SAND2008-5005C

Computer Science Research Institute

Validation & Verification and Uncertainty Quantification at Sandia

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Sandia National Laboratories
Optimization and Uncertainty Quantification

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Research Consortium for Multidisciplinary System Design Workshop
MIT, Boston, MA

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.

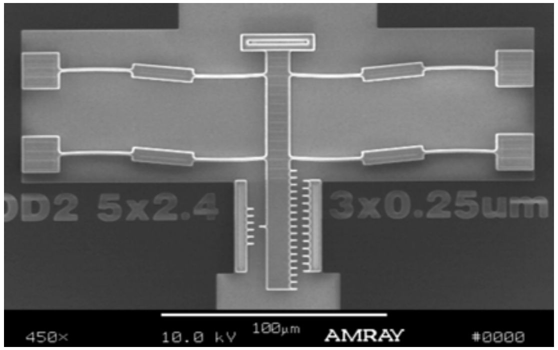
Outline

To be credible, simulations must be verified, validated with data, and deliver a best estimate of performance, together with its degree of variability or uncertainty.

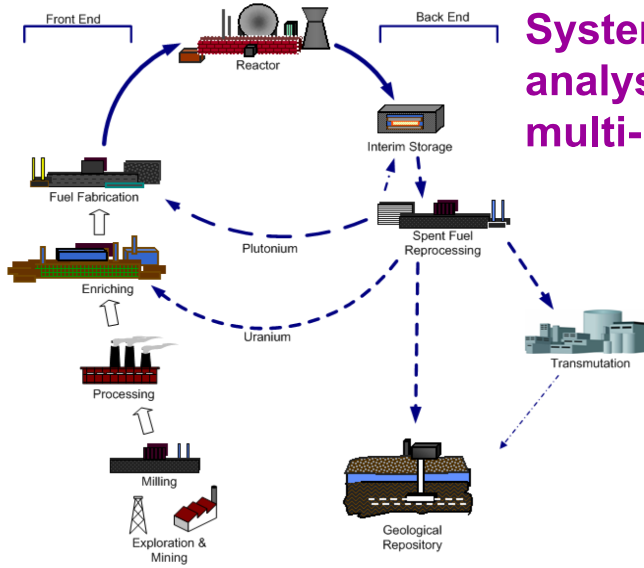
- Credible simulation and V&V
- Characterizing and propagating uncertainty for risk analysis and validation
- Intro to aleatory and epistemic UQ in DAKOTA
- Application examples:
  - UQ for CMOS7 ViArray UQ
  - Sandia's QASPR program: computational model-based system qualification

Slide credits: Mike Eldred, Laura Swiler, Tony Giunta, Joe Castro, Genetha Gray, Bill Oberkampf, Matt Kerschen, others

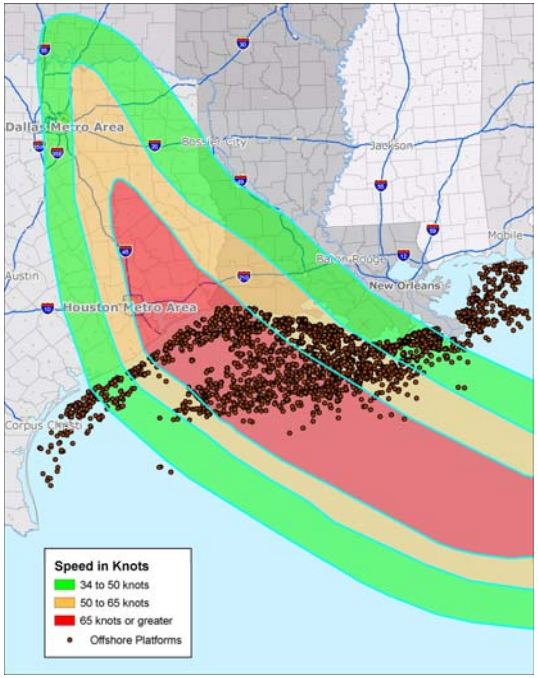
Insight from Computational Simulation



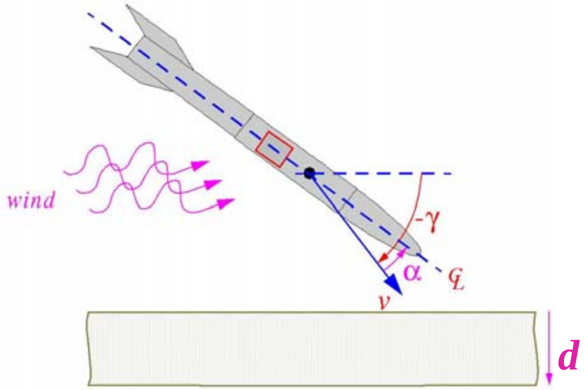
Micro-electro-mechanical systems (MEMS): quasi-static nonlinear elasticity, process modeling



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

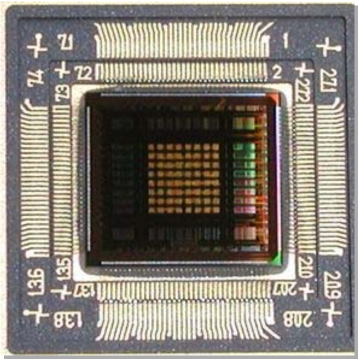


Hurricane Katrina: weather, logistics, economics, human behavior



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

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



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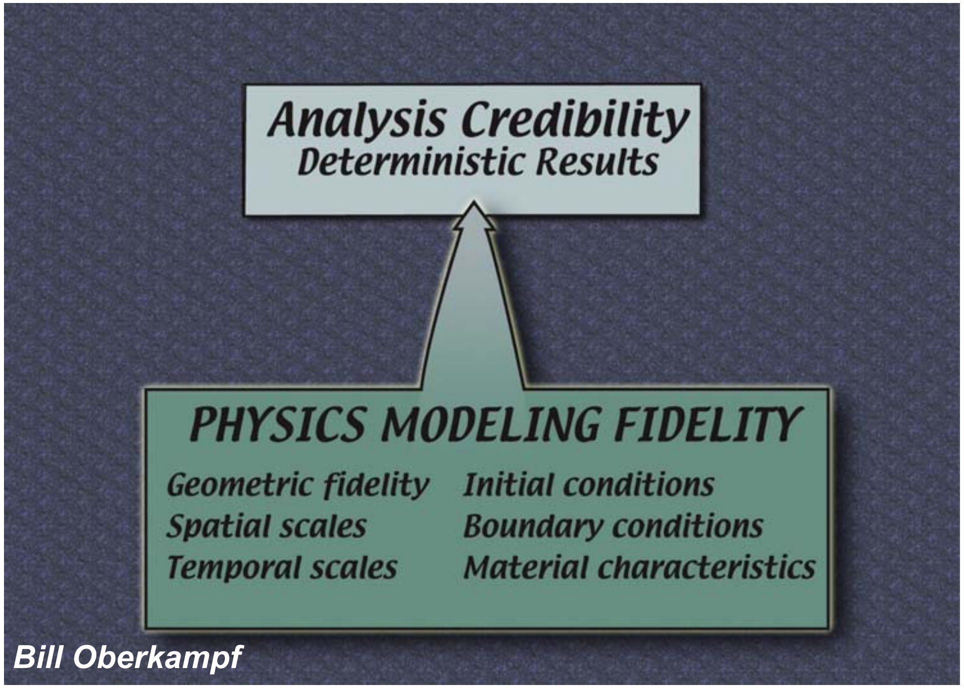
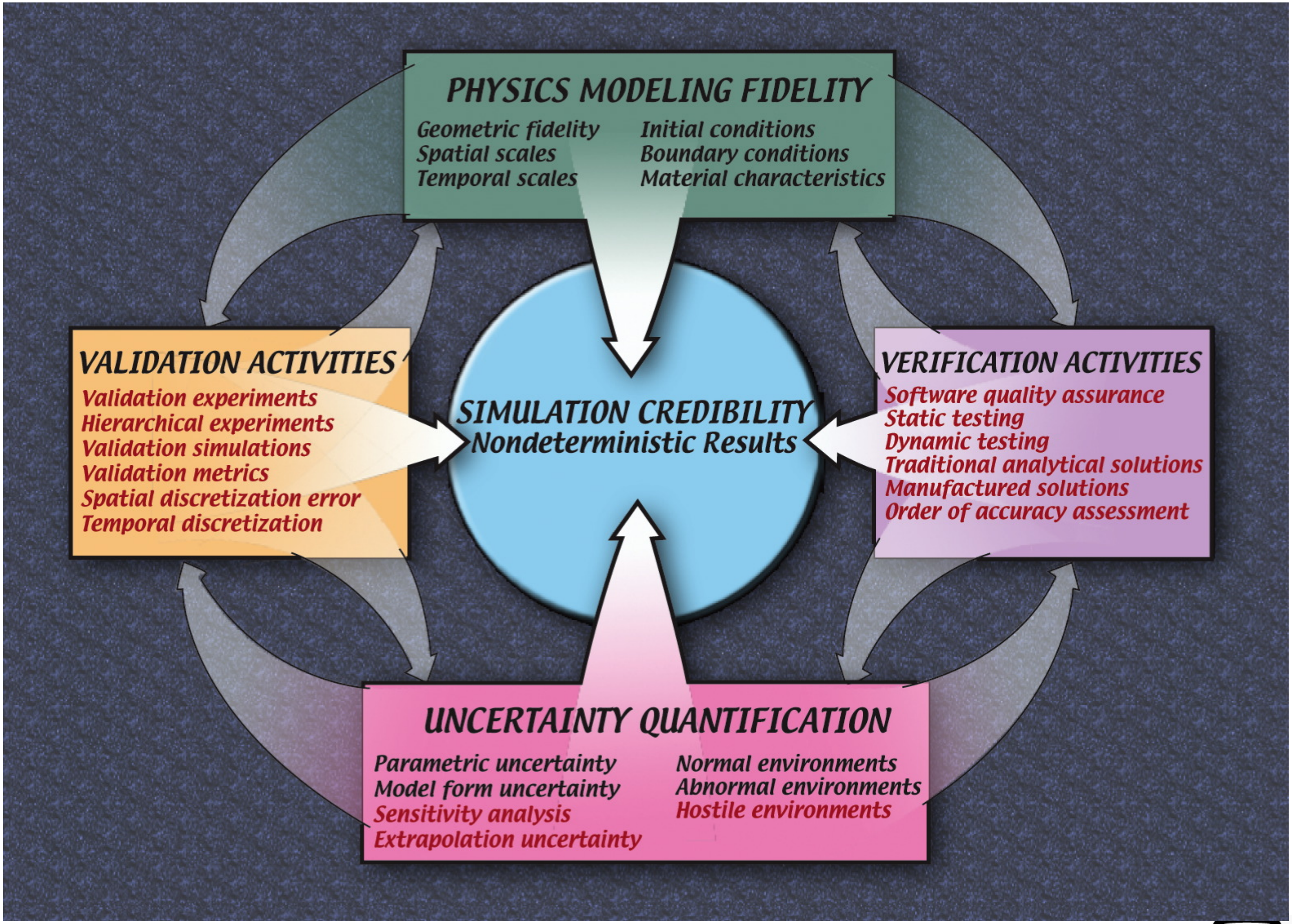
Credible Simulation

- **Ultimate purpose of modeling and simulation is (arguably) insight, prediction, and decision-making → *need credibility for intended application***



- **Historically: primary focus on *modeling fidelity***

Credible Simulation: V&V and UQ



Bill Oberkampf

Verification & Validation

- **Ultimately, quantification of margins and uncertainties (QMU):**
  How close are my uncertainty-aware code predictions to required performance?

