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UQ Algorithm Research and Advanced Deployment within the DAKOTA Project

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NRC Committee on Mathematical Foundations for V&V and UQ

Albuquerque NM

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- DAKOTA Intro
- Algorithm R&D 1: Adaptive UQ
- Algorithm R&D 2: UQ Complexity
- Advanced deployment initiatives
- Selected deployment case studies

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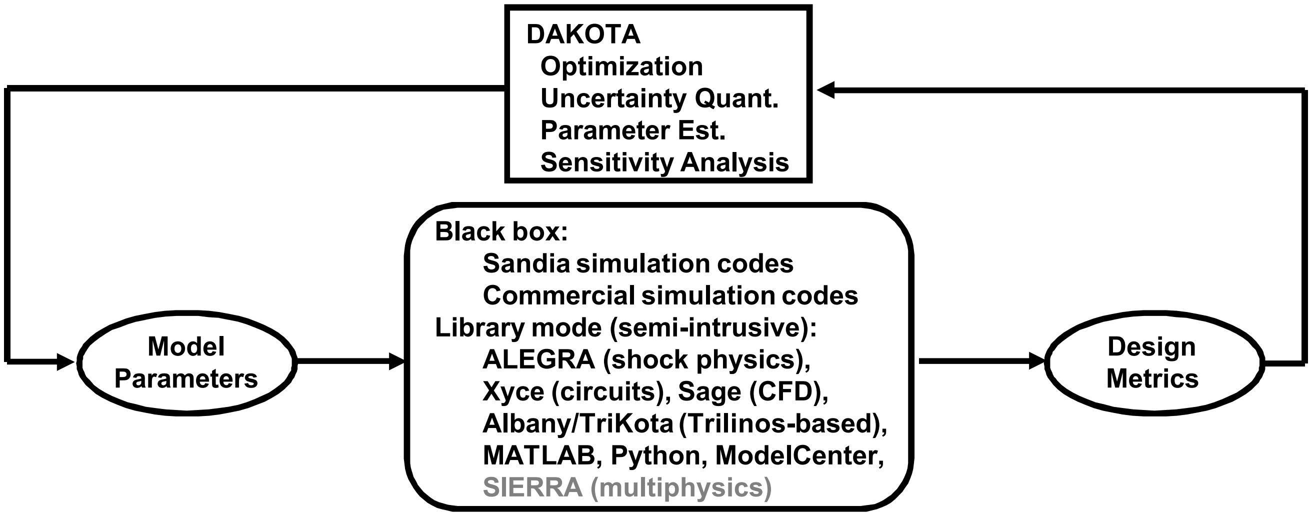
DAKOTA Software



Iterative systems analysis

Multilevel parallel computing

Simulation management

http://dakota.sandia.gov

Team: ~10 core personnel in NM/CA + TPL developers

Releases: Major/Interim, Stable/VOTD; *5.0 released 12/09*

DAKOTA Training: 8 sessions (~140 students) since 5.0;
26 sessions (~500 students) total since 2001.

2009 Outreach: Minitutorials at IMAC, SIAM CS&E;
SA/UQ short courses at NASA Langley, AFRL WPAFB.

Modern SQE: Nightly portability/regression/verification tests;
subversion, Bugzilla, TRAC, Cmake; Top 2008 SQE score

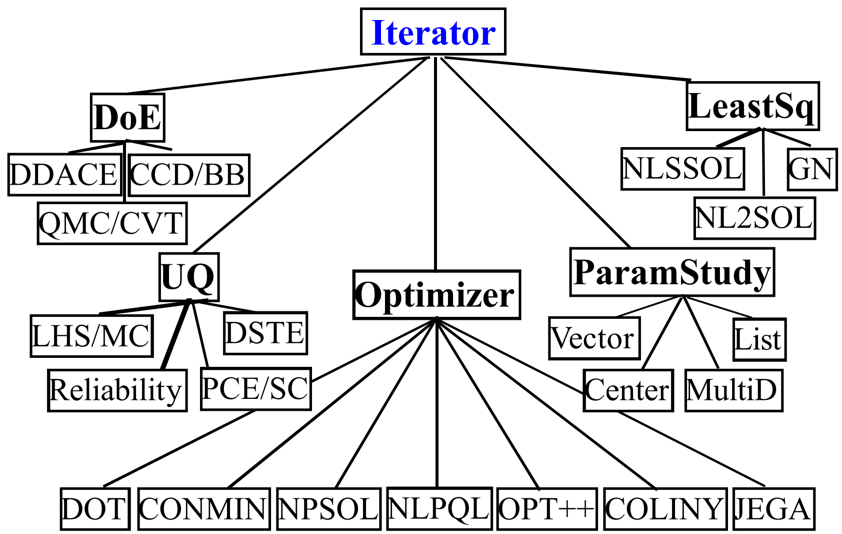
Platforms: Linux/Unix, Mac, Windows (Cygwin/MinGW → native)

GNU LGPL: free downloads worldwide
(~6500 total ext. registrations, ~3500 distributions last yr.)

Community development: open checkouts coming (→ PSAAP)

Community support: dakota-users, dakota-developers

C++ Framework



Model:

Design
- continuous
- discrete range/set

Uncertain
- normal/lognorm.
- uniform/logunif.
- triang/exp/β/Γ
- EV: I, II, III
- histogram: bin/pt
- discrete: p/b/nb/g/hg
- interval

State
- continuous
- discrete range/set

Application
- system
- fork
- direct
- grid

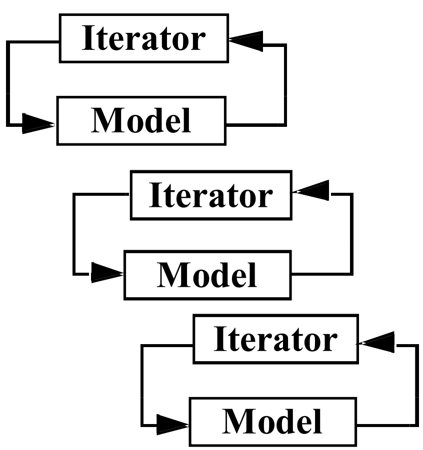
Approximation
- global
  - polynomial 1/2/3, NN, kriging, MARS, RBF
- multipoint – TANA3
- local – Taylor series
- multifidelity
- ROM

Functions
- objectives
- nonlin constraints
- least sq. terms
- generic

Gradients
- numerical
- analytic

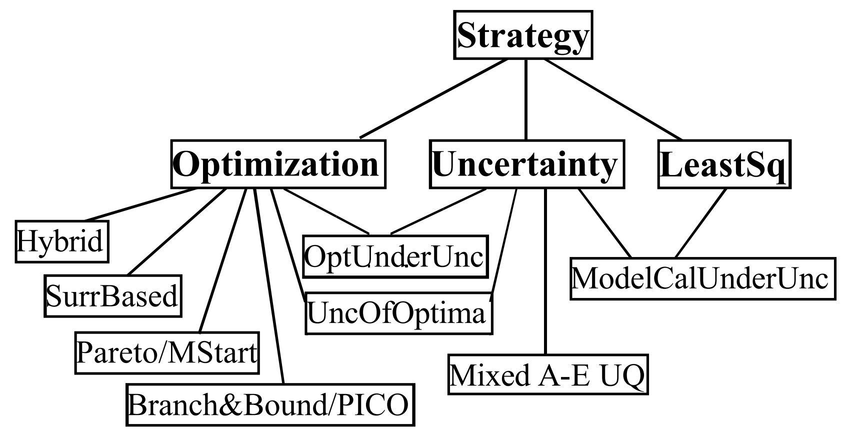
Hessians
- numerical
- analytic
- quasi

Strategy: control of multiple iterators and models



Coordination:
- Nested
- Layered
- Cascaded
- Concurrent
- Adaptive/Interactive

Parallelism:
- Asynchronous local
- Message passing
- Hybrid
- 4 nested levels with
  - Master-slave/dynamic
  - Peer/static



