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Uncertainty Quantification R&D with Applications to Nuclear Weapons

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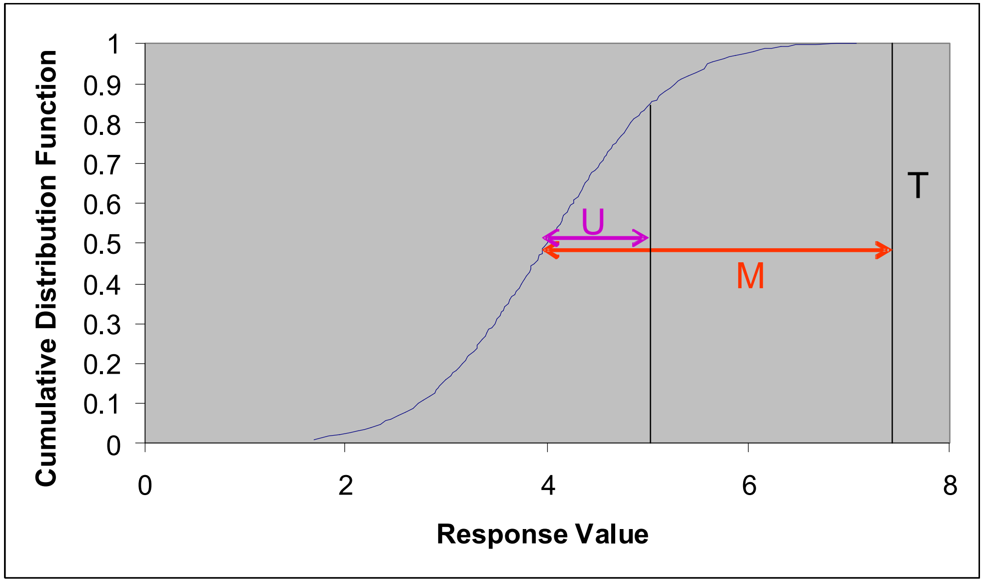
Regulatory Drivers

- In 2001, the National Nuclear Security Administration (NNSA) initiated development of a process designated Quantification of Margins and Uncertainty (QMU) for *the use of risk assessment methodologies* in the certification of the reliability and safety of the nation's nuclear weapons stockpile.

Distinguish between epistemic (incomplete knowledge, reducible), and aleatory (random) uncertainties



- JASON. *Quantifications of Margins and Uncertainties (QMU)*. JSR-04-3330. McLean, VA: The Mitre Corporation 2005.
- U.S. GAO (U.S. Government Accountability Office). *Nuclear Weapons: NNSA Needs to Refine and More Effectively Manage Its New Approach for Assessing and Certifying Nuclear Weapons*. GAO-06-261. Washington, DC: U.S. Government Accountability Office 2006.
- NNSA (National Nuclear Security Administration). *Nuclear Weapon Assessments Using Quantification of Margins and Uncertainties Methodologies*. NNSA Policy Letter: NAP-XX, Draft 5/1/07. Washington, DC: 2007.

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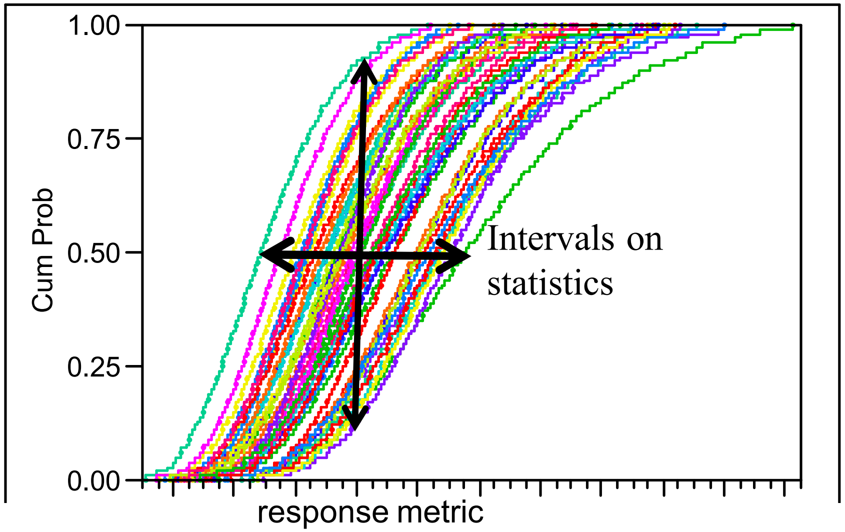

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Uncertainty Quantification Research

Challenge: Maximize accuracy of UQ results while minimizing total cost of computations

Black-Box

Workhorse

- Sampling Methods
  - Latin Hypercube Sampling
- Reliability Methods

Current R&D Focus

- Stochastic Expansion*
- Interval Analysis*
- Second-order Probability*
- Dempster-Shafer