- **Validation: *"Are we solving the right equations?"***
  - **A disciplinary science issue: is the science (physics, biology, etc.) model sufficient *for the intended application?***
  - **Involves *data and metrics;* relies on uncertainty quantification (UQ)**

- **Verification: *"Are we solving the equations correctly?"***
  - **A mathematics/computer science issue: is our mathematical formulation and software implementation of the physics model correct?**
  - ***code verification* (software correctness): SQE, especially unit/regression/ verification testing; analytic problems, method of manufactured solutions**
  - ***solution verification:* e.g., exhibits proper order of spatial/temporal/iterative convergence. Algorithms: Richardson extrapolation, finite element error estimation (ZZ, QOI)**

$$p = \frac{1}{\ln r} \ln\left(\frac{E_{grid1}}{E_{grid1}}\right)$$

$$\eta^Q \equiv \int_\Omega \boldsymbol{T}(\boldsymbol{u}_h) : (\boldsymbol{G}(\nabla \boldsymbol{z}_h) - \nabla \boldsymbol{z}_h)\, \mathrm{d}\Omega$$

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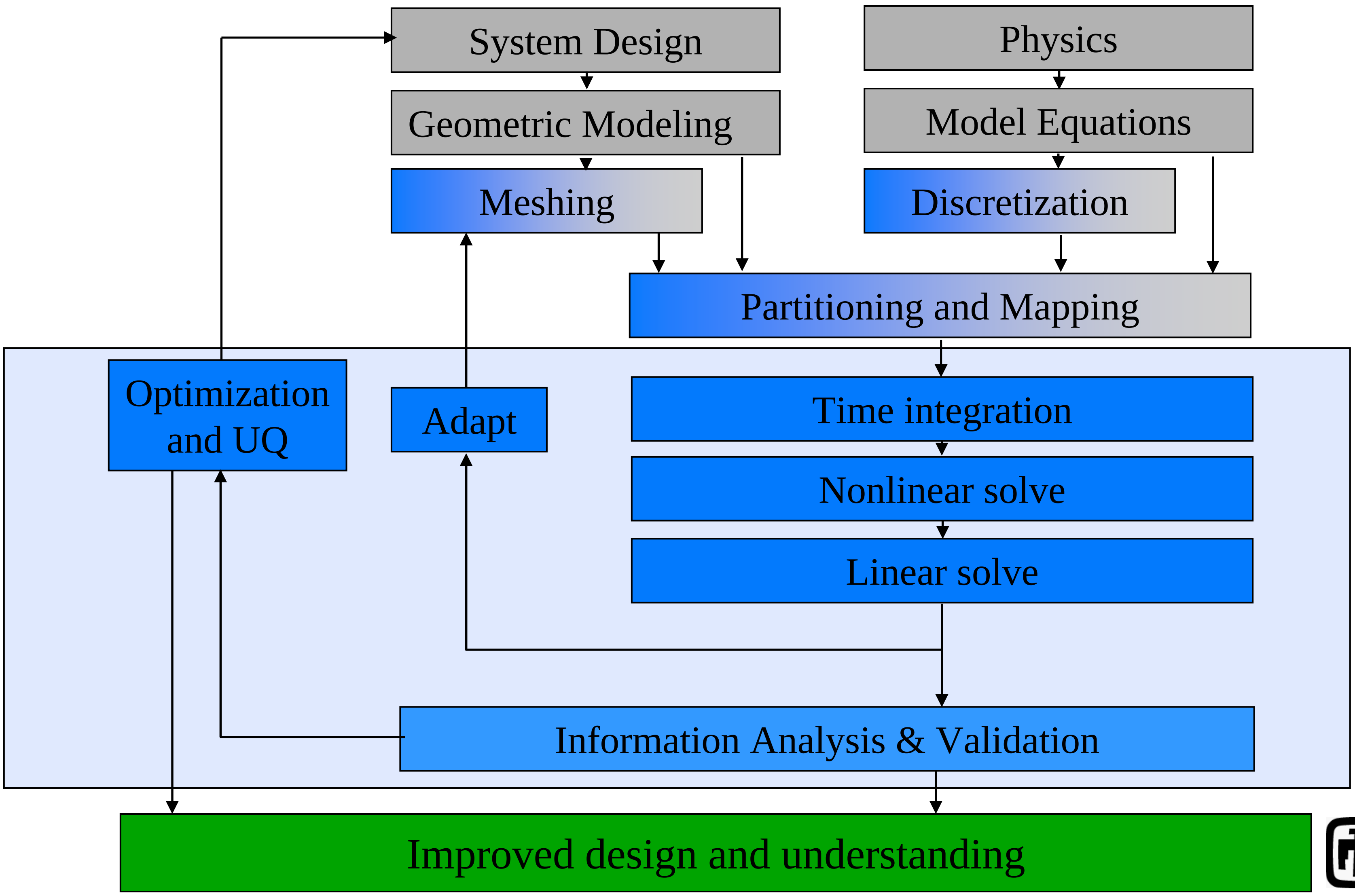
Algorithms for Computational Modeling & Simulation

Are you sure you don't need verification?!



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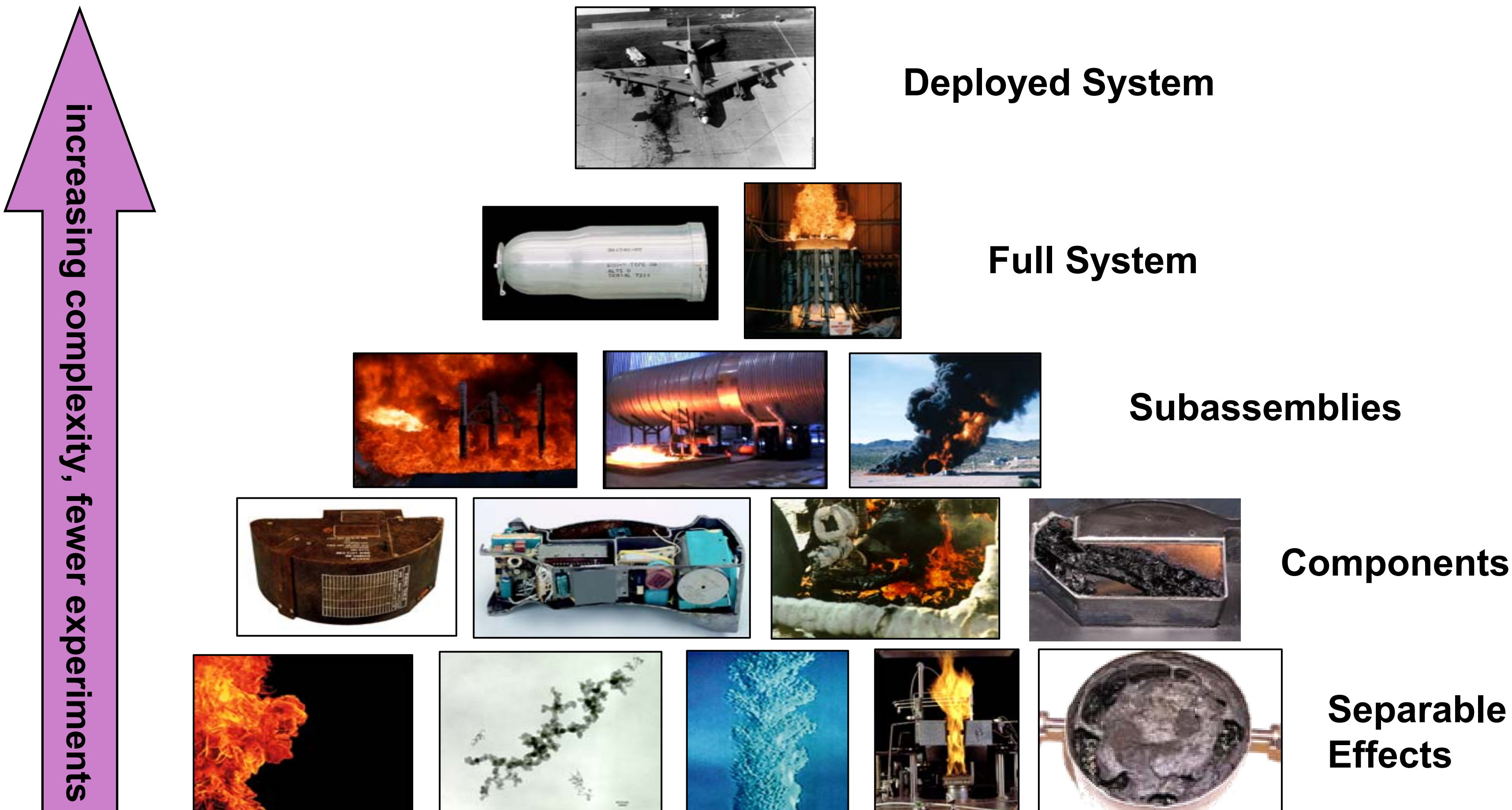
Hierarchical Validation Experiments
(Abnormal Thermal Environment)

Validation: ***"Are we solving the right equations?"*** **Based on experimental data and metrics, is the model sufficient *for the intended application?***



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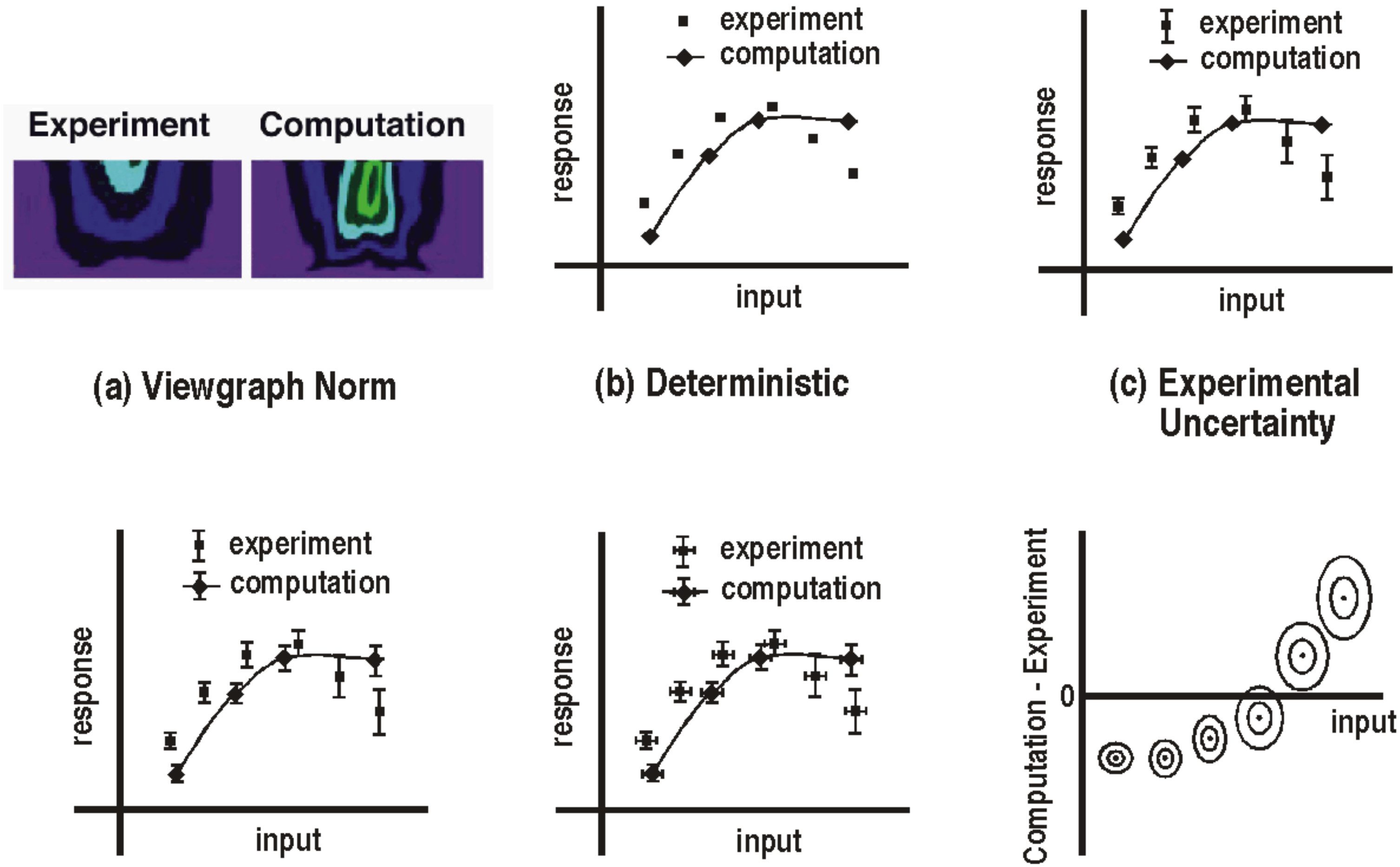
Validation Metrics: Quantitative Comparison with Experiment