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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)		gradient-enhanced EGRA	*Local:* Notre Dame, *Global:* Vanderbilt
Stochastic expansion		Tailored polynomial chaos & stochastic collocation with extended basis selections	Anisotropic sparse grid, cubature, p-adaptive, multiphysics	h-adaptive, hp-adaptive, gradient-enhanced, discrete	Stanford, Purdue, CU Boulder, USC, VPISU
Other probabilistic		Random fields/ stochastic proc.		Dimension reduction	Cornell, Maryland
Epistemic	Interval-valued/ Second-order prob. (nested sampling)	Opt-based interval estimation, Dempster-Shafer	Bayesian	Imprecise probability	LANL, Applied Biometrics
Metrics & Global SA	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		UNM

Reseach: Tailoring & Adaptivity

Adv. Deployment

Fills Gaps

Algorithm R&D in Adaptive UQ

Drivers

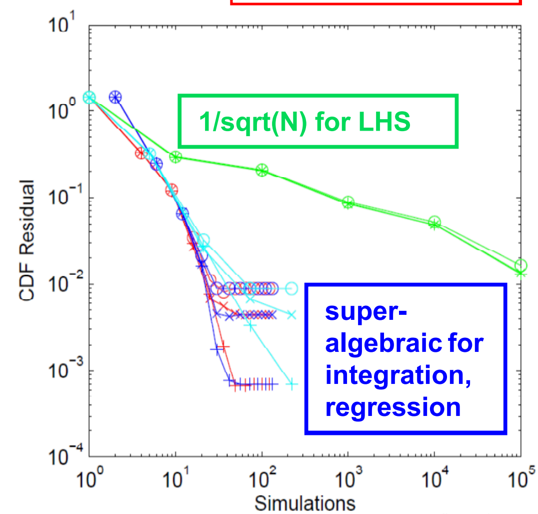
- High random dimensionality → adaptive methods, adjoint enhancement
- Complex random environments → epistemic/mixed UQ, model form/multifidelity, RF/SP, multiphysics/multiscale

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

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

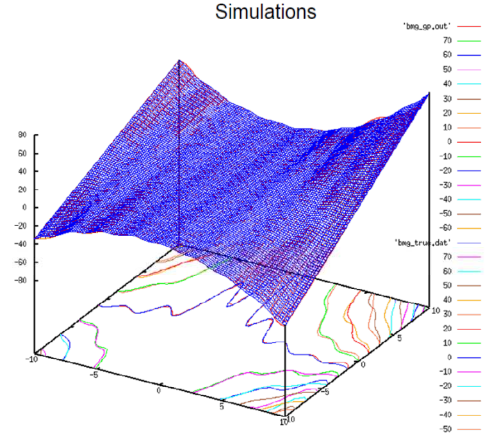
Stochastic expansions:

- *Polynomial chaos expansions (PCE)*: known basis, compute coeffs
- *Stochastic collocation (SC)*: known coeffs, form interpolants
- Adaptive approaches: emphasize key dimensions
  - Uniform/adaptive p-refinement (FY10)
  - h-/hp-adaptive collocation (FY11-12)
- Sparse adaptive global methods: scale as $m^{\log r}$ with r << n



EGRA:

- Adaptive GP refinement for tail probability estimation
- Accuracy similar to exhaustive sampling at cost similar to local reliability assessment
- Global method that scales as $\sim n^2$



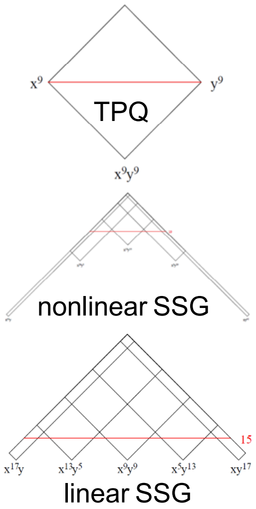
Sampling:

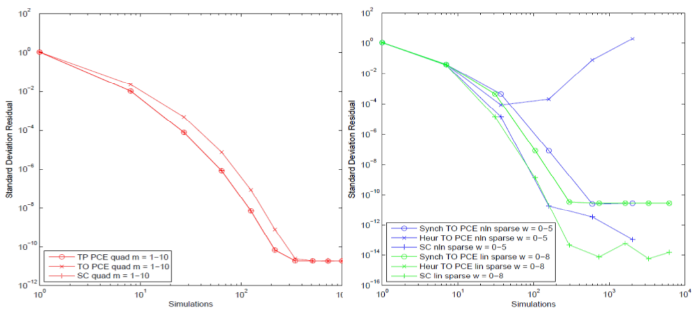
- Importance sampling (adaptive refinement)
- Incremental MC/LHS (uniform refinement)

Tailoring of Stochastic Expansions:
Fine-grained Control → Smart Adaptive Methods

Tailoring of PCE form

$$\Psi_j(\boldsymbol{\xi}) = \prod_{i=1}^{n} \psi_{m_i^j}(\xi_i)$$





Eliminate (approximate) heuristics and trial & error
Maximize performance of PCE and close / eliminate performance gap with SC

Tailoring of basis polynomials

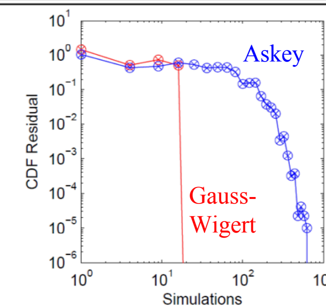
Askey family

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 $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0, \infty]$

Other PDFs:
nonlinear variable transformations
numerically-generated orthogonal polynomials

$$\begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots \\ & & \ddots & \ddots \\ 0 & & & \end{bmatrix}$$

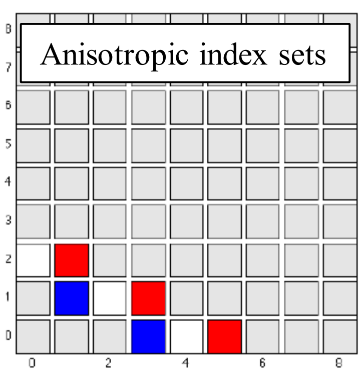
Tailored & synchronized expansion form with optimal bases

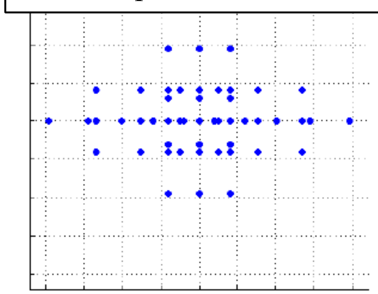


Advanced numerical integration

Anisotropic Smolyak:
(linear index set constraint)

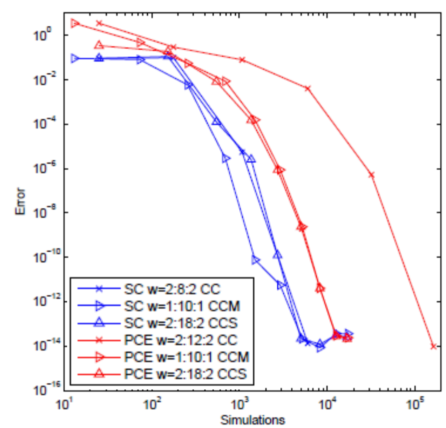
$$w\underline{\alpha} - |\alpha| < \sum_{n=1}^{d} (i_n - 1)\alpha_n \le w\underline{\alpha}$$

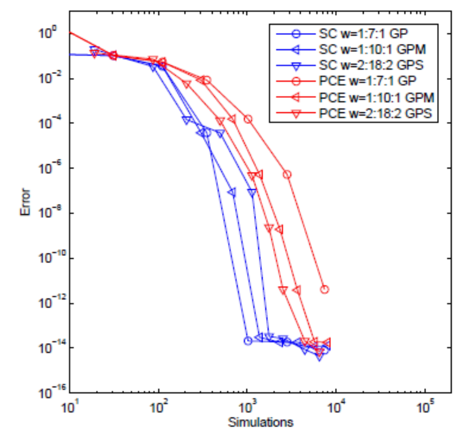




Restricted exponential growth (slow/moderate)