Implemented in DAKOTA

NOT a “one-size fits all” approach

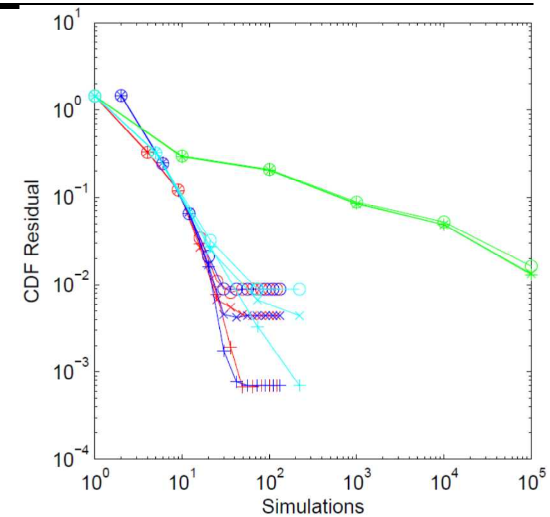
Embedded

- Automatic Differentiation (Sacado)*
- Adjoint Methods
- Stochastic Expansion (Stokhos)
- Trilinos provides growing support for embedded UQ methods

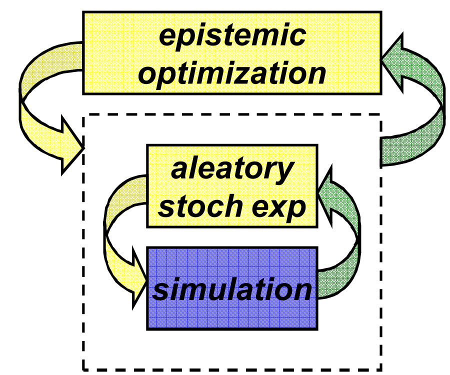
*Covered in review talks the past two years

Uncertainty Quantification Research

- **Stochastic expansion:**
  - dimension adaptive methods, anisotropic Smolyak sparse grids
  - numerically generated orthogonal polynomials
  - Sobol’ sensitivity indices (variance-based)
- **New capabilities for “mixed” epistemic/aleatory uncertainty:**
  - Estimate bounding intervals using local or global optimization methods
- **Surrogate or metamodel construction (Surfpack)**
  - Use of Gaussian process emulators in both UQ and optimization
- **Other**: Bayesian calibration, collaborations with LANL, UT; ASCR projects



Convergence Plot for Stochastic Expansion



Mixed UQ using optimization in the nested process

W87 Abnormal Thermal UQ

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W87 Abnormal: Thermal Race Margin

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QASPR Predictions of Circuit Voltages

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System Generated ElectroMagnetic Pulse

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Summary

- The CIS has an active UQ research and development program.
- Research areas:
  - embedded UQ
  - adaptive black-box methods
  - multi-scale/multi-physics UQ
  - Bayesian approaches
- UQ is not a "one size fits all" problem, R&D in a variety of methods needed.
- DAKOTA is frequently used on our high performance computers to run UQ studies for weapons applications.
- Our current milestones and UQ efforts are building up to the B-61 Life Extension Program, which is a very important deliverable for Sandia.

Innovation and Implementation in UQ

Impact for NW

Extra slides

Uncertainty Quantification Research

Challenge: Maximize accuracy of UQ results while minimizing total cost of computations

- Sampling Methods: Monte Carlo, Latin Hypercube, quasi MC
- Reliability Methods: Focus on finding the probability of failure by transforming the UQ problem to an optimization problem.
- Stochastic Expansion: Represent the uncertain output as a stochastic process, specifically as a spectral expansion in terms of suitable orthogonal polynomials (e.g. Polynomial Chaos)
- Interval Analysis: Given interval bounds on the inputs, determine interval bounds on the outputs (optimization vs. sampling)
- Second-order Probability: Epistemic “outer loop” and aleatory “inner loop”
- Dempster-Shafer: Propagate “evidence structures” on inputs to outputs. This results in two output measures: plausibility and belief.