(a) Viewgraph Norm

(b) Deterministic

(c) Experimental Uncertainty

(d) Numerical Error

(e) Nondeterministic Computation

(f) Statistical Comparison

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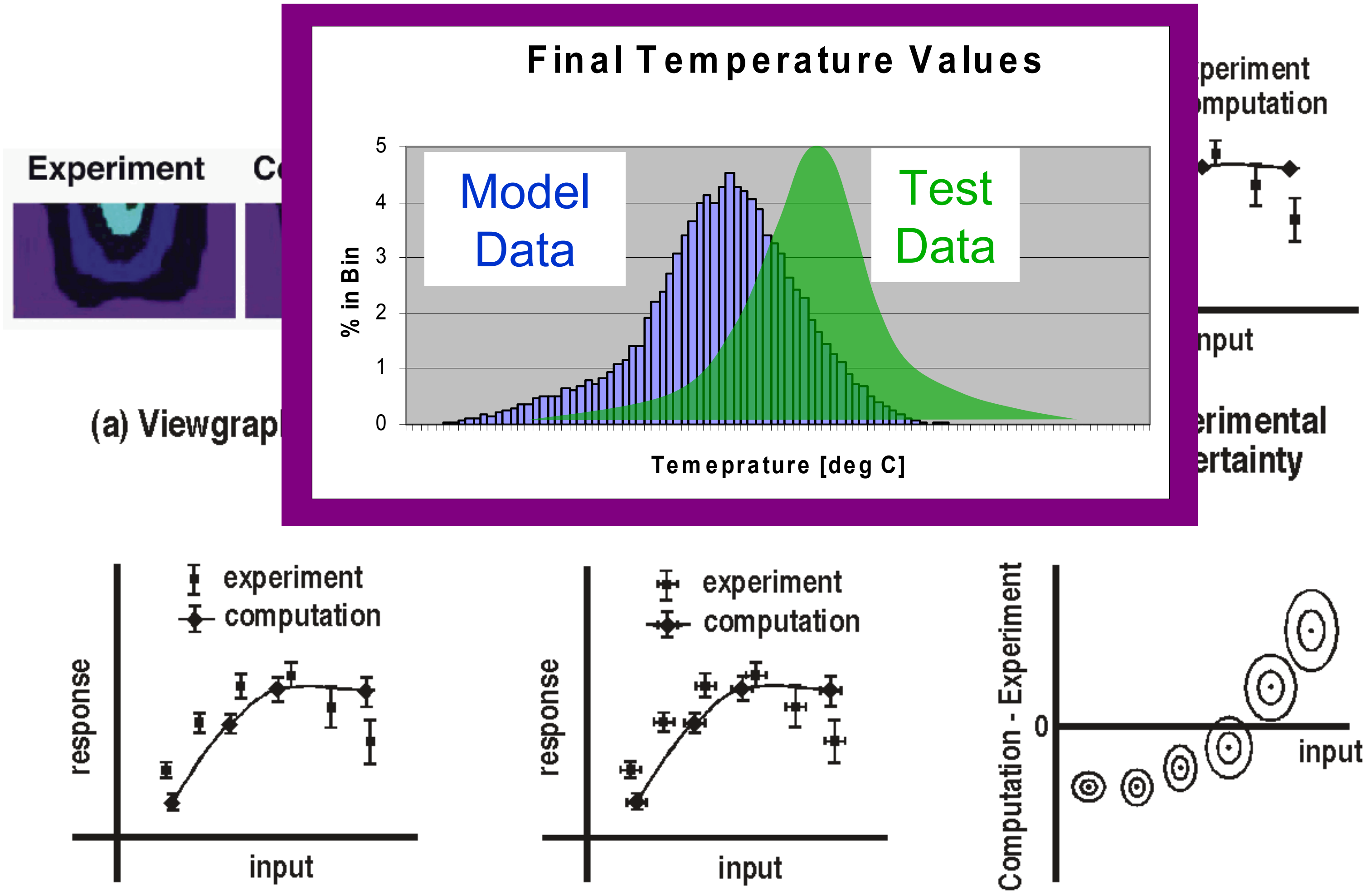
Validation Metrics: Quantitative Comparison with Experiment



(d) Numerical Error

(e) Nondeterministic Computation

(f) Statistical Comparison

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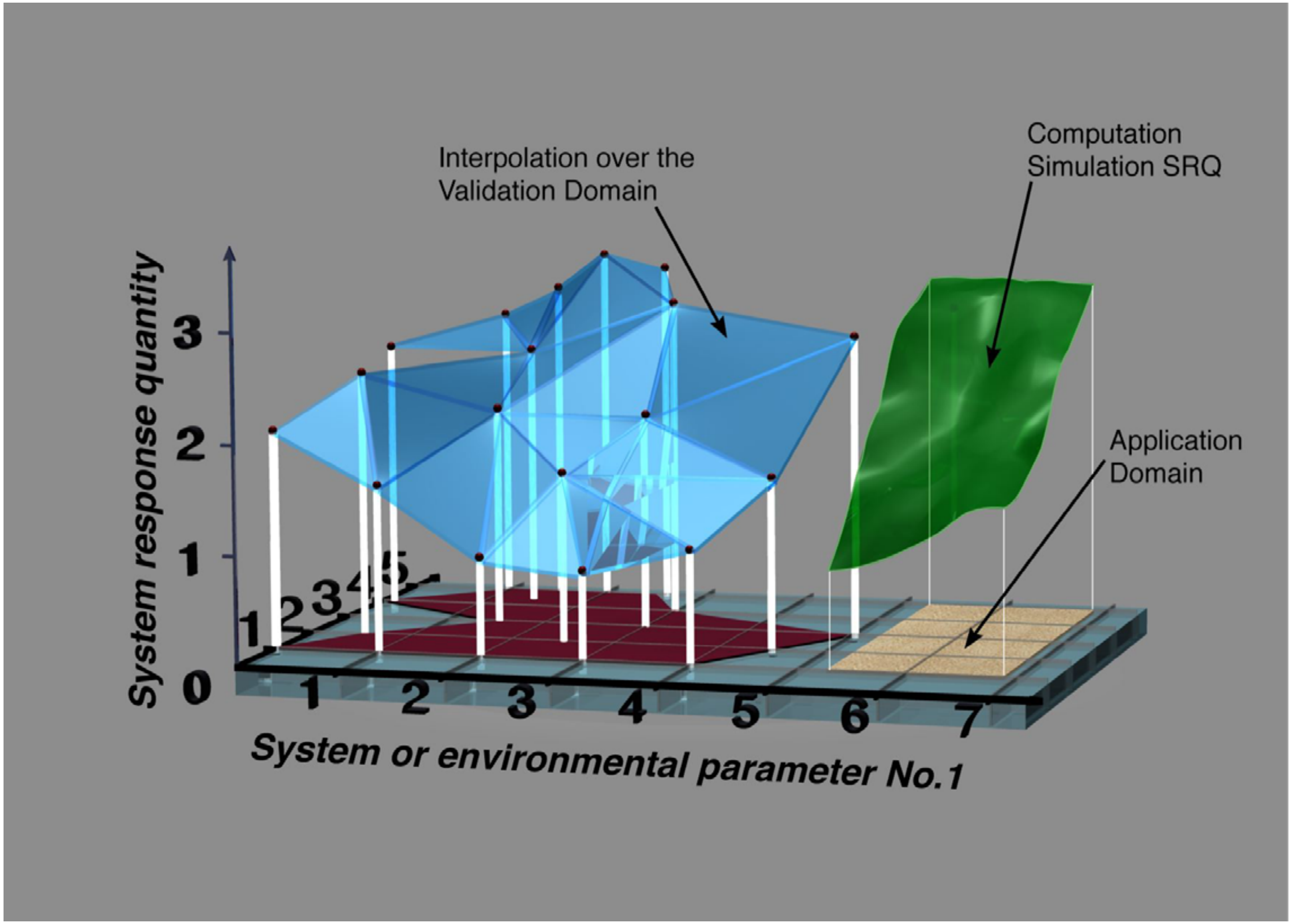
Extrapolating Beyond Validation Domain



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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
  - statistical variation, inherent randomness
  - operating environment, interference
  - initial, boundary conditions; forcing
  - geometry / structure / connectivity
  - material properties
  - manufacturing quality
- **model form / accuracy**
- **program:** requirements, technical readiness levels
- **human reliability**, subjective judgment, linguistic imprecision

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

Why Uncertainty Quantification?

- **A single optimal design or nominal performance prediction is often insufficient for**
  - **decision making / trade-off assessment**
  - **validation with experimental data ensembles**

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

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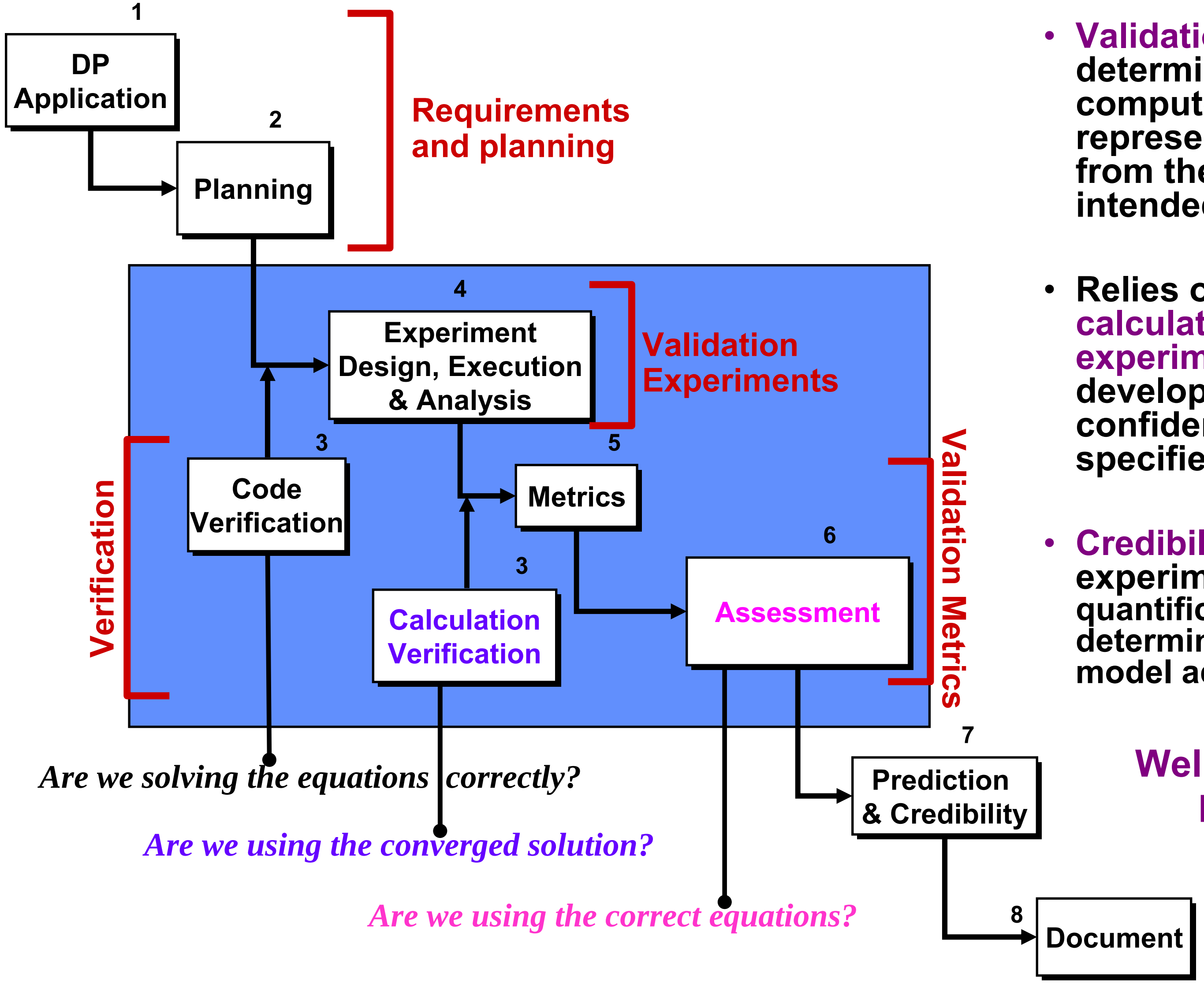
Verification & Validation: A Formal, Iterative Process



- **Validation** is "the *process* of determining the degree to which a computer model is an accurate representation of the real world from the perspective of the intended model *applications*."
- Relies on **comparing code calculations to results of physical experiments**, with the goal of developing and quantifying confidence in codes to predict a specified problem result
- **Credibility** assesses model and experiment relevance, quantification and capture of non-deterministic components, and model adequacy

Well-characterized result: BEST ESTIMATE + UNCERTAINTY

Trucano et al; SAND Report 2002-0341

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Coverage Matrix Shows Code Features Exercised in Verification Tests

Sierra Capabilities (subset)

SNL-Problem **LANL-Problem**

Sierra Capabilities (subset)	Application									Verfication Test Suite																																										
										1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
PDE terms																																																				
Conduction (diffusion term)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Capacitance (transient term)	x	x	x	x	x	x	x	x	x	x			x			x	x	x	x				x									x	x				x	x	x							x	x	x	x	x	x	x
Src (source term)	x	x									x	x	x								x	x		x	x				x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
EnclRad	x	x	x	x	x	x	x	x	x											x																																
CM (chemistry source term)													x										x																													
Thermal Conductivity																																																				
k0 (constant conductivity)	x	x	x	x	x	x	x	x	x				x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x			x	x	x
k1 (tabular T-dependant)	x	x	x	x	x	x	x	x	x																			x																				x	x			
k2 (user subroutine T-dependant, mostly)		x				x	x	x		x	x	x																																								
k3 (defined variable)																																																				
k4 (anisotropic constant)	x	x		x			x		x																																									x	x	x
k5 (anisotropic tabular T-dependant)	x	x	x	x					x																																											
Heat capacity																																																				
Cp0 (constant)	x	x	x	x	x	x	x	x	x				x					x	x				x									x	x				x	x	x							x	x			x	x	x
Cp1 (tabular T-dependant)	x	x	x	x	x	x	x	x	x							x	x																															x	x			
Cp2 (user subroutine T-dependent)		x				x		x		x																																										
Cp3 (user variable)																																																				
Density																																																				
D0 (constant)	x	x	x	x	x	x	x	x	x	x			x			x	x	x	x				x									x	x				x	x	x							x	x	x	x	x	x	x
D1 (tabular T-dependent)			x	x		x		x	x																																											
D2 (user subroutine T-dependent)		x																																																		
D3 (user variable)																																																				
D4 (volume dependant)																																																				
Source terms																																																				
G0 (constant)	x	x																			x	x							x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
G1t (tabular, time varing)	x																																																			
G1T (tabular, temp varing)																																																				
G2 (user subroutine, time or temp varing)		x									x	x	x											x	x																											
G3 (user variable)																																																				
Temperature boundary conditions																																																				
T-0 (constant)	x				x	x	x				x	x	x	x	x					x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
T-1t (tabular, time dependent)					x																																															
T-2 (user subroutine)						x	x						x																																							
Flux boundary conditions																																																				
Q-0 (constant)																		x	x		x	x							x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x
Q-1t (tabular, time dependant)			x																																																	
Q-1T (tabular, temp dependant)																																																				
Q-2 (user subroutine)				x					x	x						x	x																																		x	
Convective boundary conditions																																																				
h-0 (constant)	x	x	x	x	x	x															x	x							x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
h-1t (tabular, time dependent)			x																																																	
h-1T (tabular, temp dependent)																																																				
h-2 (user subroutine)																																																				
Tref-0 (constant ref temp)	x	x	x	x	x	x															x	x							x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
Tref-1t (tabular, time dependent, ref temp)	x																																																			
Tref-1T tabular, temp depentdent, ref temp)																																																				
Tref-2 (user subroutine, ref temp)																																																				
Tref-B (bulk fluid element)			x	x																																																
Radiation boundary conditions																																																				
e-0 (constant emissity)	x	x	x	x																																																
e-1 (tabular, T-dependent)			x	x																																																
e-2 (user subroutine, T dependent)		x																																																		
Trad-0 (constant radiation temperature)	x	x	x	x																																																
Trad-1t (tabular, time dependent rad temp)	x																																																			

Fills Gap

Matrix helps prioritize gaps, create new verification problems to fill most important, w.r.t. intended use.