- Synchronize with Gaussian linear growth
- Exploit point nesting without sacrificing integrand uniformity





Initial Adaptive Methods

$$f_{PC}(\boldsymbol{x}) = f_0 + \sum_{i=1}^{n} \sum_{\boldsymbol{\alpha} \in \mathcal{I}_i} f_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(x_i) + \sum_{1 \le i_1 < i_2 \le n} \sum_{\boldsymbol{\alpha} \in \mathcal{I}_{i_1,i_2}} f_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(x_{i_1}, x_{i_2}) + \dots + \sum_{1 \le i_1 < \dots < i_s \le n} \sum_{\boldsymbol{\alpha} \in \mathcal{I}_{i_1,\dots,i_s}} f_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(x_{i_1}, \dots, x_{i_s}) + \dots + \sum_{\boldsymbol{\alpha} \in \mathcal{I}_{1,2,\dots,n}} f_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(x_1, \dots, x_n)$$

$$SU^T_{j_1,\dots,j_t} = \sum_{(i_1,\dots,i_s) \in \mathcal{J}_{j_1,\dots,j_t}} SU_{i_1,\dots,i_s}$$

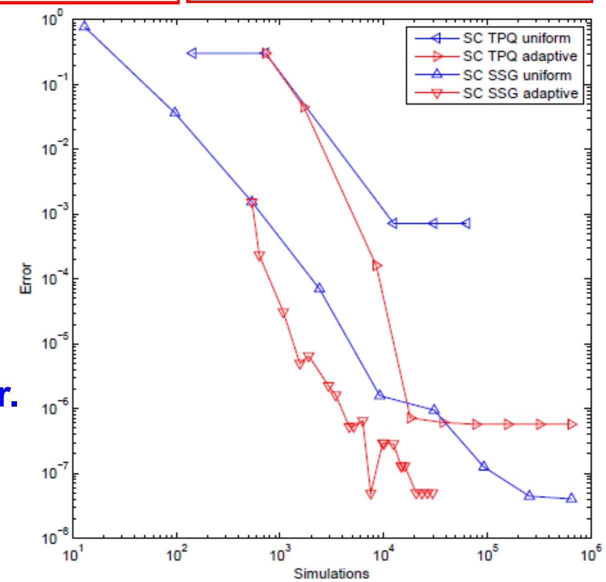
$$SU_{i_1 \dots i_s} = \sum_{\boldsymbol{\alpha} \in \mathcal{I}_{i_1,\dots,i_s}} f^2_{\boldsymbol{\alpha}} \, \mathrm{E}\left[\Psi^2_{\boldsymbol{\alpha}}\right] / D_{PC}$$

Uniform and adaptive p-refinement:

- **Uniform: isotropic TPQ/SSG**
  - **convergence: 2-norm of change in resp. covariance**
- **Dimension adaptive: anisotropic TPQ/SSG**
  - **Start from low-order isotropic or set of 1-D experiments**
  - **PCE/SC: analytic VBD → Sobol' indices**
  - **PCE: spectral coefficient decay**
  - **PCE/SC: *a posteriori* error/conv. rate est. (in QOI!)**
  - **Main effects → aniso TPQ, aniso SSG w/ linear index constr.**

$$w\underline{\alpha} - |\alpha| < \sum_{n=1}^{d} (i_n - 1)\alpha_n \le w\underline{\alpha}$$

  - **Interactions → aniso SSG w/ nonlinear index constraint**



h-adaptive:

- **Discretize based on error est.** (detect discontinuity/singularity)
  - **Najm, Karniadakis, Zabaris, Aluru, et al.**
  - **Identify/resolve important *regions* (not just dimensions)**

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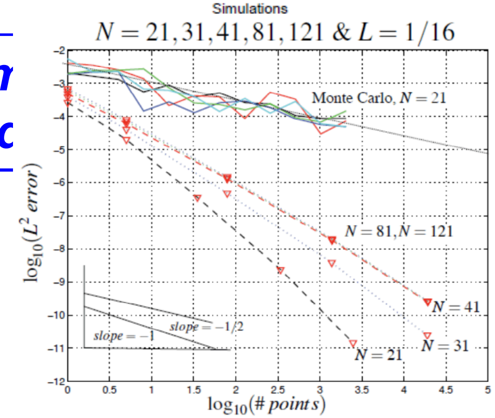
hp-adaptive:

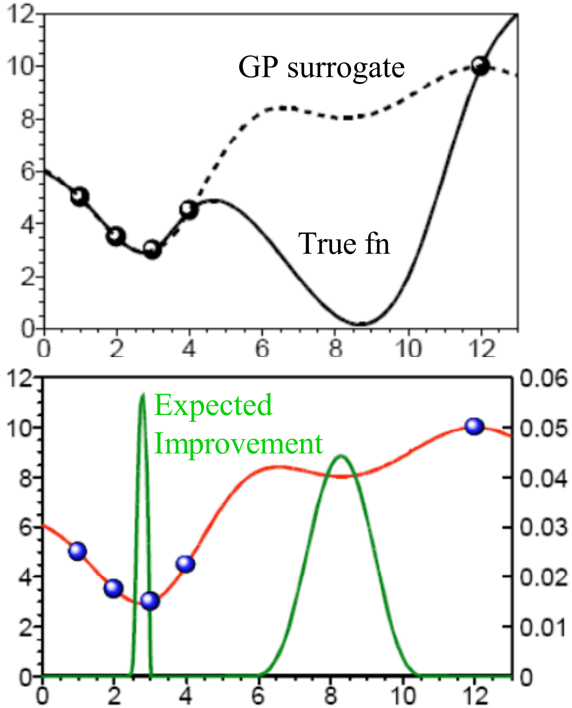
- **Ultimate goal is to do both:**
  - **p-adaptive for performance (convergence rate)**
  - **h-adaptive for robustness (discontinuity/singularity)**



AN ANISOTROPIC SPARSE GRID STOCHASTIC COLLOCATION METHOD FOR PARTIAL DIFFERENTIAL EQUATIONS WITH RANDOM INPUT DATA, Nobile, Tempone, and Webster, *SIAM J. NUMER. ANAL.*, 2008