We have all of these methods implemented in the DAKOTA optimization/UQ toolkit

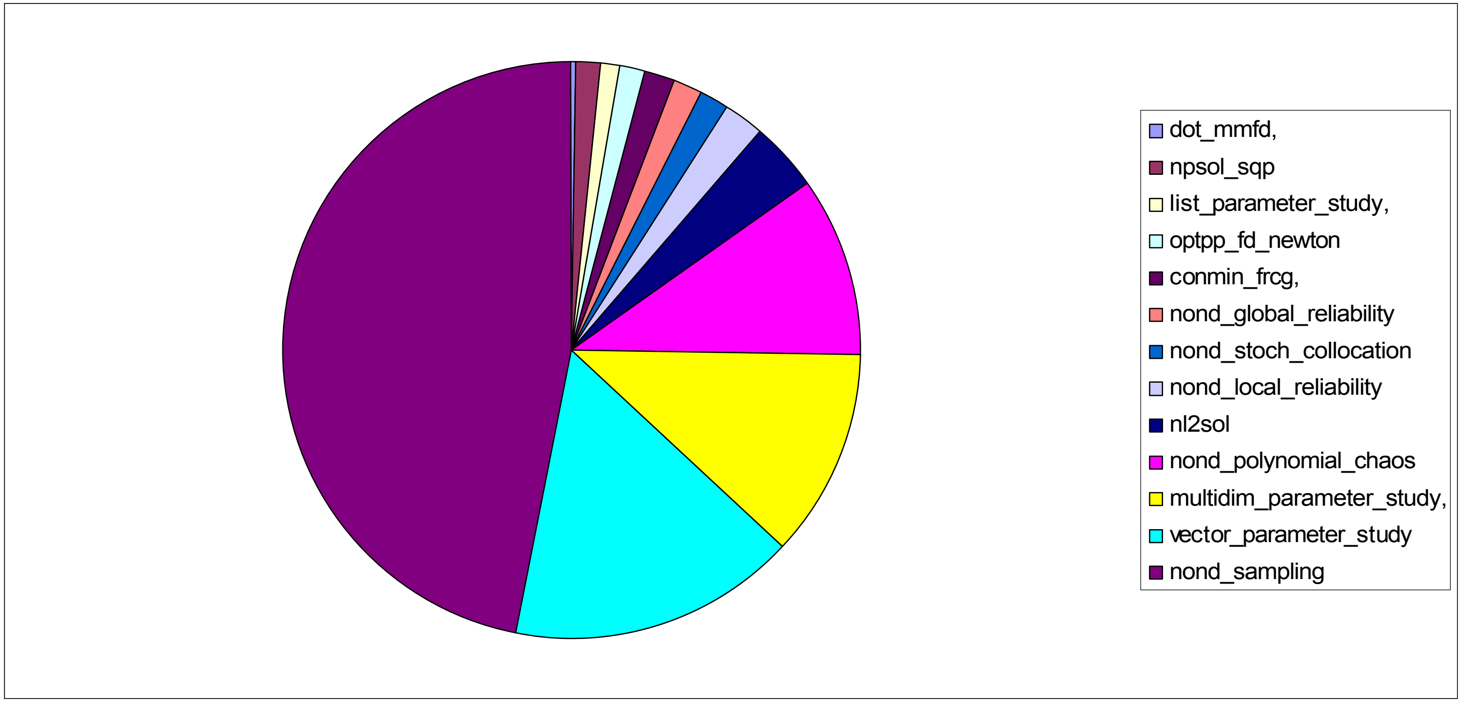
Selected UQ Recent Publications

- **Sampling Methods:** Swiler, L.P. and West, N.J., "Importance Sampling: Promises and Limitations," AIAA 2010-2850 at *51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference,* Orlando, FL, Apr 12-15, 2010.
- **Reliability Methods:** Bichon, B.J., Eldred, M.S., Swiler, L.P., Mahadevan, S., and McFarland, J.M., "Efficient Global Reliability Analysis for Nonlinear Implicit Performance Functions," *AIAA Journal*, Vol. 46, No. 10, October 2008, pp. 2459-2468.
- **Stochastic Expansion:** Eldred, M.S., "Recent Advances in Non-Intrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Analysis and Design," paper AIAA-2009-2274 in Proceedings of the 50th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Palm Springs, CA, May 4-7, 2009.
- **Interval Analysis:** Eldred, M.S., Swiler, L.P., and Tang, G., "Mixed Aleatory-Epistemic Uncertainty Quantification with Stochastic Expansions and Optimization-Based Interval Estimation," (in review) *Reliability Engineering and System Safety (RESS)*.
- **Second-order Probability:** Jakeman, J., Eldred, M.S., and Xiu, D., "A Numerical Approach for Quantification of Epistemic Uncertainty," *Journal of Computational Physics (JCP),* Vol. 229, No. 12, June 2010, pp. 4648-4663.
- **Dempster-Shafer:** Tang, G., Swiler. L.P., and Eldred, M.S., "Using Stochastic Expansion Methods in Evidence Theory for Mixed Aleatory-Epistemic Uncertainty Quantification," in *51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference* Orlando, FL, Apr 12-15, 2010.

Sandia, led by CIS, has an active research agenda in UQ.

DAKOTA Usage by Method

- **92% of DAKOTA invocations on SNL clusters over 2 month period (Jan-Feb. 2010) were UQ or parameter studies**



External DAKOTA Use:

- **Unique external download *registrations*** over project life: 6411
- ***Actual source and binary downloads*** May 2009 – April 2010: 3419

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Introduction:
Risk-informed Decision Making, QMU, and UQ

In order to support risk-informed decision making using modeling and simulation, the following key elements are required:

- ***Predictive simulations:*** **verified and validated for application of interest**
- ***Quantified uncertainties:*** **the effect of random variability is fully understood**