Categories of Uncertainty

Often useful algorithmic distinctions, but not always a clear division

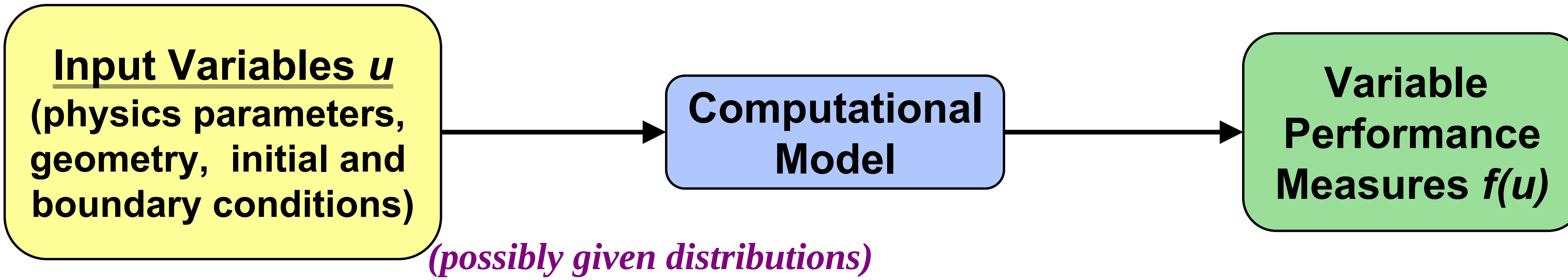
- **Aleatory** ***(think probability density function)***
  - **Inherent variability (e.g., in a population)**
  - **Irreducible uncertainty – can't reduce it by further knowledge**

- **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**

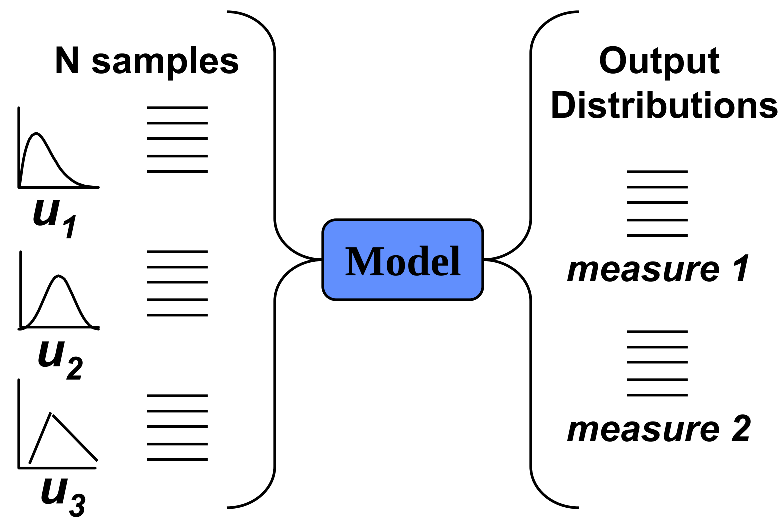
Uncertainty Quantification

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



Potential Goals:

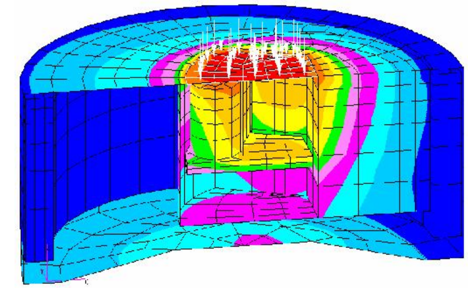
- based on uncertain inputs, determine variance of outputs and probabilities of failure (reliability metrics)
- identify parameter correlations/local sensitivities, robust optima
- identify inputs whose variances contribute most to output variance (global sensitivity analysis)
- quantify uncertainty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

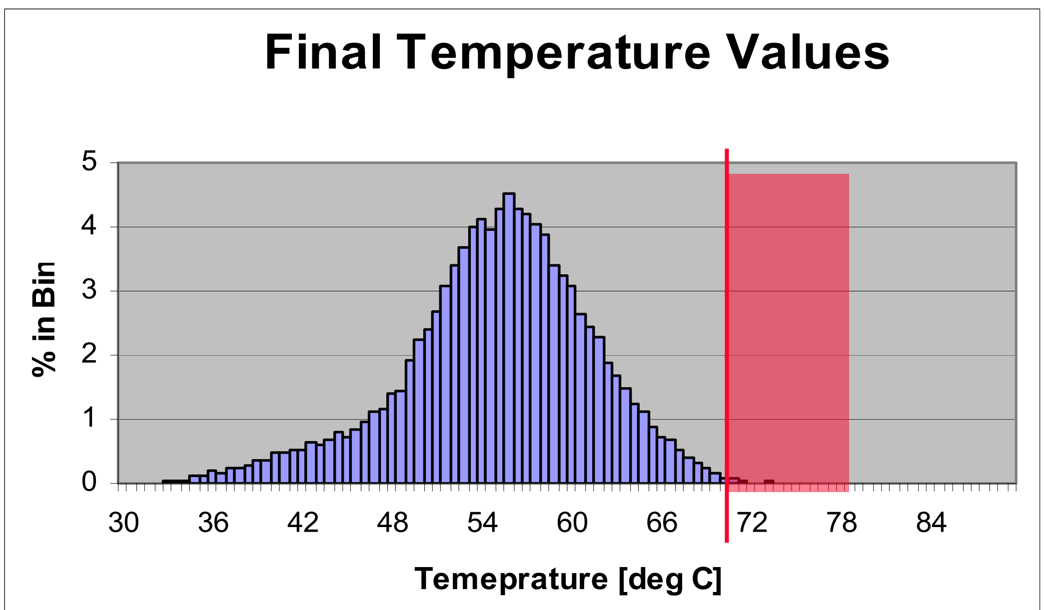


Typical method: Monte Carlo Sampling

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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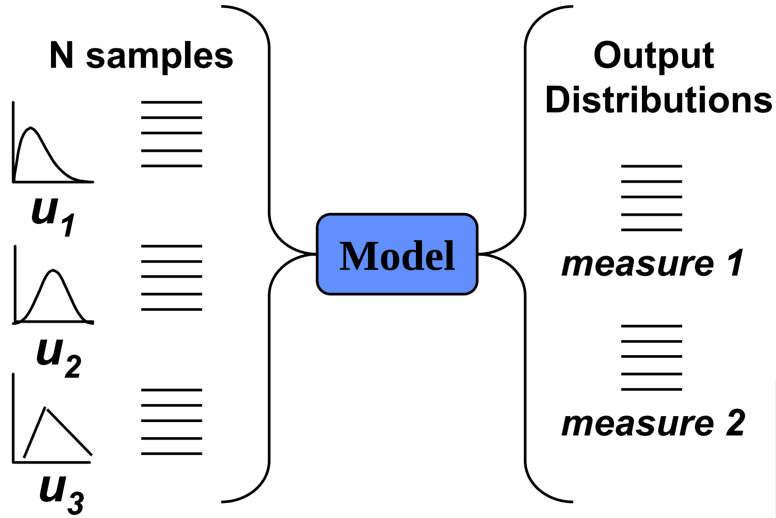
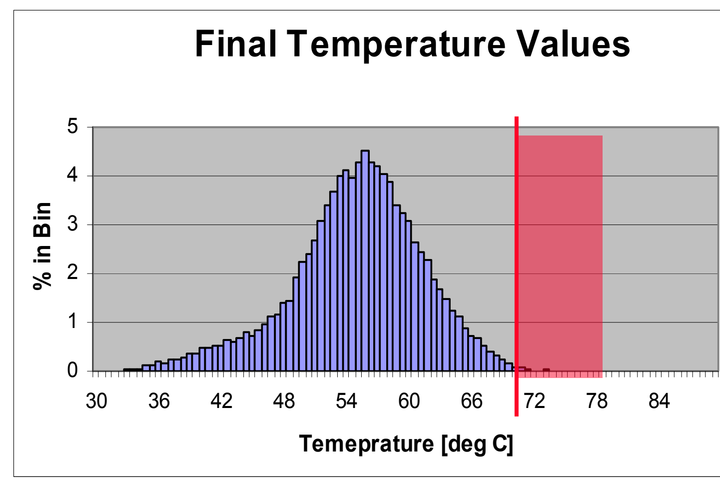
UQ: Sampling Methods

Given __distributions__ of $u_1,\ldots,u_N$, UQ methods…



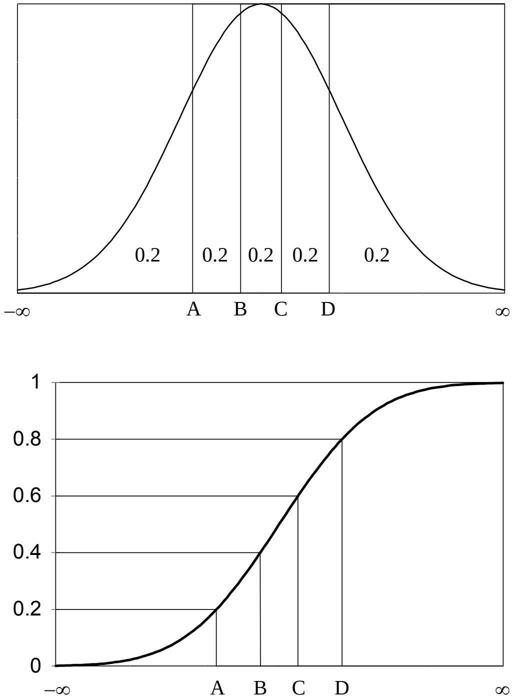
…calculate statistical info on outputs $T(u_1,\ldots,u_N)$



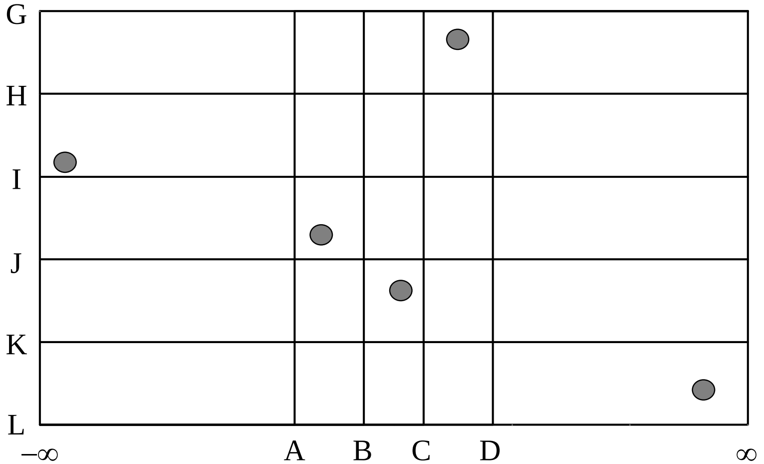
- **Monte Carlo sampling**
- **Quasi-Monte Carlo**
- **Centroidal Voroni Tessalation (CVT)**
- **Latin Hypercube sampling**

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**



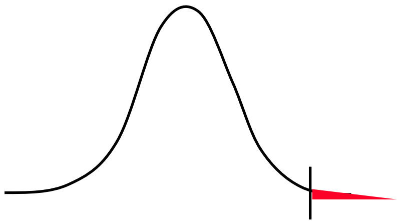
Intervals Used with a LHS of Size n = 5 in Terms of the pdf and CDF for a Normal Random Variable