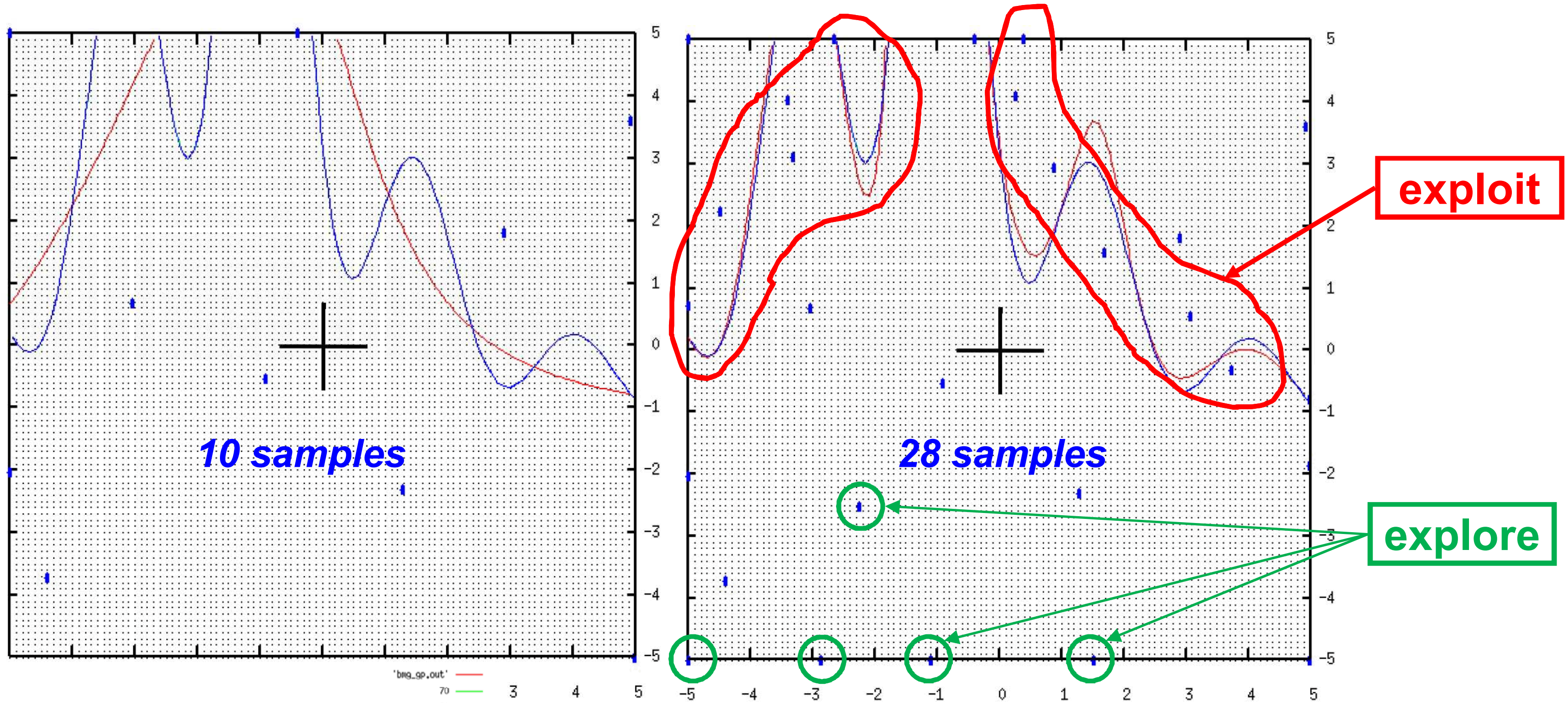
Efficient Global Reliability Analysis (EGRA)

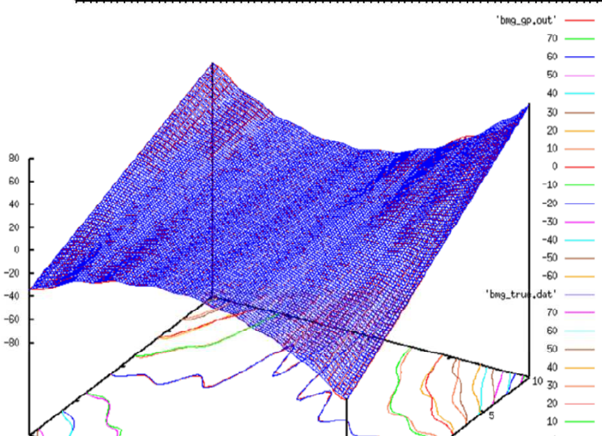
- **Address known failure modes of local reliability methods:**
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP
- **Based on EGO (surrogate-based global opt.), which exploits special features of GPs**
  - Mean and variance predictions: formulate expected improvement (EGO) or expected feasibility (EGRA)
  - Balance explore and exploit in computing an optimum (EGO) or locating the limit state (EGRA)



From Jones, Schonlau, Welch, 1998

Efficient Global Reliability Analysis





Reliability Method	Function Evaluations	First-Order p_f (% Error)	Second-Order p_f (% Error)	Sampling p_f (% Error, Avg. Error)
No Approximation	70	0.11797 (277.0%)	0.02516 (-19.6%)	—
x-space AMV^2+	26	0.11797 (277.0%)	0.02516 (-19.6%)	—
u-space AMV^2+	26	0.11777 (277.0%)	0.02516 (-19.6%)	—
u-space TANA	131	0.11797 (277.0%)	0.02516 (-19.6%)	—
LHS solution	10k	—	—	0.03117 (0.385%, 2.847%)
LHS solution	100k	—	—	0.03126 (0.085%, 1.397%)
LHS solution	1M	—	—	0.03129 (truth , 0.339%)
x-space EGRA	35.1	—	—	0.03134 (0.155%, 0.433%)
u-space EGRA	35.2	—	—	0.03133 (0.136%, 0.296%)

Accuracy similar to exhaustive sampling at cost similar to local reliability assessment

Extend Scalability through Adjoint Derivative-Enhancement

PCE:

- **Linear regression with derivatives**
  - Gradients/Hessians → addtnl. eqns.

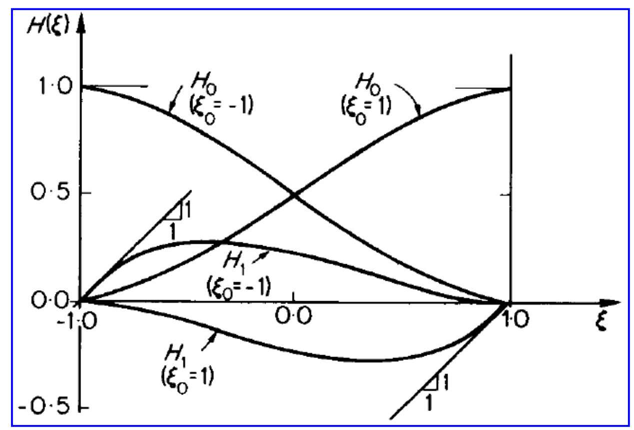
$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \pi_{0,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_{n_\xi}}(\vec{\xi}_i) \\ \vdots & \vdots & & \vdots \end{bmatrix} \begin{pmatrix} \vdots \\ \vec{u}^{(m,j)} \\ \vec{u}^{(m+1,j)} \\ \vdots \\ \vec{u}^{(m+n_\xi,j)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \vec{u}_i \\ \frac{\partial \vec{u}_i}{\partial \xi_1} \\ \vdots \\ \frac{\partial \vec{u}_i}{\partial \xi_{n_\xi}} \\ \vdots \end{pmatrix}$$

SC:

- **Gradient-enhanced interpolants**
  - Cubic Lagrange splines (discretization → h-adaptive)
  - Hermitian polynomials

$a_j^i = 1$ for $i = 1$

$$a_j^i = \begin{cases} \prod_{l=j-1,\, l\neq j}^{j+2} \frac{x - x_l^i}{x_j^i - x_l^i} & \text{if } x \in \left[x_j^i, x_{j+1}^i\right], \quad j = 2,\dots,m_i - 2 \\ \prod_{l=j+1}^{j+2} \frac{x - x_l^i}{x_j^i - x_l^i} & \text{if } x \in \left[x_j^i, x_{j+1}^i\right], \quad j = 1 \\ \prod_{l=j-1,\, l\neq j}^{j+1} \frac{x - x_l^i}{x_j^i - x_l^i} & \text{if } x \in \left[x_j^i, x_{j+1}^i\right], \quad j = m_i - 1 \\ 0 & \text{otherwise} \end{cases}$$



EGRA:

- **Gradient-enhanced kriging/cokriging**
  - Interpolates function values and gradients
  - Scaling: n^2 → n

database $\{\mathbf{x},\mathbf{y}\}$ & initial $(\Delta x, \theta)$

Step A:

$$R_{12} = R(\mathbf{x}^1, \mathbf{x}^2) = \prod_{j=1}^{d} \exp\left(-\theta_j \left|\mathbf{x}_j^1 - \mathbf{x}_j^2\right|^2\right)$$

$$\hat{\beta} = (\mathbf{1}^T \mathbf{R}^{-1} \mathbf{1})^{-1} \mathbf{1}^T \mathbf{R}^{-1} \mathbf{y} \qquad \mathbf{R} = \begin{bmatrix} R_{11} & \cdots & R_{1n} \\ \vdots & \ddots & \vdots \\ R_{n1} & \cdots & R_{nn} \end{bmatrix}$$

$$\hat{\sigma}_z^2 = \frac{1}{n}(\mathbf{y} - \mathbf{1}\hat{\beta})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{1}\hat{\beta})$$