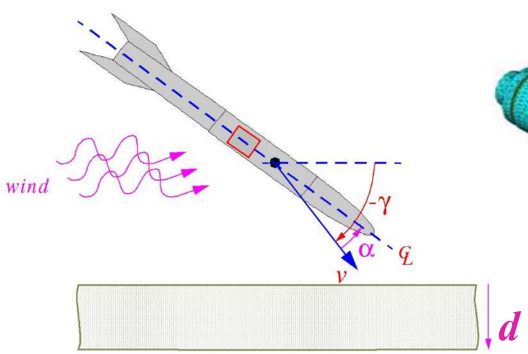
Formal DOE process for Quantification of Margins and Uncertainties (QMU): process of providing *best estimate* + *uncertainty* in the decision context

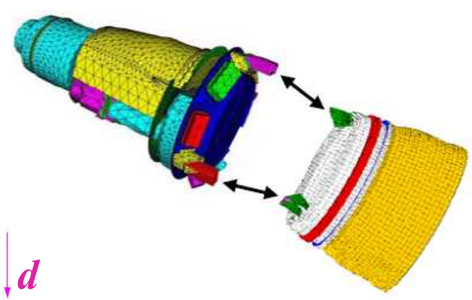
Uncertainty Quantification

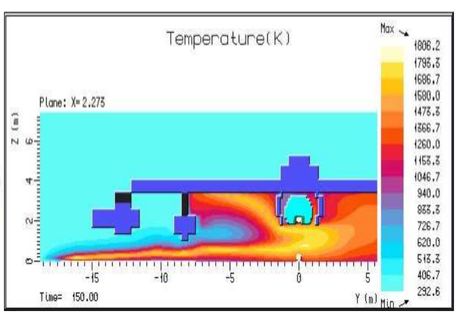
Critical component of QMU: credible M&S capability for stockpile stewardship

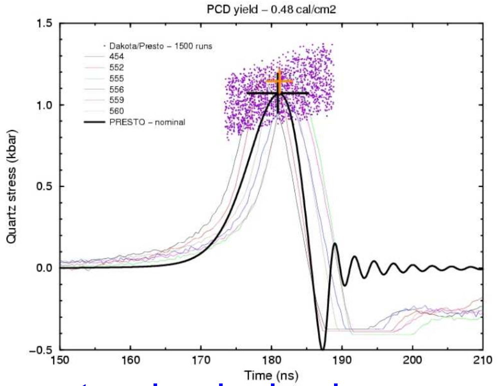
Uncertainty can be categorized to be one of two different types:

- **Aleatory/irreducible:** inherent variability with sufficient data → probabilistic models
- **Epistemic/reducible:** uncertainty from lack of knowledge → nonprobabilistic models









Uncertainty applications: penetration, joint mechanics, abnormal environments, shock physics, …

Uncertainty Quantification Algorithms @ SNL: New methods bridge robustness/efficiency gap

	Production	New	Under dev.	Planned	Collabs.
Sampling	Latin Hypercube, Monte Carlo	Importance, Incremental		Bootstrap, Jackknife	FSU
Reliability	*Local:* Mean Value, First-order & second-order reliability methods (FORM, SORM)	*Global:* Efficient global reliability analysis (EGRA)			*Local:* Notre Dame, *Global:* Vanderbilt
Stochastic expansion		Traditional & Tailored polynomial chaos & stochastic collocation	Golub-Welsch numerical polynomials (arbitrary input PDFs)	anisotropic sparse grid, cubature, adaptivity	USC, VPISU, Stanford, CU Boulder, Purdue, Illinois
Other probabilistic		Random fields/ stochastic proc.		Dimension reduction	Cornell, Maryland
Epistemic	Second-order probability (nested sampling)	Dempster-Shafer, Opt-based interval estimation	Bayesian	Imprecise probability	LANL, Applied Biometrics
Metrics	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		UNM

Additional Tailoring

Highlights of Foundational UQ

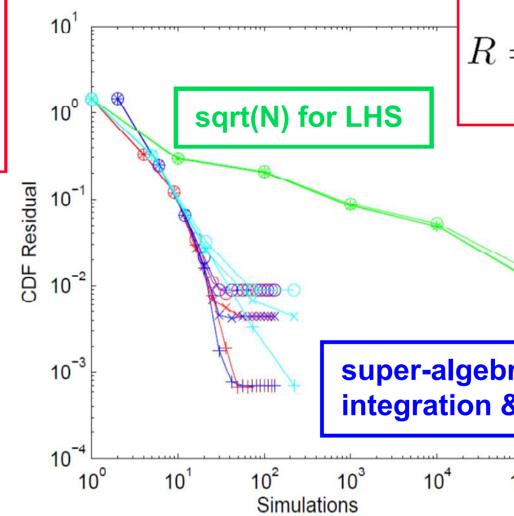
Stochastic expansions:

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

- *Polynomial chaos expansions (PCE)*: known basis, compute coefficients
- (Lagrange) *Stochastic collocation (SC)*: known coefficients, form interpolant

$$R = \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

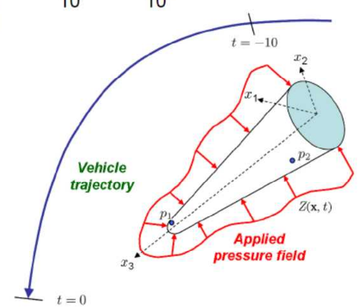
- Tailoring → fine-grained algorithmic control:
  - Synchronize PCE form with numerical integration
  - Optimal basis & Gauss pts/wts for arbitrary input PDFs
  - Anisotropic approaches: emphasize key dimensions
- h/p-adaptive collocation (FY09-FY10)



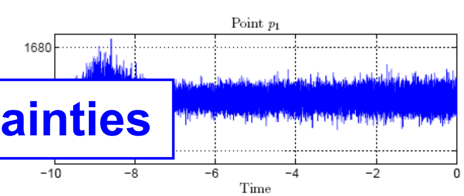
Epistemic UQ:

- Refinements to GP-based adaptive approaches → EGO, EGRA, *EGIE* (global opt-based interval est.)
- PCE/SC extensions for epistemic variables

Random Fields / Stochastic Processes (RF/SP):



- New library: Parallel Environment for Creation Of Stochastics (PECOS)
- Complex random environments (fluctuating pressure field for reentry)
  - Gaussian stationary RF/SP (iFFT: Shinozuka-Deodatis, Grigoriu)
  - Non-Gaussian, non-stationary RF/SP; K-L, memory saving approaches



Smart adaptive methods for handling complex uncertainties

Generalized Polynomial Chaos Expansions

Approximate response w/ spectral proj. using orthogonal polynomial basis fns

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

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

- Nonintrusive: estimate α_j using sampling (expectation), pt collocation (regression), tensor-product quadrature or Smolyak sparse grids (numerical integration)

Wiener-Askey Generalized PCE

- Tailor basis: optimal basis selection leads to exponential conv 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 type/order/range: TP or TO PCE, h/p-adapt based on PCE error est.
  - Dimension p-refinement: anisotropic quadrature/sparse grid
  - Dimension h-refinement: discretization of random domain

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Stochastic Collocation
(based on Lagrange interpolation)

$$L_i = \prod_{\substack{j=1 \\ j\neq i}}^{m} \frac{x - x_j}{x_i - x_j}$$

Instead of estimating coeffs for known basis fns,
form interpolants for known coefficients

$$R = \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

$$\boldsymbol{R} = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n}\right)$$

Form sparse interpolant using Σ of tensor products (same as forming sparse grid)

Key is use of same Gauss points/weights from the orthogonal polynomials
for specified input PDFs → same exponential convergence rates

Advantages relative to PCE:

- Simpler (no expansion order)
- Adapts to integration approach / collocation pt set:
  doesn't over-/under-integrate a (nonsynchronized) expansion
- Estimating moments of any order is easy: $E[R^k] = \Sigma\, r^k_j\, w_j$
  (formation of interpolant only reqd for CDF sampling)
- No intrusive variant:
  intrusive approach decouples into collocation

$$\mu_R = \sum_{j=1}^{N_p} r_j w_j$$

$$\sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2$$

Disadvantages relative to PCE:

- Requires structured data sets: quadrature/sparse grid (cubature?), no random sets
- Expansion variance not guaranteed positive, no analytic VBD

Tailoring of Polynomial Chaos Expansions

$$R = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi})$$ ⇒ $$\Psi_j(\boldsymbol{\xi}) = \prod_{i=1}^{n} \psi_{m_i^j}(\xi_i)$$ ⇒ **Multi-index length & content**

Tensor-product

$$\begin{aligned}
\Psi_0(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_0(\xi_2) &&= 1\\
\Psi_1(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_0(\xi_2) &&= \xi_1\\
\Psi_2(\boldsymbol{\xi}) &= \psi_2(\xi_1)\,\psi_0(\xi_2) &&= \xi_1^2 - 1\\
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\Psi_5(\boldsymbol{\xi}) &= \psi_2(\xi_1)\,\psi_1(\xi_2) &&= (\xi_1^2 - 1)\xi_2\\
\Psi_6(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_2(\xi_2) &&= \xi_2^2 - 1\\
\Psi_7(\boldsymbol{\xi}) &= \psi_1(\xi_1)\,\psi_2(\xi_2) &&= \xi_1(\xi_2^2 - 1)\\
\Psi_8(\boldsymbol{\xi}) &= \psi_2(\xi_1)\,\psi_2(\xi_2) &&= (\xi_1^2 - 1)(\xi_2^2 - 1)
\end{aligned}$$

$$N_t = 1 + P = \prod_{i=1}^{n} (p_i + 1)$$

Total-order

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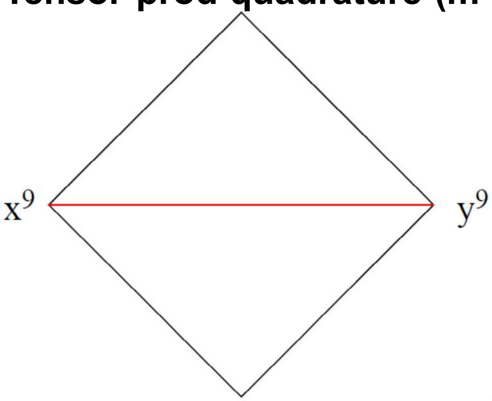
\Psi_5(\boldsymbol{\xi}) &= \psi_0(\xi_1)\,\psi_2(\xi_2) &&= \xi_2^2 - 1
\end{aligned}$$