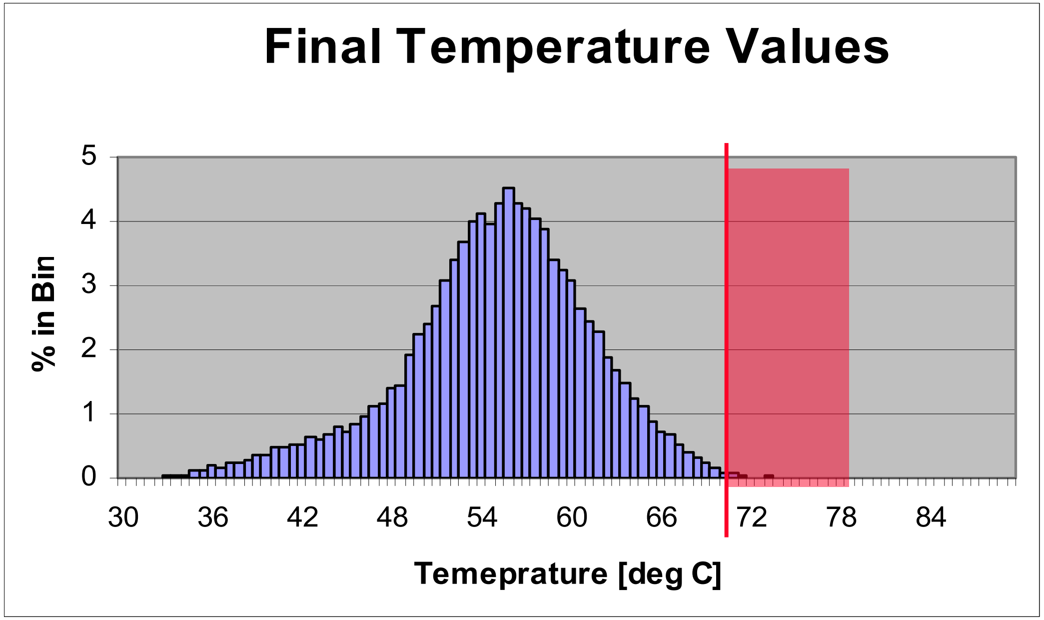


A Two-Dimensional Representation of One Possible LHS of size 5 Utilizing X1 (normal) and X2 (uniform)

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…**

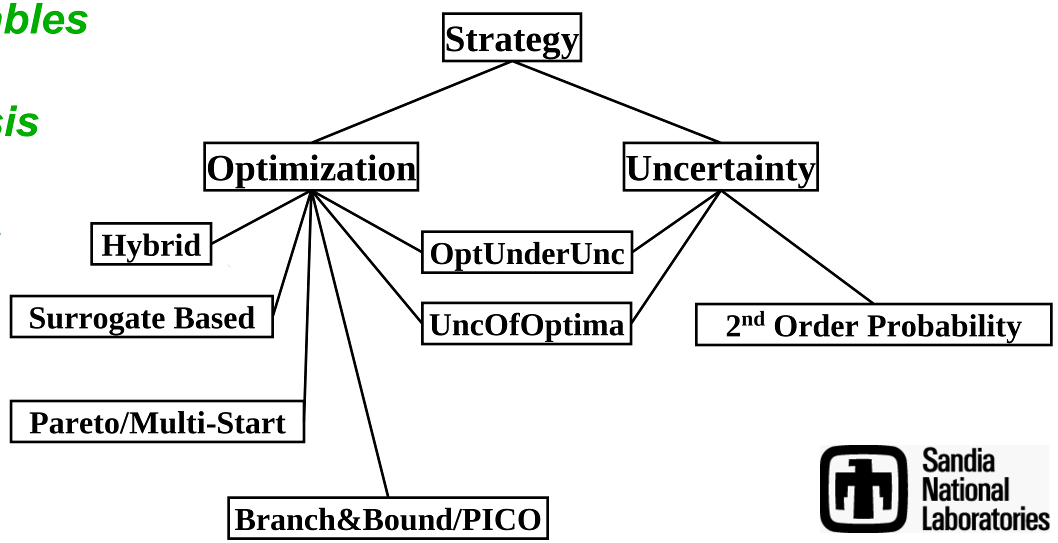
- **Or directly determine input variables which give rise to failure behaviors by solving an optimization problem.**

Alternatives to Sampling

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

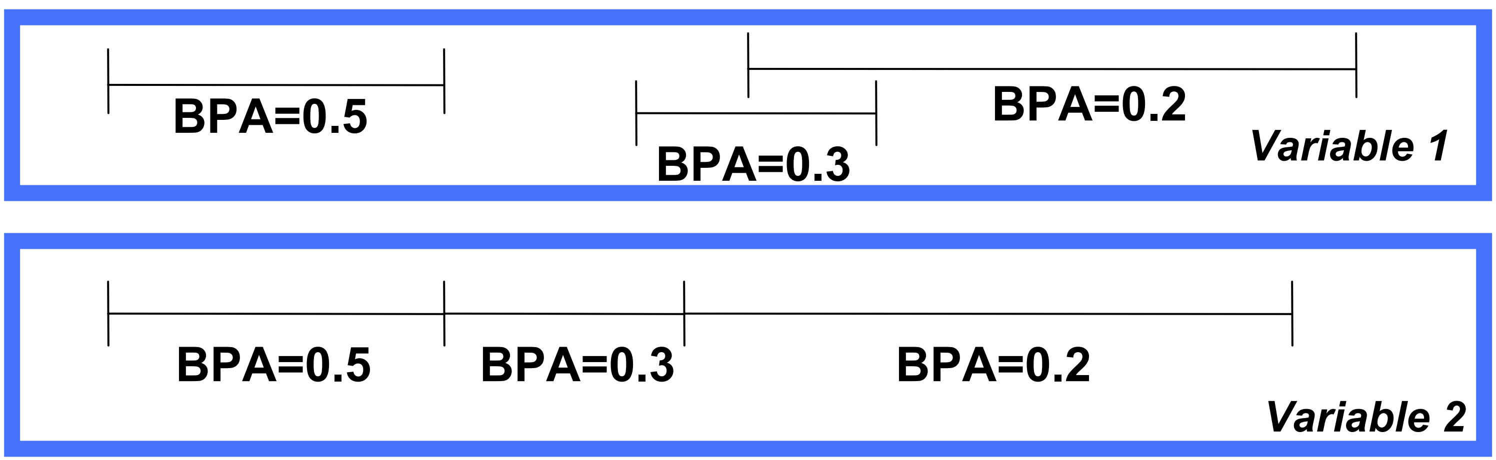
- **for a modest number of random variables, polynomial chaos expansions may converge considerably faster to statistics of interest**
- **if principal concern is with failure modes (tail probabilities), consider global reliability methods**

Upcoming (Mike): DAKOTA enables more efficient UQ by combining optimization, uncertainty analysis methods, and surrogate (meta-) modeling in a single framework.



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**



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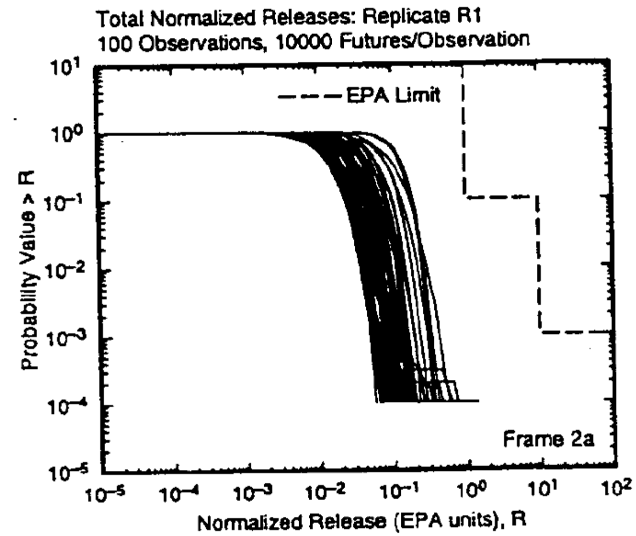
Propagating Epistemic UQ

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).

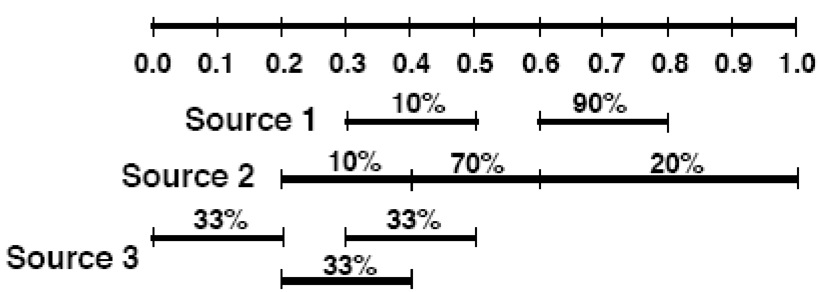


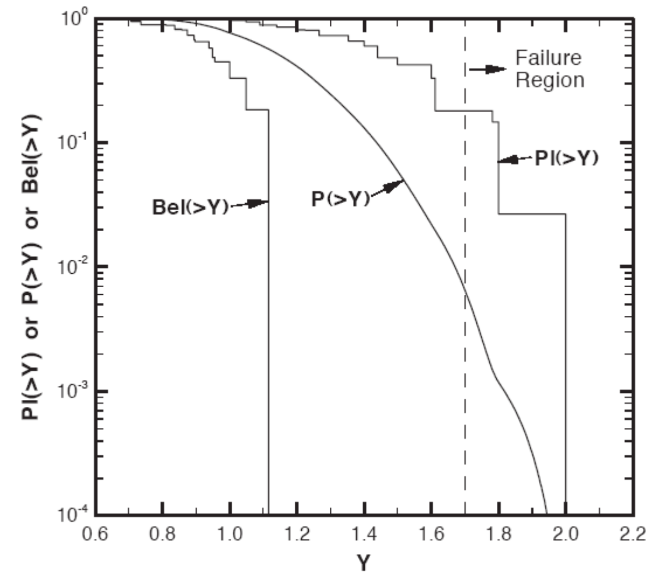
Dempster-Shafer theory of evidence

- Basic probability assignment (interval-based)

New

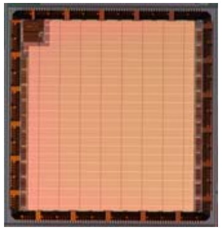
- Solve opt. problems (currently sampling-based) to compute belief/plausibility for output intervals



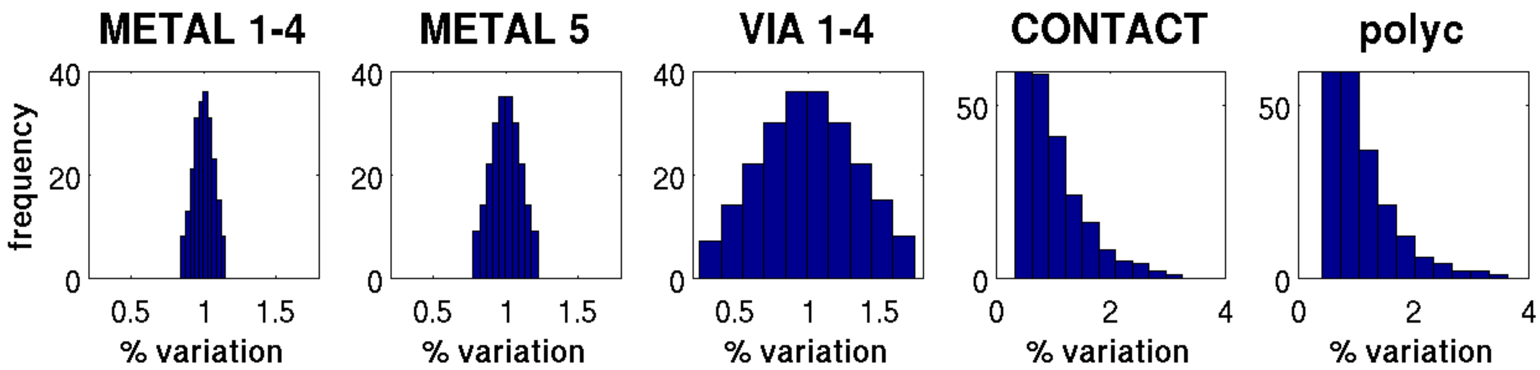


Circuit UQ Analysis

Use DAKOTA with Xyce circuit simulator to perform pre-fabrication uncertainty analysis of new CMOS7 ViArray



- ViArray: generic ASIC implementation platform
- Target applications: guidance, satellite, command & control
- Assess voltage droop/spike during photocurrent event
- Consider effect of process variation in each ‘layer’ on supply voltages; representative distributions:



- Truncated normals used for METAL and VIA; truncated lognormals used for CONTACT and polyc.