Step B:

$$\min : IMSE = \hat{\sigma}_z^2 \left[\int_\Omega 1 d\mathbf{x} - trace\left[\begin{pmatrix} 0 & \mathbf{1}^T \\ \mathbf{1} & \mathbf{R} \end{pmatrix}^{-1} \int_\Omega \begin{pmatrix} 1 & \mathbf{r}^T \\ \mathbf{r} & \mathbf{r}\mathbf{r}^T \end{pmatrix} d\mathbf{x}\right]\right]$$

update $(\Delta x, \theta)$

Algorithm R&D in UQ Complexity

Drivers

- High random dimensionality → adaptive methods, adjoint enhancement
- Complex random env. → mixed UQ, model form/multifidelity, RF/SP, multiphysics/multiscale

Stochastic sensitivity analysis

- Aleatory or combined expansions including nonprobabilistic dimensions *s* → sensitivities of moments w.r.t. design and/or epistemic parameters

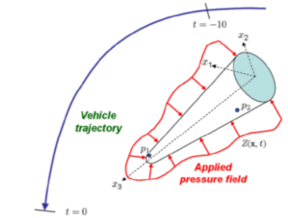
$$R(\xi, s) = \sum_{j=0}^{P} \alpha_j(s)\Psi_j(\xi)$$

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

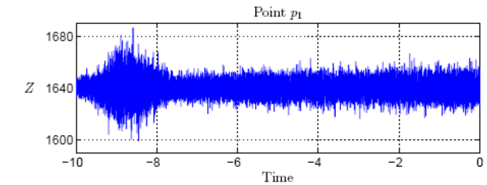
Design and Model Calibration Under Uncertainty

Mixed Aleatory-Epistemic UQ

- SOP, IVP, and DSTE approaches that are more accurate and efficient than traditional nested sampling



Random Fields / Stochastic Processes (Encore, PECOS)



Multiphysics (multiscale) UQ:

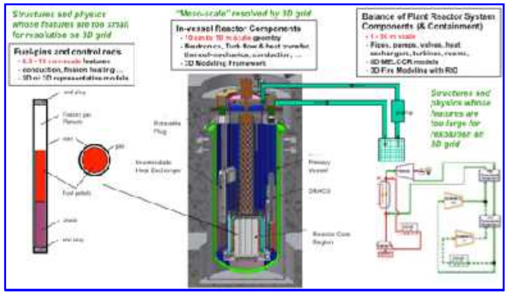
- Invert UQ & multiphysics loops → transfer UQ stats among codes

Bayesian Inference:

- Collaborations w/ LANL (GPM), UT (Queso), Purdue/MIT (gPC)

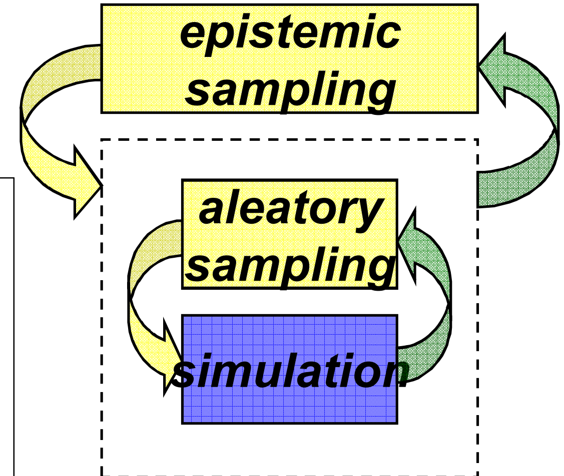
Model form:

- Multifidelity UQ (hierarchy), Bayesian model averaging (ensemble)



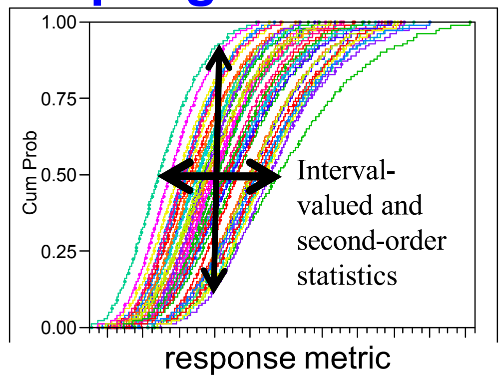
Mixed Aleatory-Epistemic UQ: IVP, DSTE, and SOP

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



Traditional approach: nested sampling

- Expensive sims → under-resolved sampling (especially @ outer loop)
- Under-prediction of credible outcomes



Algorithmic approaches

- Interval-valued probability (IVP), *aka* probability bounds analysis (PBA)
- Dempster-Shafer theory of evidence (DSTE)
- Second-order probability (SOP), *aka* probability of frequency

Increasing epistemic structure (stronger assumptions)

Address accuracy and efficiency

- Inner loop: stochastic exp. that are epistemic-aware (aleatory, combined)
- Outer loop:
  - IVP, DSTE: opt-based interval estimation, global (EGO) or local (NLP)
  - SOP: nested stochastic exp. (nested expectation is only post-processing in special cases)

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

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

Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

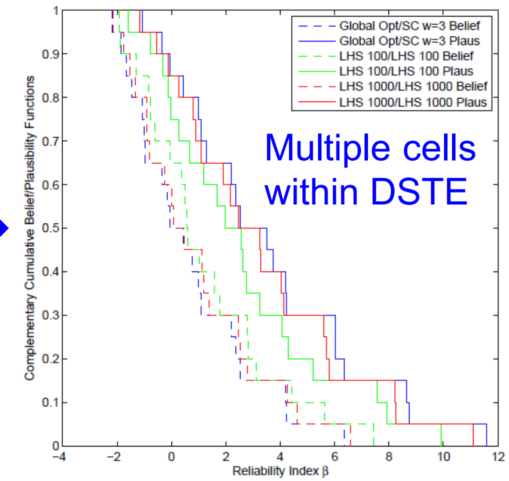
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals

Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β
EGO	SC SSG w = 1	Aleatory	(84/91, 0/0)	[75.0002, 374.999]	[-2.26264, 11.8623]
EGO	SC SSG w = 2	Aleatory	(372/403, 0/0)	[75.0002, 374.999]	[-2.18735, 11.5900]
EGO	SC SSG w = 3	Aleatory	(1260/1365, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
EGO	SC SSG w = 4	Aleatory	(3564/3861, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 1	Aleatory	(21/77, 21/77)	[75.0000, 375.000]	[-2.26264, 11.8623]
NPSOL	SC SSG w = 2	Aleatory	(93/341, 93/341)	[75.0000, 375.000]	[-2.18735, 11.5901]
NPSOL	SC SSG w = 3	Aleatory	(315/1155, 315/1155)	[75.0000, 375.000]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 4	Aleatory	(891/3267, 891/3267)	[75.0000, 375.000]	[-2.18732, 11.5900]

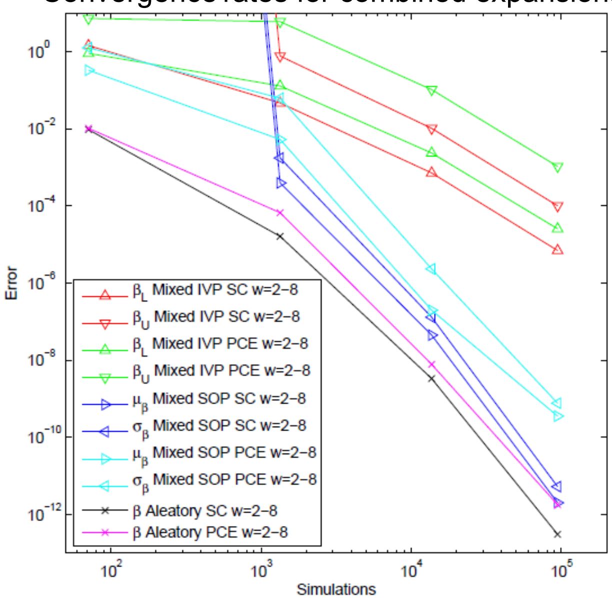
IVP nested LHS sampling: converged to 2-3 digits by 10^8 evals