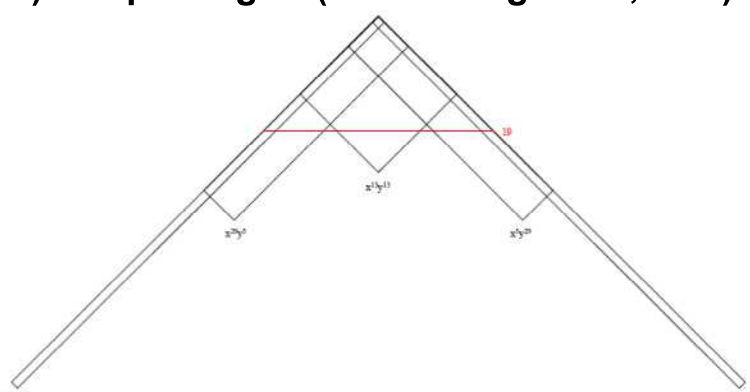
$$N_t = 1 + P = 1 + \sum_{s=1}^{p} \frac{1}{s!} \prod_{r=0}^{s-1} (n + r) = \frac{(n+p)!}{n!\,p!}$$

Monomial coverage

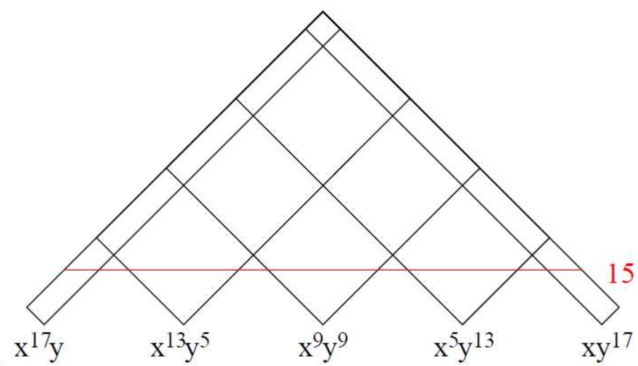
Tensor-prod quadrature (m=5)



Sparse grid (nonlinear growth, w=4)



Sparse grid (linear growth, w=4)



Traditional PCE: **total-order p = m-1**
Tailored PCE: **tensor-product p = m-1**

Traditional PCE: **heuristic total-order**
Tailored PCE: **synchronized total-order**

UQ Remarks

UQ R&D: New methods bridge critical gap → reliability of LHS at much lower cost

Comparison of Stochastic Expansion Methods

- Nonintrusive PCE: known basis, compute coefficients (sampling, regression, TPQ, SSG)
- SC: known coefficients, compute interpolant (TPQ, SSG)
- SC outperforms traditional PCE using numerical integration due, at least in part, to nonoptimal PCE expansion/integration synchronization
- Tailoring of PCE closes, and in some cases eliminates, performance gap
  - TPQ: tailored tensor-product PCE identical to SC
  - Nonlinear SSG: tailored total-order PCE more reliable than heuristics & more efficient than trial & error, but performance falls well short of SC
  - Linear SSG: linear growth for Gaussian non-/weakly-nested reduces integrable monomial set not appearing in expansion and closes gap with SC. Don't use nonlinear growth unless fully nested!
- In no direct comparison does nonintrusive PCE outperform SC. PCE motivated by flexibility in collocation sets (i.e., Genz cubature, unstructured/random sets supporting fault tolerance).
- TPQ more efficient for 2 dim, TPQ ~ SSG for 3 dim, SSG more efficient for 4 dim or more

Current directions:

- Additional tailoring and fine-grained algorithmic control
  - Numerically generated orthogonal polynomials for arbitrary input PDFs (Golub-Welsch)
  - Sparse grids: anisotropy in level w
- Stochastic error estimation & h-p adaptive collocation methods

OUU and Mixed UQ Remarks

Stochastic sensitivity analysis:

- 0^{th}-order combined or 1^{st}-order uncertain expansions → enables OUU, MCUU, Mixed UQ

Optimization Under Uncertainty

- Bi-level, sequential, and multifidelity OUU formulations
- 1^{st}-order uncertain more reliable: effective in bi-level & sequential approaches
- 0^{th}-order combined can be more efficient → explored use as low fidelity UQ surrogate
- Sequential is competitive; quasi-2^{nd}-order linkage assists convergence of iteration
- Multifidelity coerces LF UQ to HF optimum; competitive with cheapest LF UQ (MVFOSM)