ViArray: Benefits of UQ

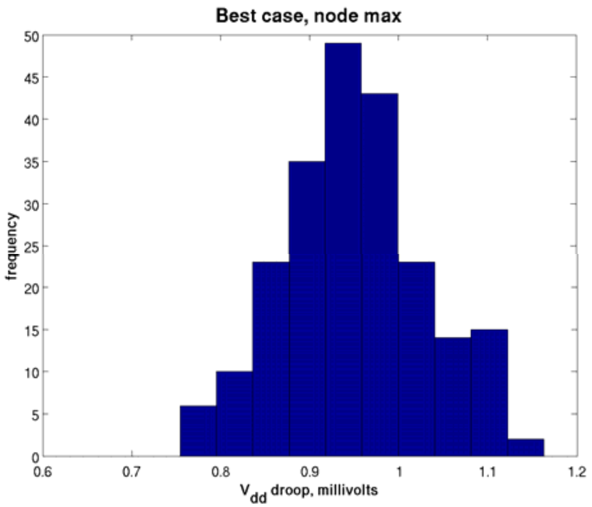
- One ensemble of UQ calculations used to determine most sensitive parameters and output ranges: determined that sensitivity depends on final chip configuration

- Suspicious UQ results led to correcting simulation failures not observed at nominal parameters

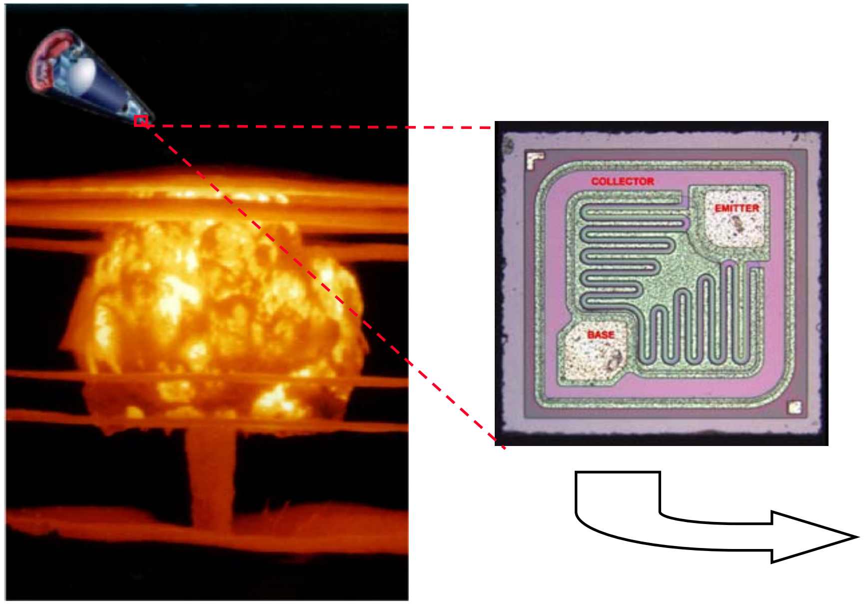
- Gave process engineers and circuit designers insight into possible circuit behaviors

- Sensitivity could help guide data collection

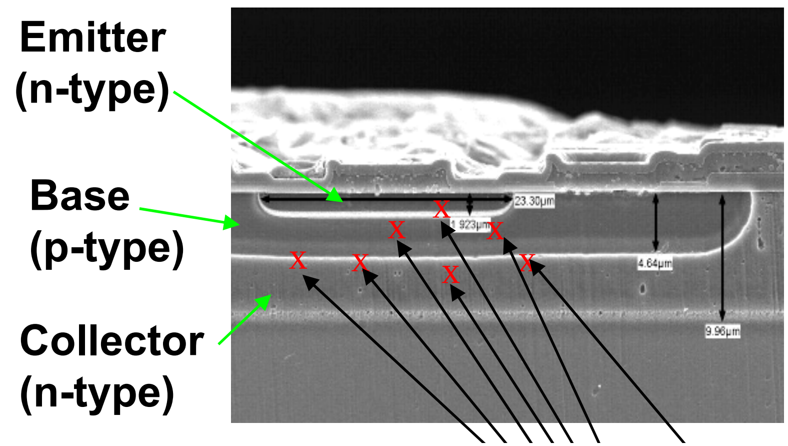
- Ongoing work: assess interaction of package parasitics with on-chip parasitics, V&V for photocurrent generation models



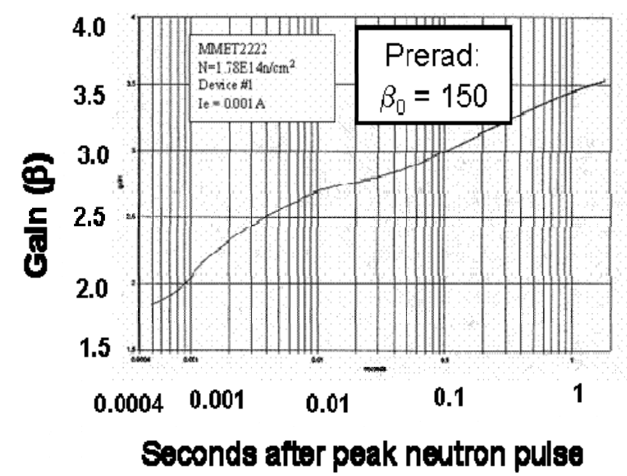
Neutron Radiation Exposure Degrades Electronics



neutrons create damage



damage degrades gain



- Military requirement: certify to hostile environment

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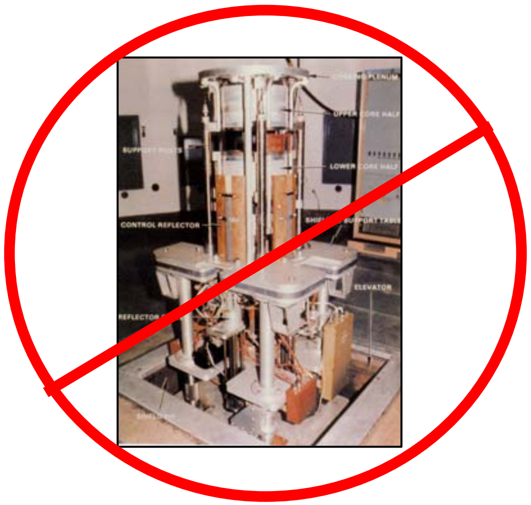
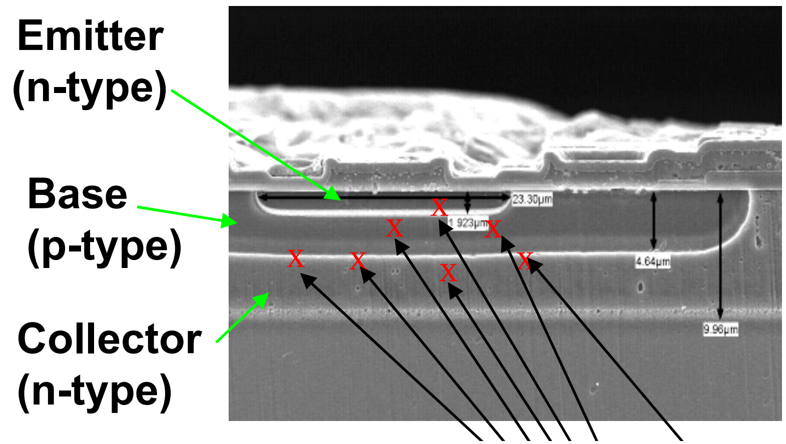
Neutron Radiation Exposure Degrades Electronics

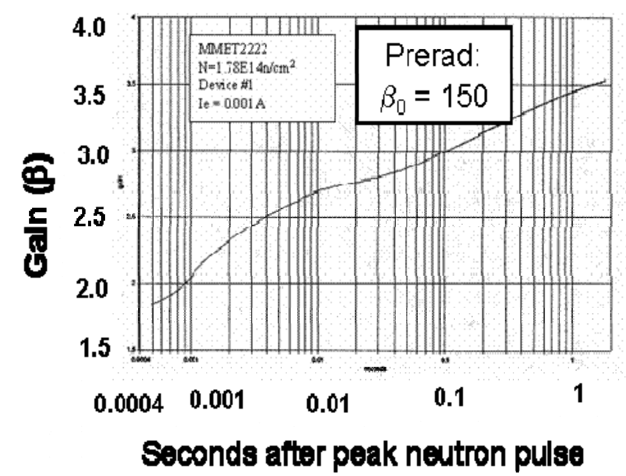


pass/fail testing

neutrons create damage



damage degrades gain



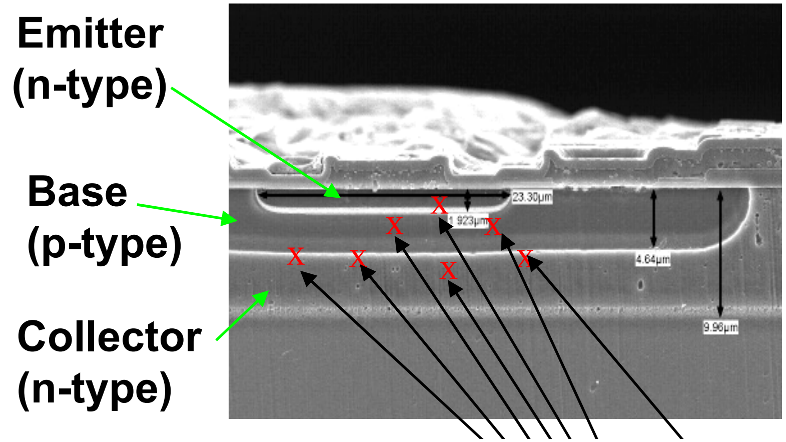
- **Military requirement: certify to hostile environment**
- **SPR dismantled end of FY06 to improve security posture**

Neutron Radiation Exposure Degrades Electronics

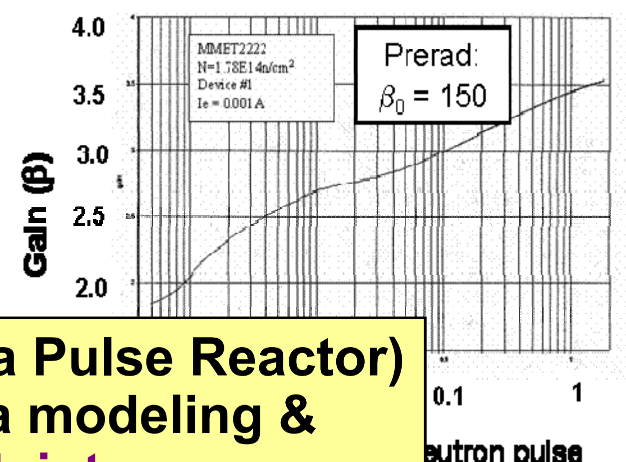
QASPR
QUALIFICATION ALTERNATIVES TO SPR

quantified uncertainty

neutrons create damage



damage degrades gain



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

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

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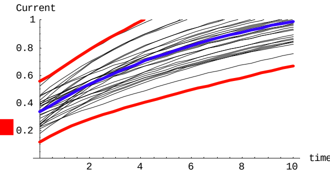
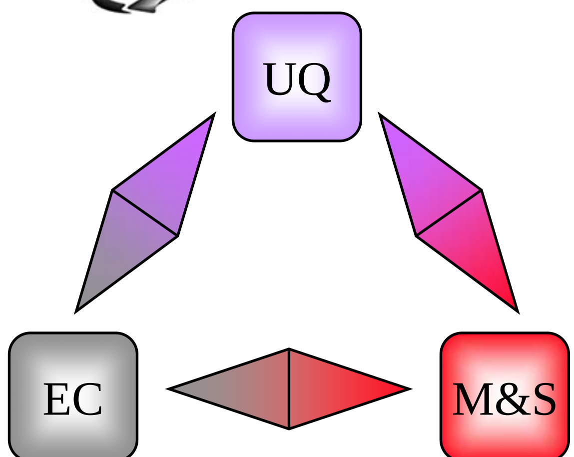
QASPR: Science-Based Engineering Methodology For Qualification

Risk Informed Decisions ⟵ ⟶ **Qualification Evidence**



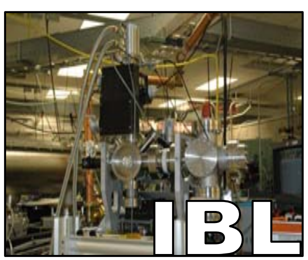
uncertainty quantification



validation

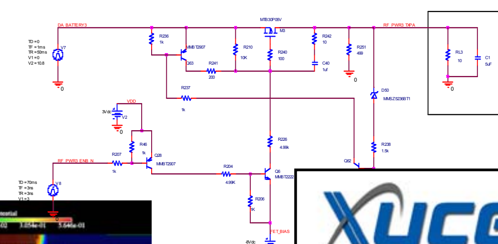
select experiments in alternate facilities