LHS 100	LHS 100	N/A	$(10^4/10^4, 0/0)$	[80.5075, 338.607]	[-2.14505, 8.64891]
LHS 1000	LHS 1000	N/A	$(10^6/10^6, 0/0)$	[76.5939, 368.225]	[-2.19883, 11.2353]
LHS 10^4	LHS 10^4	N/A	$(10^8/10^8, 0/0)$	[76.4755, 373.935]	[-2.16323, 11.5593]

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



Convergence rates for combined expansions



L^∞ metrics: IVP mixed, DSTE mixed

L^2 metrics: Aleatory, SOP mixed

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

Current:

- **Global or local opt. for epistemic intervals**
  → accuracy *or* scaling w/ epistemic dimension
- **Global or local UQ for aleatory statistics**
  → accuracy *or* scaling w/ aleatory dimension

Future:

- ***adaptive* and *adjoint-enhanced* global methods**
  → accuracy *and* scaling

ASCR: Multi-Physics and Network-Coupled UQ

- Component-level UQ via stochastic expansions
- Stochastic dimension reduction at component interfaces (generate new bases orthogonal to (implied) output PDFs)
- Strongly coupled solver technology for coupled stochastic problems

Component 1

$$v_2 = G_1(v_1, p_1) = g_1(u_1(v_1), p_1) \;\; \text{s.t.} \;\; f_1(u_1, v_1, p_1) = 0$$

Component 2

$$v_1 = G_2(v_2, p_2) = g_2(u_2(v_2), p_2) \;\; \text{s.t.} \;\; f_2(u_2, v_2, p_2) = 0$$

v_1 v_2

Nonlinear elimination

Equations

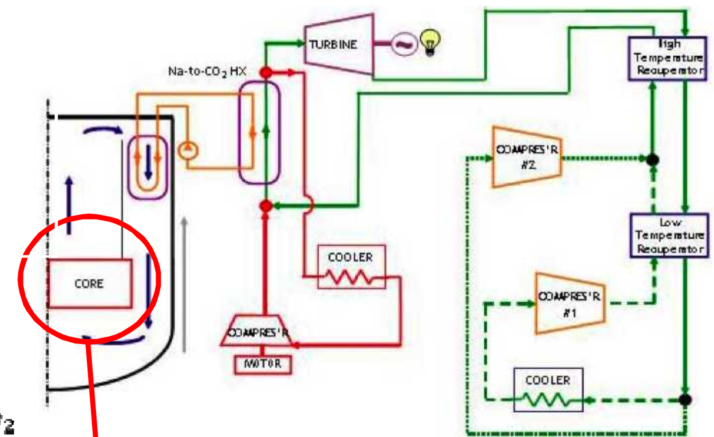
$$v_2 - G_1(v_1, p_1) = 0$$
$$v_1 - G_2(v_2, p_2) = 0$$

Newton Step

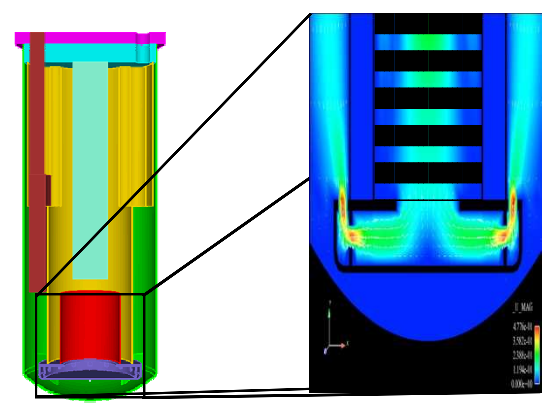
$$\begin{bmatrix} -dG_1/dv_1 & 1 \\ 1 & -dG_2/dv_2 \end{bmatrix} \begin{bmatrix} \Delta v_1 \\ \Delta v_2 \end{bmatrix} = - \begin{bmatrix} v_2 - G_1(v_1, p_1) \\ v_1 - G_2(v_2, p_2) \end{bmatrix}$$

$$\frac{dG_i}{dv_i} = -\frac{\partial g_i}{\partial u_i} \left(\frac{\partial f_i}{\partial u_i} \right)^{-1} \frac{\partial f_i}{\partial v_i}$$

$$\left. \begin{aligned} \frac{1}{\langle \Psi_j^2 \rangle} \langle (\hat{v}_2(\xi) - \hat{G}_1(\xi)) \Psi_j(\xi) \rangle &= 0 \\ \frac{1}{\langle \Psi_j^2 \rangle} \langle (\hat{v}_1(\xi) - \hat{G}_2(\xi)) \Psi_j(\xi) \rangle &= 0 \end{aligned} \right\} \implies \left. \begin{aligned} v_{2j} - G_{1j} &= 0 \\ v_{1j} - G_{2j} &= 0 \end{aligned} \right\}, \quad j = 0, \ldots, P$$



Low-fidelity Network Plant Model



High-fidelity Multi-physics Component Model (Core)