Mixed Aleatory-Epistemic UQ

- SOP approaches that are more accurate (crisp bounds from optimizers) and efficient (exponential conv. rates from stoch. exp.) than traditional nested sampling
  - Inner loop: epistemic-aware stochastic expansions; Outer loop: global opt.-based interval estimation
- EGO with PCE/SC aleatory expansions → intervals using $O(10^2) - O(10^3)$ evals. were significantly more accurate that those from $O(10^8)$ simulations w/ nested sampling
- Uncertain/aleatory expansions were again more effective than combined expansions
  - Resolving aleatory stats for selected instances of *s* one at a time appears more efficient than globally resolving these stats for all values of *s* all at once (insufficient usage to offset construction)
- To further reduce expense or to scale to larger problems, can currently relax from global/global to use local at either/both levels → approx. intervals. Future: adaptive collocation.

Deployment and Support

Access

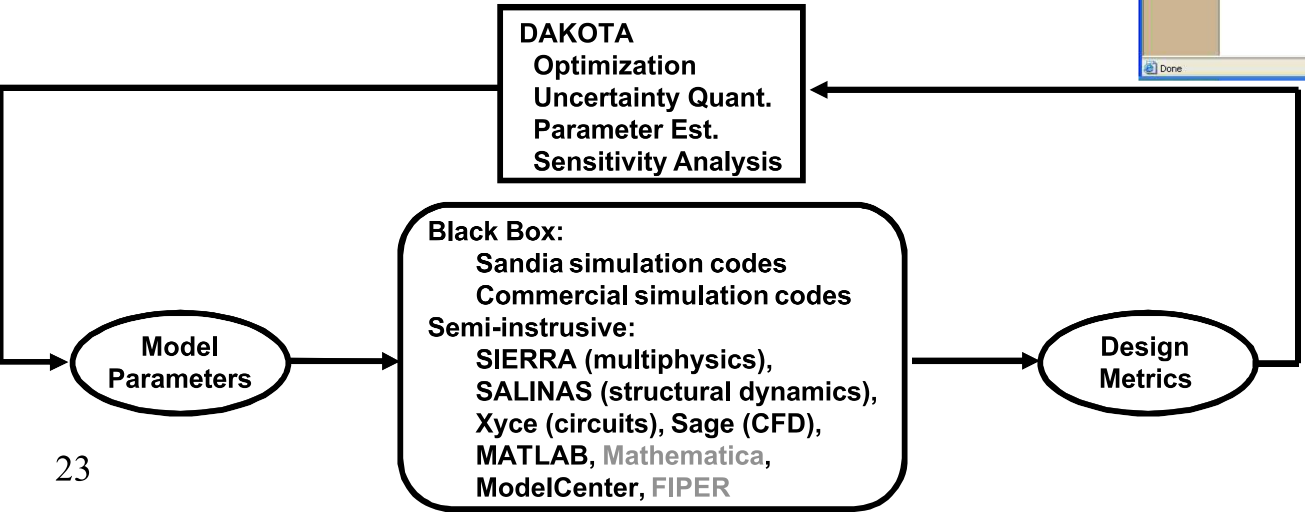
- Internal/external downloads from http://www.cs.sandia.gov/dakota
- GNU GPL – freely available worldwide (>6000 registered users)
- Releases: Major, Interim, Stable, VOTD [5.0 released Dec. 2009]
- Manuals: Users, Reference, Developers
- GUI: JAGUAR 2.0, Java-based "smart" GUI that adapts to DAKOTA input spec, deployed Dec. 2009

Platforms

- Linux, Solaris, AIX, Windows (Cygwin/MINGW), Mac
- MPICH, MVAPICH, OpenMPI on IP, GM, IB

SQE

- Nightly platform builds + ~850 serial/parallel tests
- Top SQE score in 2008 ASC assessment



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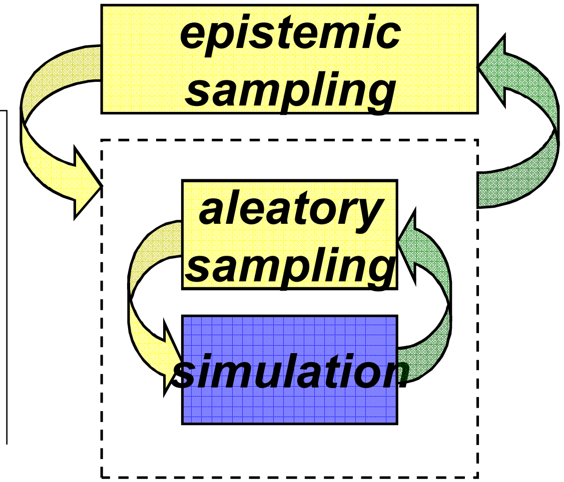
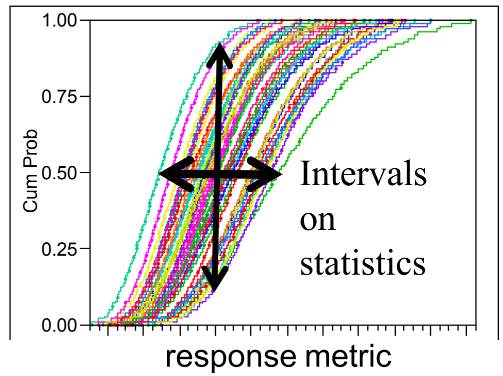
Mixed Aleatory-Epistemic UQ:
Second-Order Probability using Stochastic Expansions