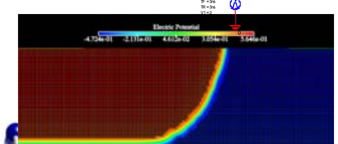
γ,n – 100 ms
long pulse

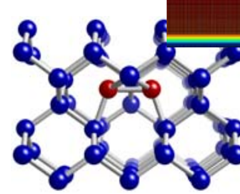


ion – 100 μs
short pulse

high performance, multi-fidelity, predictive computational modeling







Xyce PARALLEL ELECTRONIC SIMULATOR

CHARON

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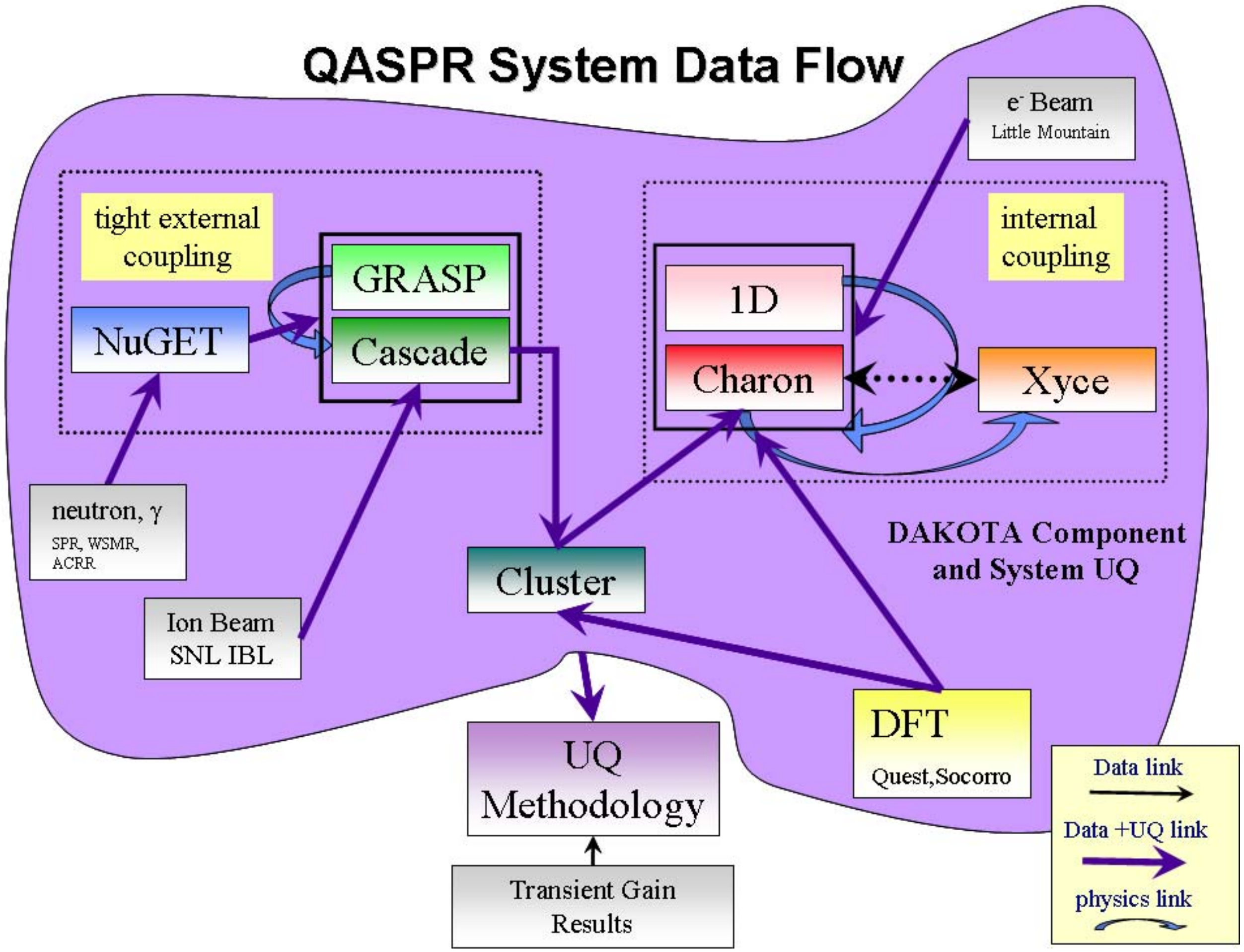
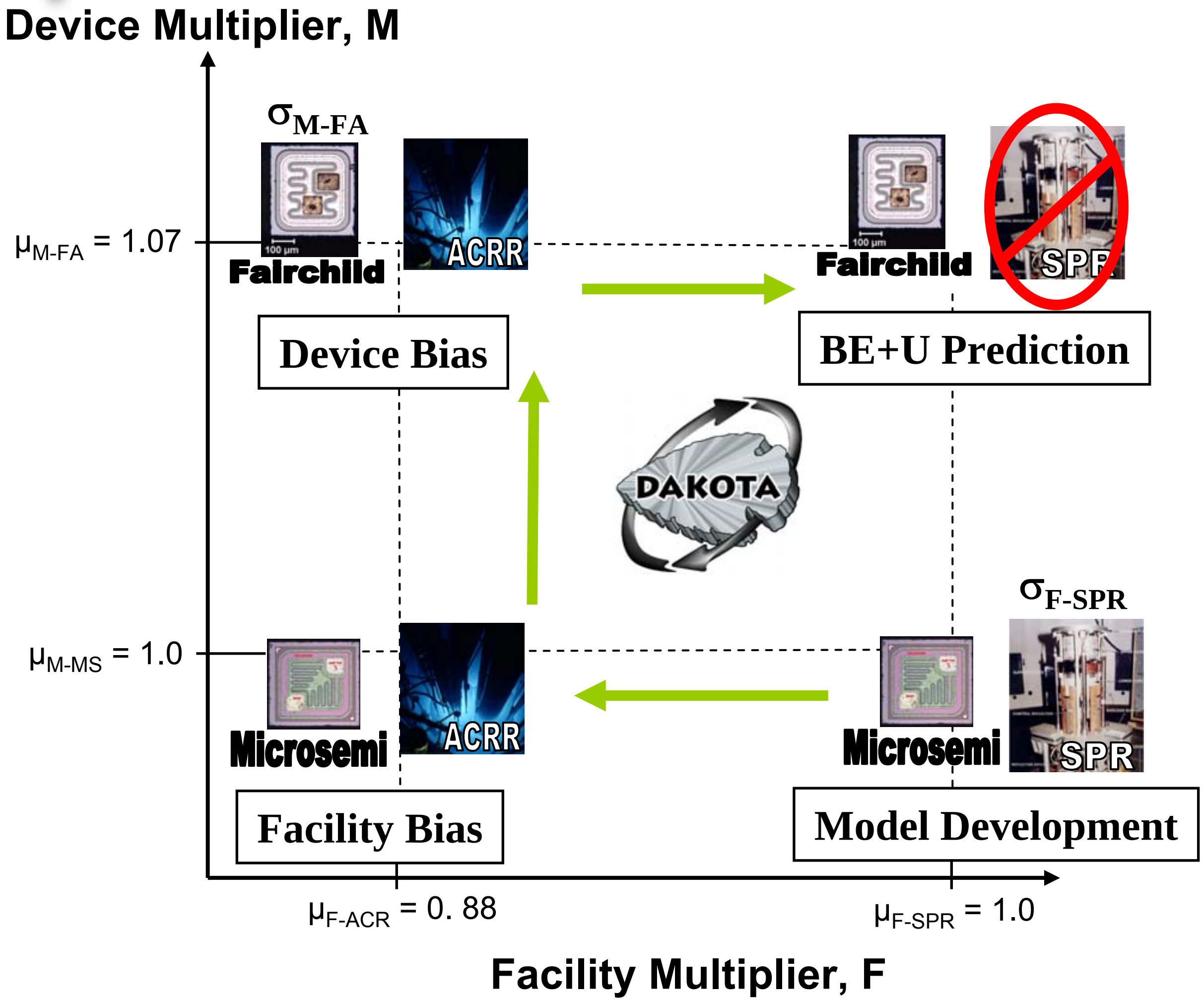
V&V for QASPR Components



- 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

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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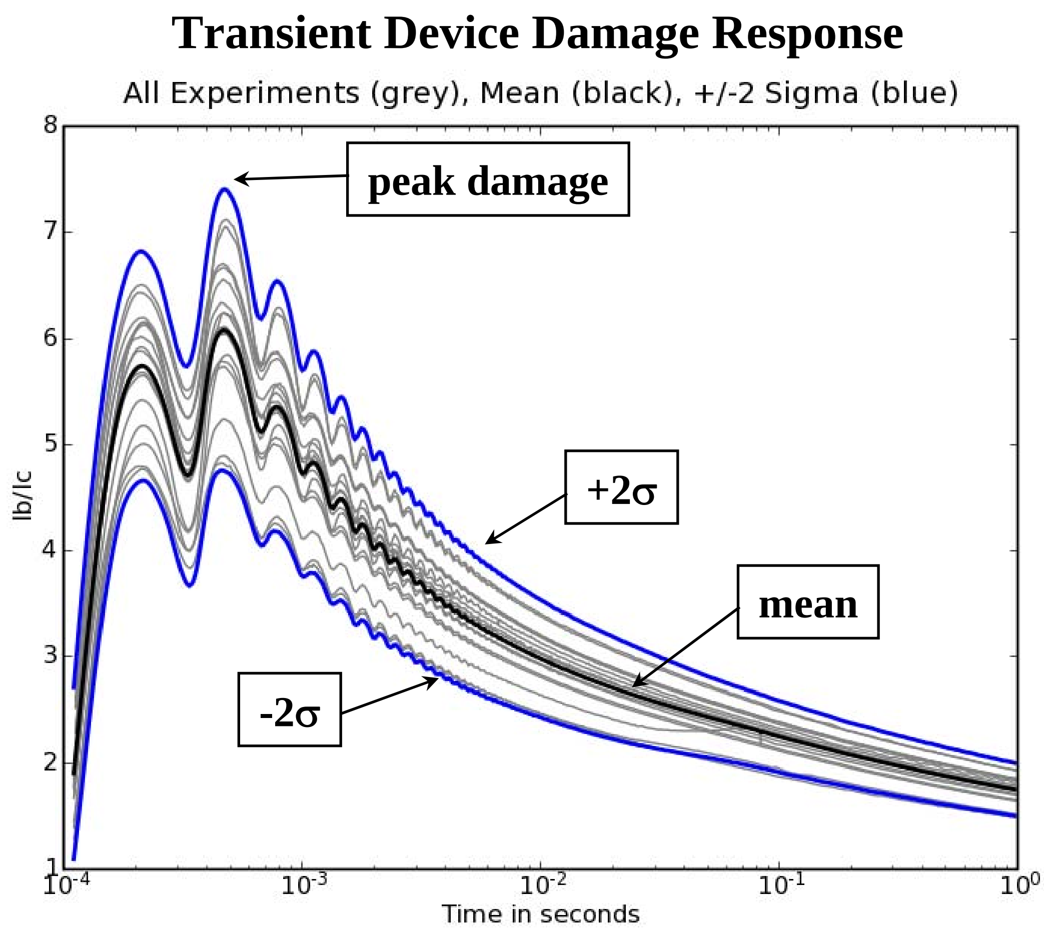
Model Validation: Blind Prediction

- 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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Model Validation: Blind Prediction

- **Fairchild response data within SPR hidden**
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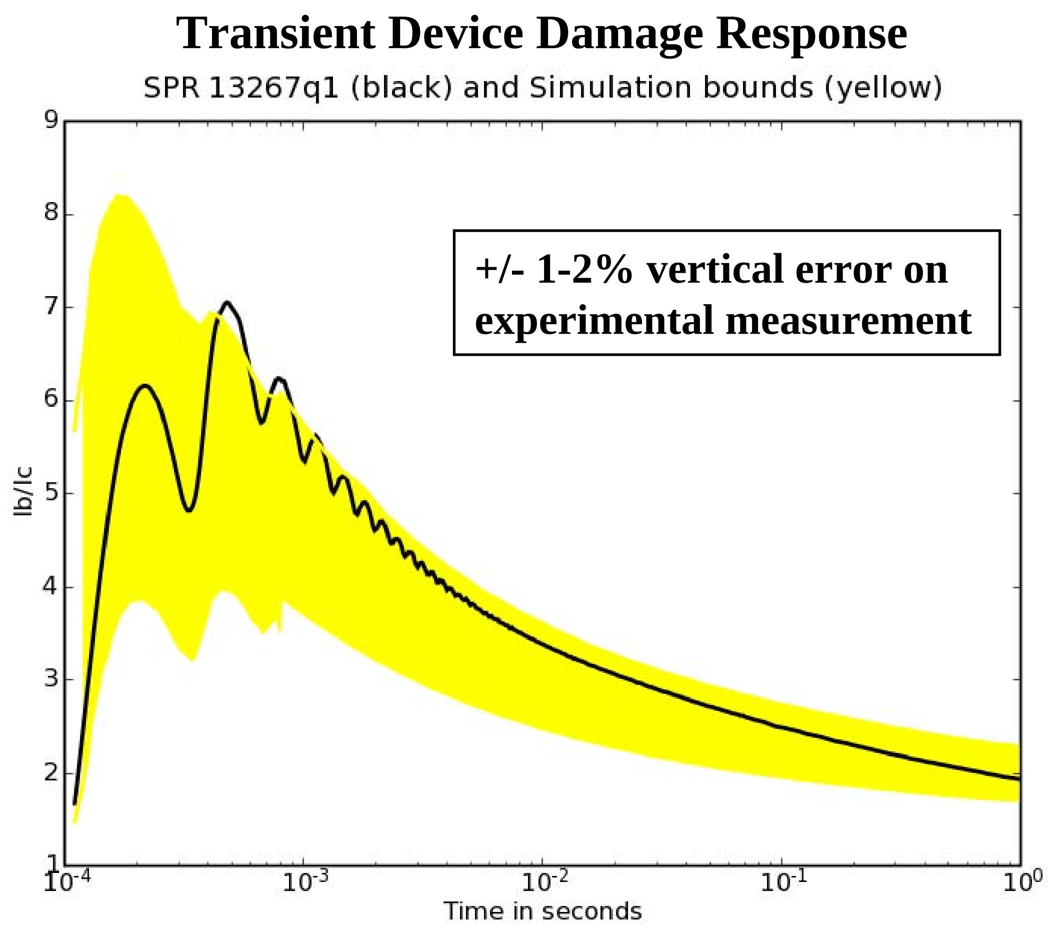

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Model Validation: Blind Prediction