Graphics courtesy: Rod Schmidt, BRISC project

Proposed Multi-scale UQ research: LDRD, ASCR

Deployment

Address core usability barriers

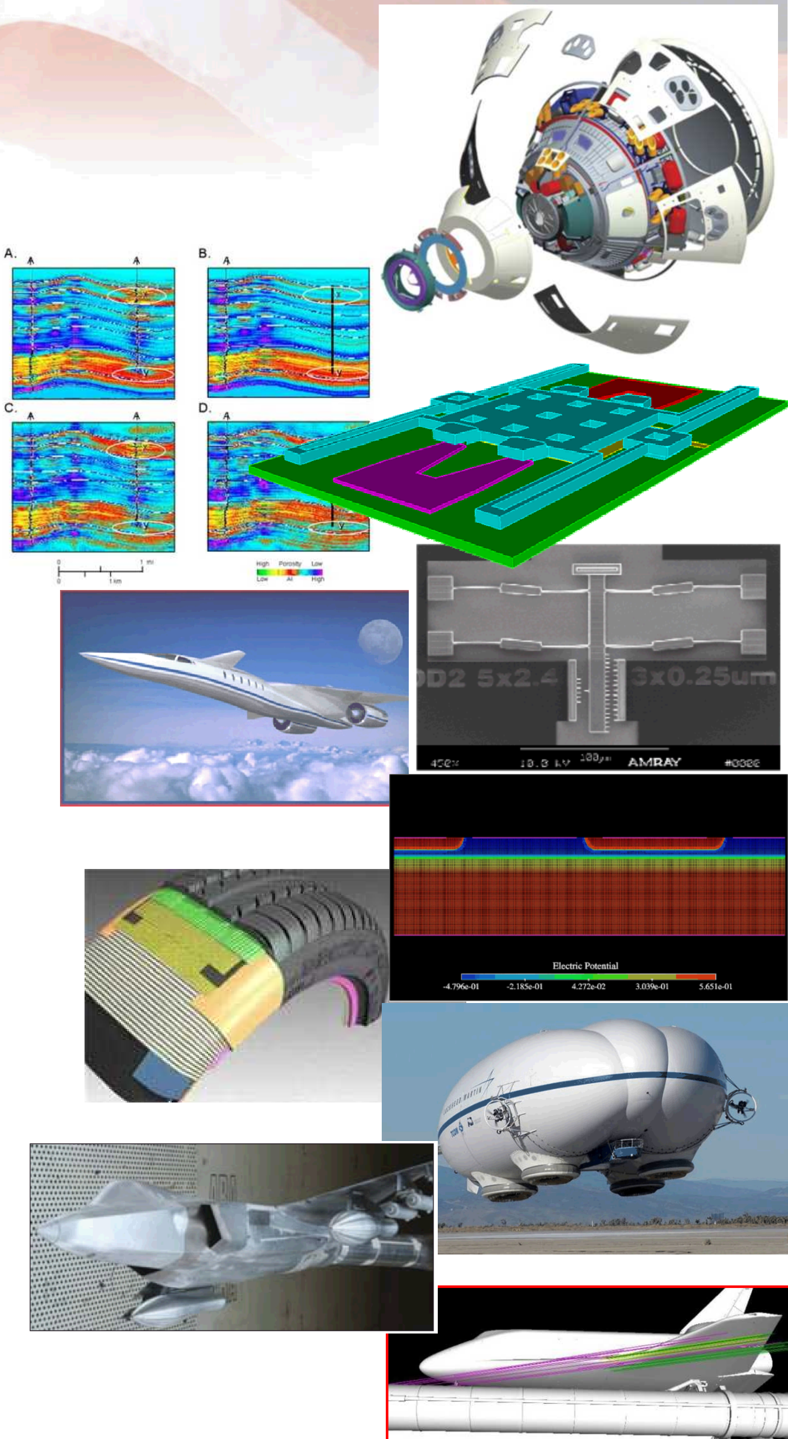
- JAGUAR
- Library embedding

Impact Sandia missions

- Technology insertion
  - ASC milestones
  - Early adopters

Partnerships

- Government: LLNL, LANL, ORNL, INL, NASA, DOD
- Industry: Lockheed Martin, Goodyear, Exxon Mobil
- University: MIT, Cornell, CU Boulder, Vanderbilt, USC, FSU, Notre Dame, VPISU, UNM
  - CSRI students/postdocs, faculty sabbaticals
  - ASC PSAAP: UT Austin (Bayesian), Purdue (cubature), UIUC (adaptive collocation), Caltech (global opt.), Michigan (gradient-enhanced interpolation), Stanford (adaptive collocation)

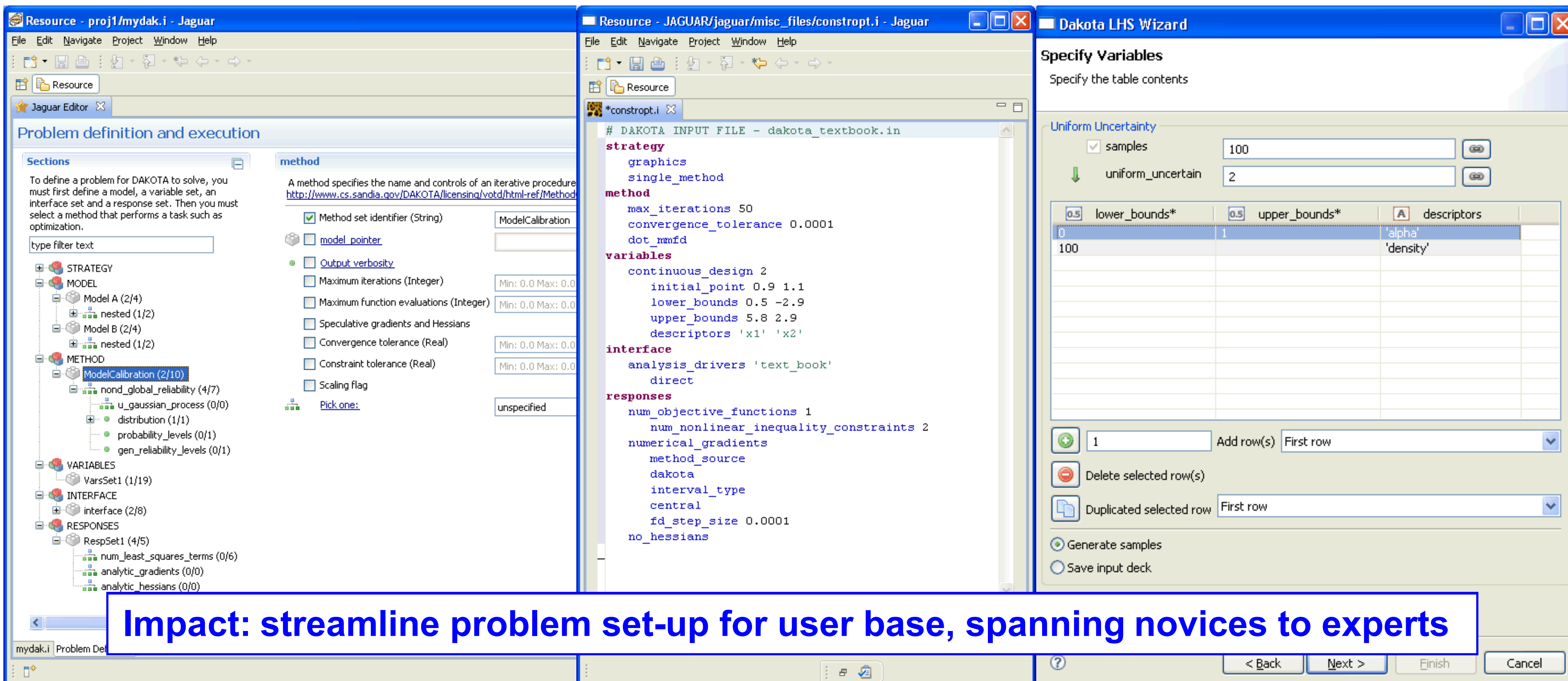


Advanced Deployment: JAGUAR User Interface

- Eclipse-based rendering of full DAKOTA input spec.
- Automatic syntax updates
- Tool tips, Web links, help
- Symbolics, sim. interfacing

- Flat text editor for experienced users
- Keyword completion
- Automatically synchronized with GUI widgets

- Simplified views for high-use applications ("Wizards")



Impact: streamline problem set-up for user base, spanning novices to experts

Advanced Deployment: Embedding

Make DAKOTA natively available within application codes

- Streamline problem set-up, reduce complexity, and lower barriers
  - A few additional commands within existing simulation input spec.
  - Eliminate analysis driver creation & streamline analysis (e.g., file I/O)
  - Simplify parallel execution
- Integrated options for simulation intrusion

SNL Embedding

- Existing: Xyce, Sage, Albany (TriKOTA)
- New: ALEGRA, SIERRA (TriKOTA)

External Embedding

- Existing: ModelCenter, university applications
- New: QUESO (UT Austin), R7 (INL)
- Expanding our external focus:
  - GPL → LGPL; svn restricted → open network

ModelEvaluator Levels

Non-intrusive

ModelEvaluator: systems analysis

- All residuals eliminated, coupling satisfied
- DAKOTA optimization & UQ

Intrusive to coupling

ModelEvaluator: multiphysics

- Individual physics residuals eliminated; coupling enforced by opt/UQ
- DAKOTA opt/UQ & MOOCHO opt.