Epistemic uncertainty (aka: subjective, reducible, lack of knowledge uncertainty): insufficient information to specify probability distributions



Second-order probability

- Traditional approach: nested sampling
- Expensive sims → under-resolved sampling (especially @ outer loop)
- Epistemic variables may insert or augment aleatory variables



Address accuracy and efficiency

- Inner loop: stochastic exp which are epistemic-aware (0th-order combined. 1st-order prob.)
- Outer loop: opt-based interval estimation, adaptive GP-based exploiting min/max data reuse

$$\begin{array}{ll} \text{minimize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \end{array}$$

$$\begin{array}{ll} \text{maximize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \end{array}$$

SC SSG Aleatory: converged to 5-6 digits by 527 evals.

EGO	SC SSG w = 1	Aleatory	(119, 0)	[75.0002, 374.999]	[-2.26264, 11.8623]
EGO	SC SSG w = 2	Aleatory	(527, 0)	[75.0002, 374.999]	[-2.18735, 11.5900]
EGO	SC SSG w = 3	Aleatory	(1785, 0)	[75.0002, 374.999]	[-2.18732, 11.5900]
EGO	SC SSG w = 4	Aleatory	(5049, 0)	[75.0002, 374.999]	[-2.18732, 11.5900]

Nested sampling: 2-3 digits by 10^8 evals.

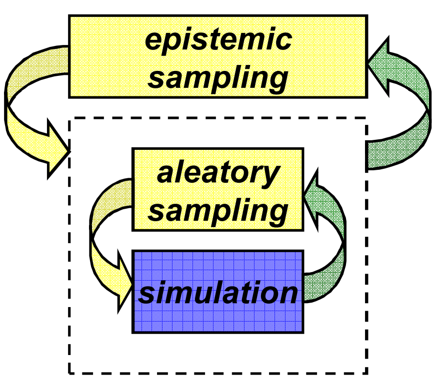
LHS 100	LHS 100	N/A	$(10^4, 0)$	[80.5075, 338.607]	[-2.14505, 8.64891]
LHS 1000	LHS 1000	N/A	$(10^6, 0)$	[76.5939, 368.225]	[-2.19883, 11.2353]
					[-2.16323, 11.5593]

Impact: render mixed UQ studies practical for large-scale applications

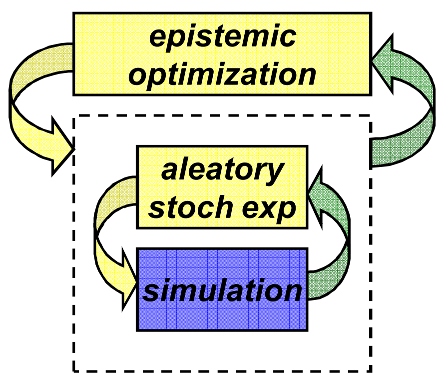
Fully converged area interval = [75., 375.], β interval = [−2.18732, 11.5900]

Research Innovations

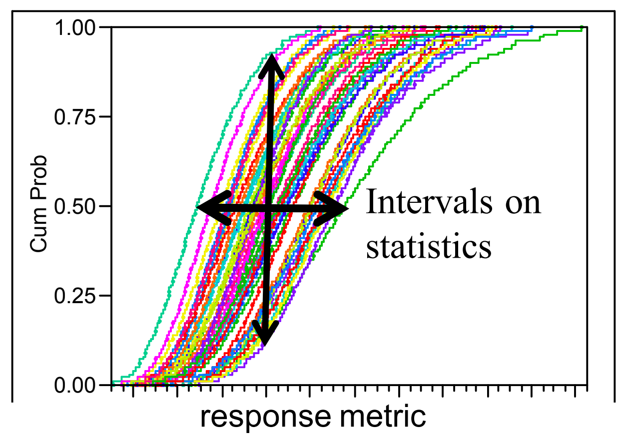
CHALLENGE	SOLUTION
Represent epistemic uncertainty	Apply stochastic expansion methods to interval variables using Legendre basis
Curse of dimensionality	Dimension-adaptive stochastic expansion methods
Curse of dimensionality	Anisotropic Smolyak sparse grids
Estimate outer loop bounding interval	Local gradient-based methods can now leverage analytic moments and their sensitivities with respect to epistemic parameters.
Estimate outer loop bounding interval	Global nongradient-based optimization approaches to interval estimation with data reuse among minimization and maximization solves, using GP emulators



Workhorse SOP



Research SOP



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