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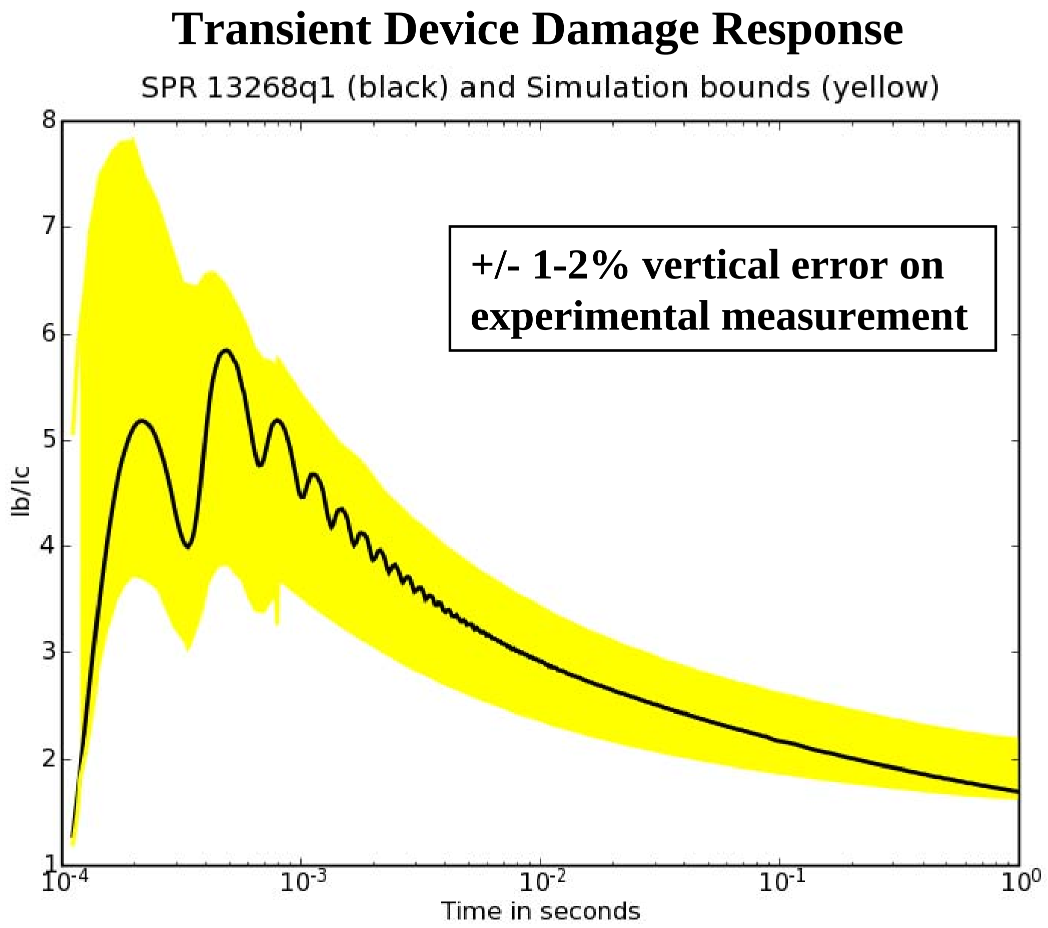

UQ algorithms have a critical role in system validation

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Model Validation: Blind Prediction

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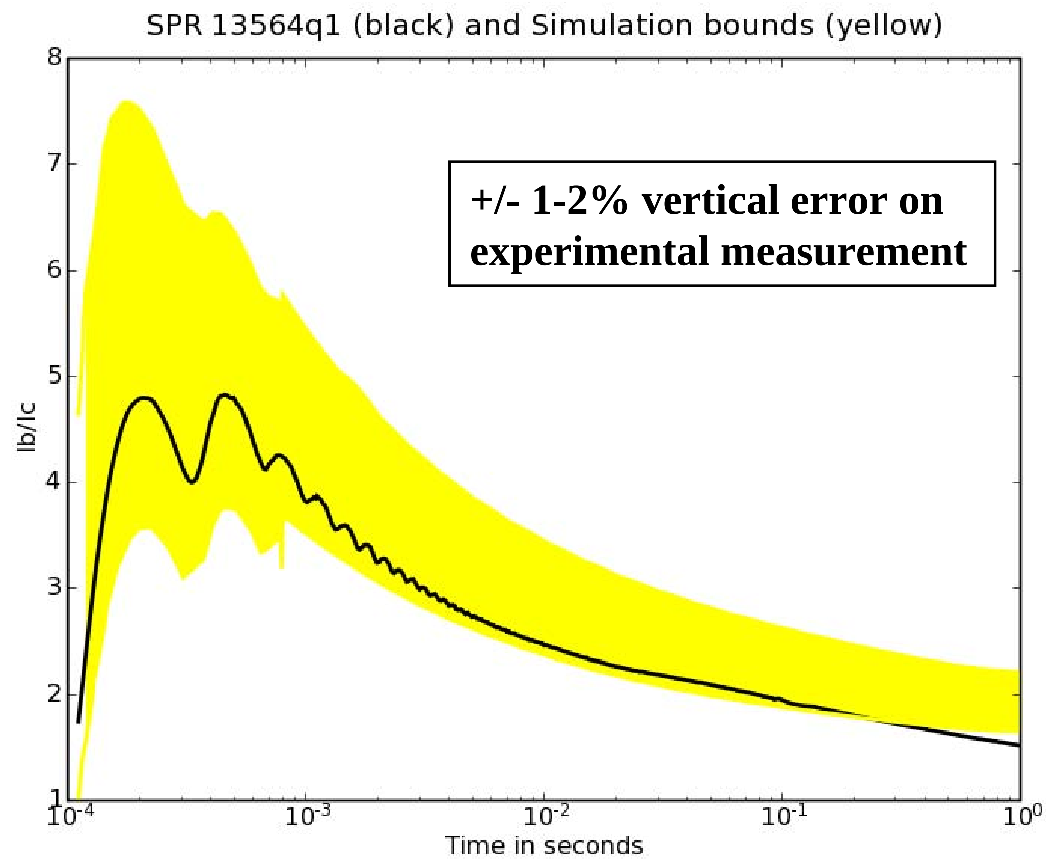
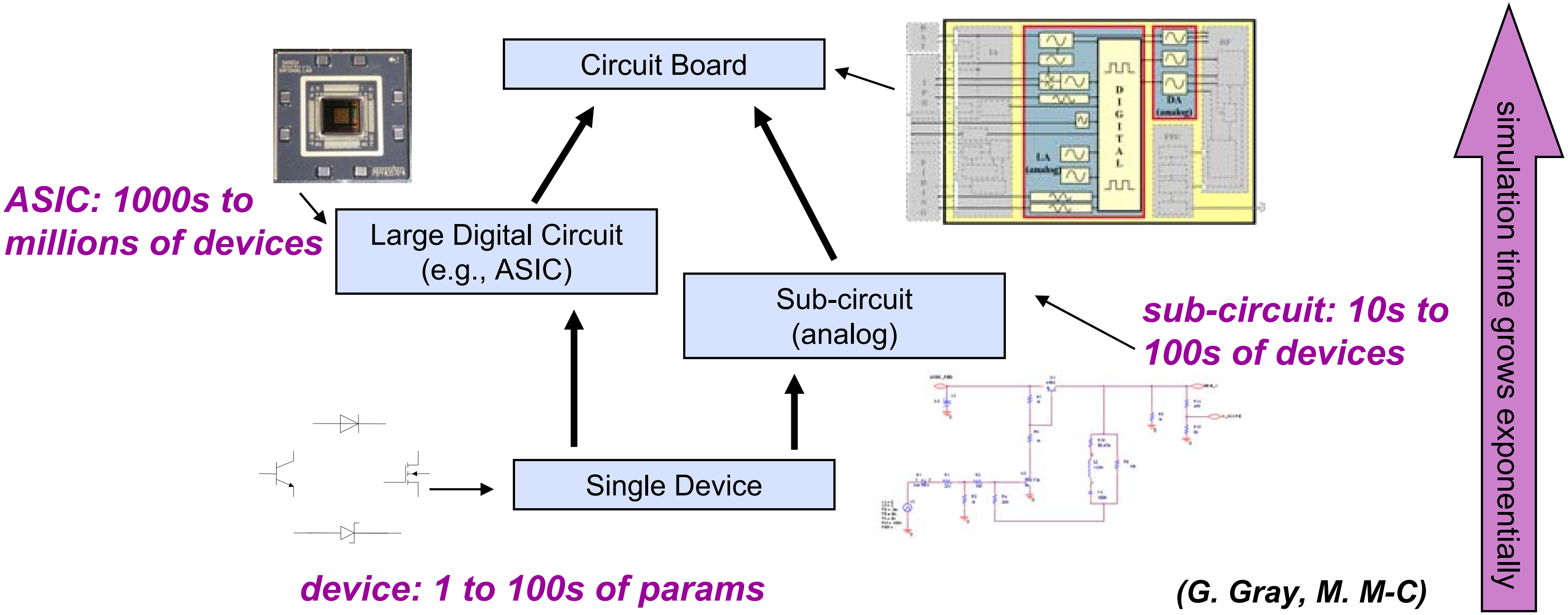
Transient Device Damage Response



UQ algorithms have a critical role in system validation

Electrical Modeling Complexity

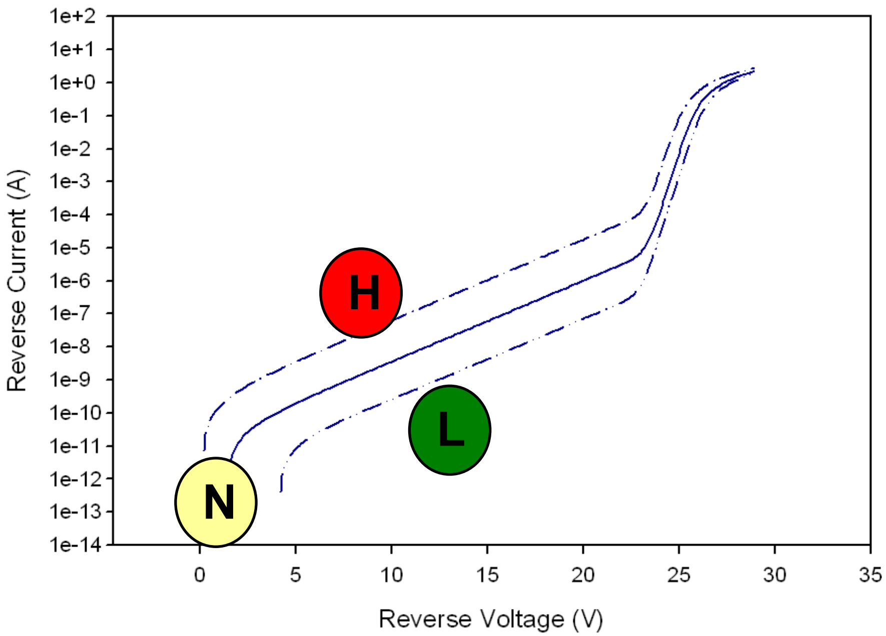
complex device models + replicates in circuits



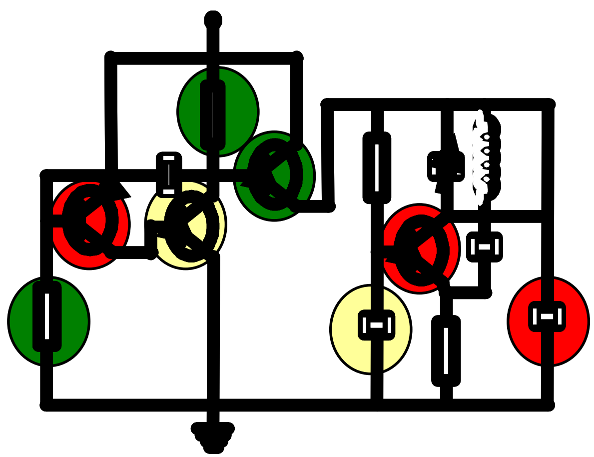
- **simple devices: 1 parameter, typically physical and measurable**
- **e.g., resistor @ 100Ω +/- 1%**
- **resistors, capacitors, inductors, voltage sources**

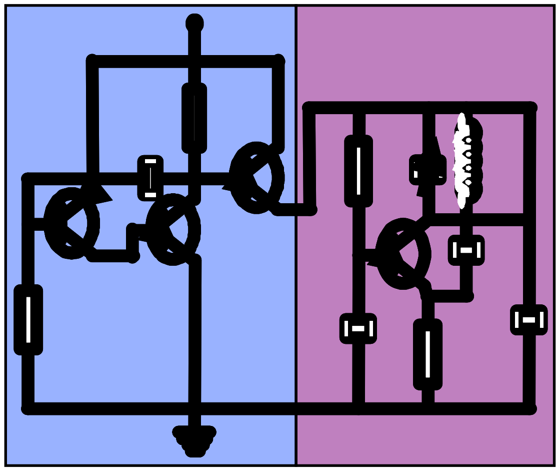
- **complex devices: many parameters, some physical, others "extracted" (calibrated)**
- **multiple modes of operation**
- **e.g., zener diode: 30 parameters, 3 bias states; many transistor models (forward, reverse, breakdown modes)**

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

To be credible, simulations must be verified, validated with data, and deliver a best estimate of performance, together with its degree of variability or uncertainty.

- **Formal V&V process helps certify credible simulation**
- **Uncertainty quantification algorithms are essential in validation and calibration under uncertainty**
- **Complex, large-scale simulations demand research in advanced efficient UQ methods**

Thank you for your attention!

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