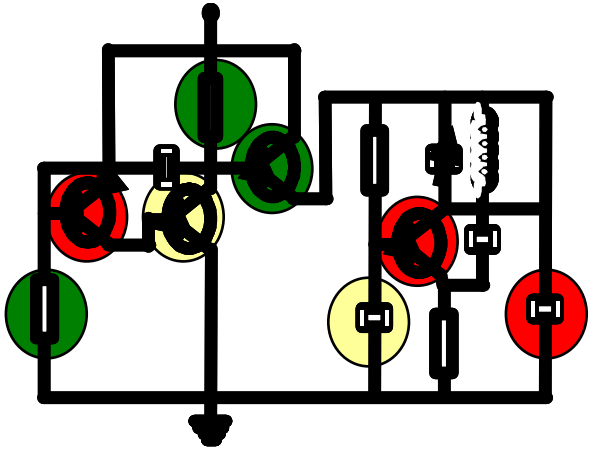
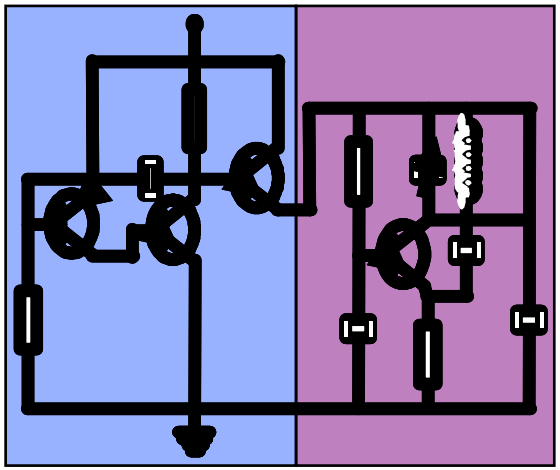
# UQ: Mitigate Explosion of Factors!




- Consider bounding parameter sets?
- Exploit natural hierarchy or network structure?
- Use surrogate/macro-models as glue between levels?
- *Need approaches curbing the curse of dimensionality*





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# Summary

***Advanced algorithms enable robust, efficient uncertainty quantification for validating models with experimental data and making credible predictions.***

- **Credible simulations must deliver best estimate + uncertainty.**
- **Uncertainty quantification algorithms are essential in validation and calibration under uncertainty**
- **Complex/large-scale/multi-scale/multi-physics simulations demand research in advanced efficient UQ methods**

**Thank you for your attention!**

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**http://www.sandia.gov/~briadam**

**http://www.cs.sandia.gov/DAKOTA**

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# Abstract

**Uncertainty Quantification Algorithms and Software Enabling V&V**

**Computational simulations are increasingly used for risk-informed decision making in the presence of uncertainties. To be credible, they must deliver not only a best estimate of performance, but also its degree of variability or uncertainty. Uncertainty quantification (UQ) algorithms compute the effect of uncertain input variables on simulation response metrics of interest, enabling model validation and subsequent credible risk assessment.**

**I will survey UQ algorithms research addressing both aleatory (inherent) and epistemic (lack-of-knowledge) uncertainties. For example, advanced reliability analysis and polynomial chaos expansion methods available in Sandia's DAKOTA toolkit offer substantial efficiency advantages over ubiquitous Monte Carlo sampling. Application to electrical circuit calibration and validation in the QASPR (Qualification Alternatives to Sandia's Pulsed Reactor) program will demonstrate UQ algorithms in an extrapolation context and motivate the need to develop hierarchical UQ techniques for systems analysis.**