Intrusive to physics

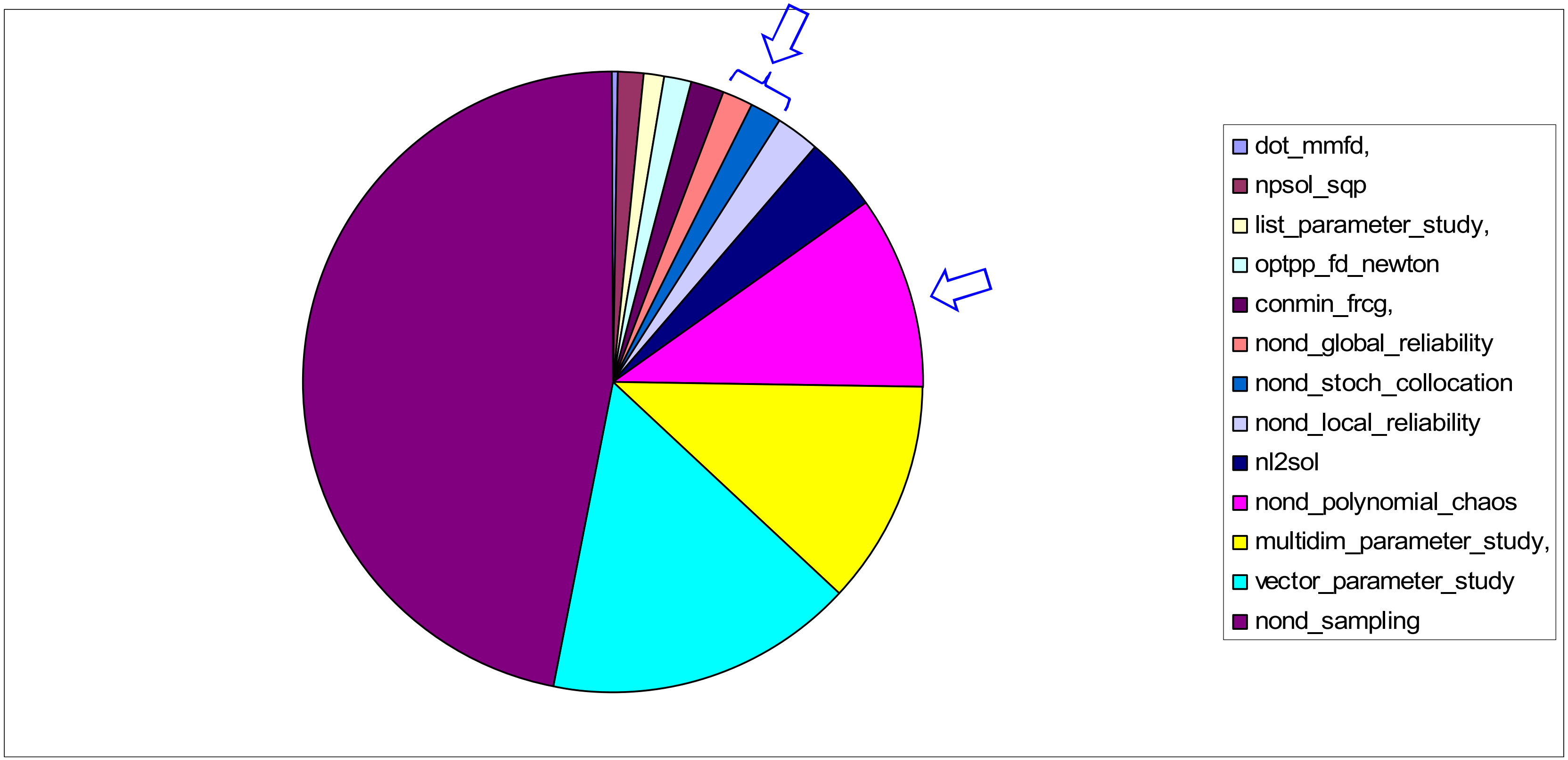
ModelEvaluator: single physics

- MOOCHO opt., Stokhos UQ, NOX, LOCA

Impact: eliminate custom set-up and support fully integrated opt. and UQ studies

DAKOTA Usage by Method

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



New PCE/SC/EGRA are starting to eat into traditional LHS dominance

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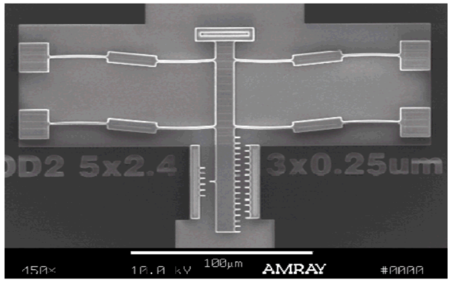
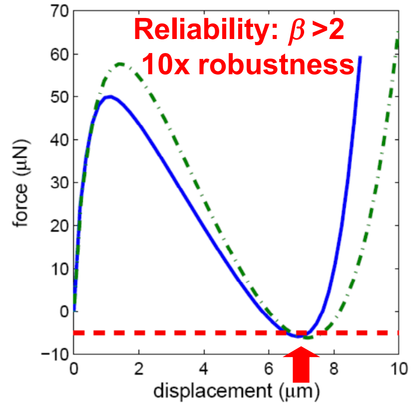
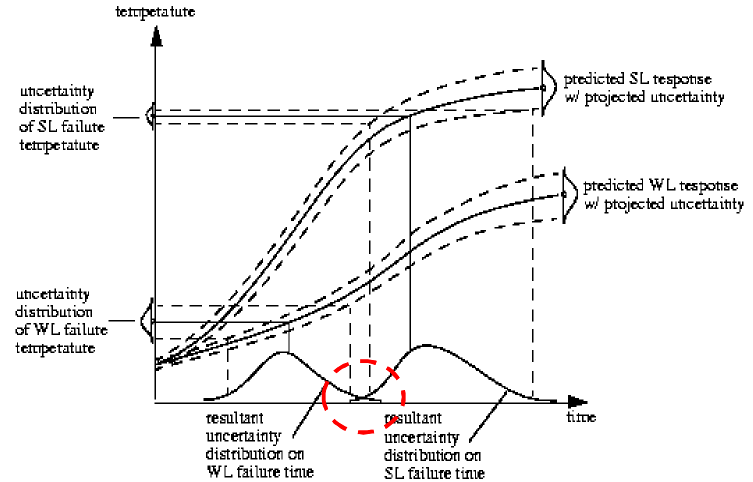
Deployment of Advanced Methods



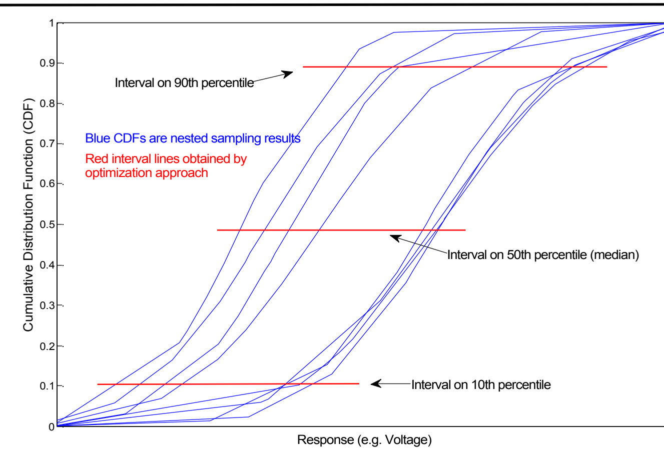


- Solution-verified reliability analysis with adjoint-based error estimation → AMR, error correction
- Robust and reliable designs for bi-stable MEMS



- Abnormal thermal (fire) with PCE
- Exponential convergence demonstrated

- Abnormal mechanical (drop) with EGRA
- Accuracy comparable to exhaustive sampling demonstrated at reduced cost



- Mixed aleatory-epistemic UQ for QASPR
- Device (Charon) and circuit (Xyce) models
- More fully resolved interval estimates

Concluding Remarks

R&D in Adaptive UQ Methods → curse of dimensionality

- Stochastic expansions: PCE, SC
  - Tailoring to maximize performance → foundation for uniform/adaptive p-/h-/hp-refinement
  - Adjoint enhancement
- EGRA + Adjoint enhancement
- Adaptive/incremental sampling

R&D in UQ Complexity → mixed uncertainties, multiphysics/multiscale

- Stochastic sensitivity analysis → enables OUU/MCUU and mixed UQ
- Mixed UQ with IVP/SOP/DSTE → greater accuracy/efficiency than nested sampling
  - Inner loop: stochastic expansions (aleatory or combined)
  - Outer loop: opt-based interval est.; global with data reuse (robust) or local with SSA (scalable)
- Multi-* → Multi-physics UQ, Multi-scale UQ, Multifidelity/Model Form UQ
- Random fields/Stochastic processes, Bayesian inference

Advanced deployment → mission impact using advanced UQ methods

Current emphases

Additional Resources

References

- **Full list of research publications: http://www.cs.sandia.gov/dakota/publications.html**
- **Selected research highlights: http://www.cs.sandia.gov/dakota/research.html**
- **Selected application examples: http://www.cs.sandia.gov/dakota/applications.html**
- **DAKOTA UQ method documentation: http://www.cs.sandia.gov/dakota/documentation.html (see Ch. 6 of Users Manual)**

Software Downloads

- **DAKOTA: http://www.cs.sandia.gov/dakota/download.html**
- **Related packages: http://www.cs.sandia.gov/dakota/packages.html**

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