Overview of Uncertainty Quantification Algorithm R&D in the DAKOTA Project

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Survey of nonintrusive UQ methods:

- Sampling
- Local and global reliability
- Stochastic expansions: polynomial chaos, stochastic collocation

Build on these algorithmic foundations:

- Mixed aleatory-epistemic UQ, Opt/model calibration under uncertainty

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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	recursive emulation, TGP	*Local:* Notre Dame, *Global:* Vanderbilt
Stochastic expansion		PCE and SC with uniform & dimension-adaptive p-/h-refinement	local h-refinement, gradient-enhanced	hp-adaptive, discrete, multi-physics	Stanford, Purdue, Austr. Natl., FSU
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, UT Austin
Metrics & Global SA	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		LANL

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Research: Adaptive Refinement, Basis Enhancement

Adv. Deployment

Fills Gaps

Algorithm R&D in Adaptive UQ

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

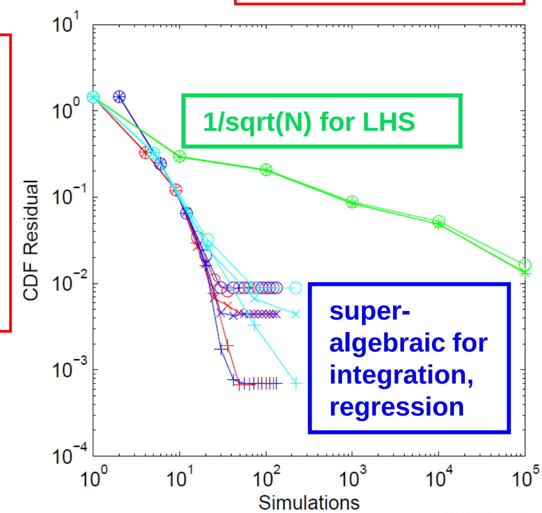
$$R = \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

Drivers

- Efficient/robust/*scalable* core → adaptive methods, adjoint enhancement
- Complex random environments → epistemic/mixed UQ, model form/multifidelity, RF/SP, multiphysics/multiscale

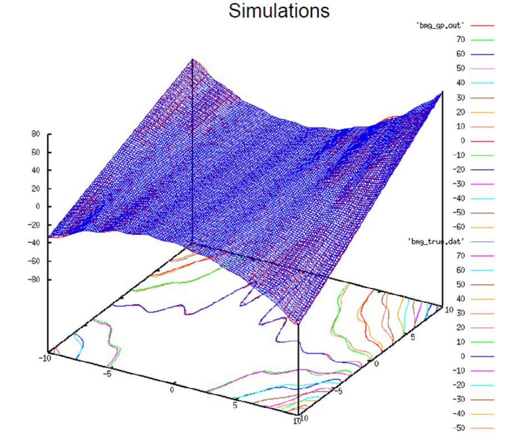
Stochastic expansions:

- *Polynomial chaos expansions (PCE)*: known basis, compute coeffs
- *Stochastic collocation (SC)*: known coeffs, form interpolants
- Adaptive approaches: emphasize key dimensions
  - Uniform/dim-adaptive p-refinement: iso/aniso/generalized sparse grids
  - Dimension-adaptive h-refinement with grad-enhanced interpolants
- 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 ~n^2



Sampling:

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

Algorithm R&D in UQ Complexity

Drivers

- Efficient/robust/*scalable* core → 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

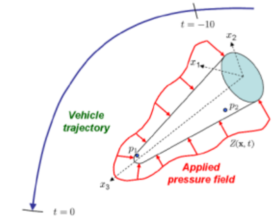
$$R(\xi, s) = \sum_{j=0}^{P} \alpha_j(s)\Psi_j(\xi)$$

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

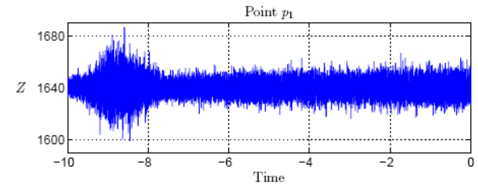
Design and Model Calibration Under Uncertainty

Mixed Aleatory-Epistemic UQ

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

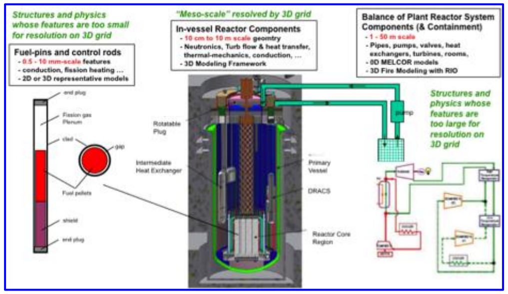


Random Fields / Stochastic Processes (Encore, PECOS)



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), model averaging/selection (ensemble)

Reliability Methods for UQ

UQ with Reliability Methods

Mean Value Method

$$\mu_g = g(\mu_{\mathbf{x}})$$

$$\sigma_g^2 = \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}})$$

$$\bar{z} \rightarrow p, \beta \begin{cases} \beta_{cdf} = \dfrac{\mu_g - \bar{z}}{\sigma_g} \\ \beta_{ccdf} = \dfrac{\bar{z} - \mu_g}{\sigma_g} \end{cases}$$

$$\bar{p}, \bar{\beta} \rightarrow z \begin{cases} z = \mu_g - \sigma_g \bar{\beta}_{cdf} \\ z = \mu_g + \sigma_g \bar{\beta}_{ccdf} \end{cases}$$

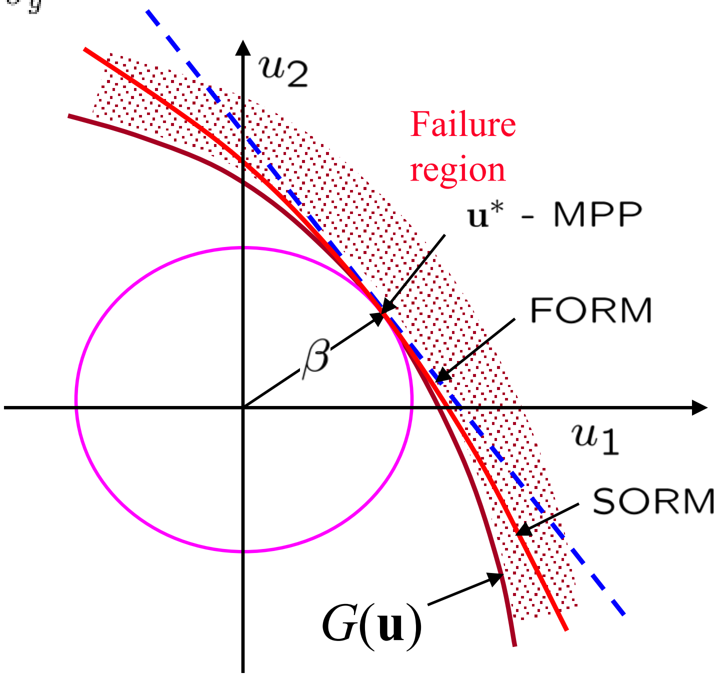
Rough statistics

MPP search methods

Reliability Index Approach (RIA)

$$\begin{array}{ll} \text{minimize} & \mathbf{u}^T\mathbf{u} \\ \text{subject to} & G(\mathbf{u}) = \bar{z} \end{array}$$

Find min dist to G level curve
Used for fwd map $z \rightarrow p/\beta$



Performance Measure Approach (PMA)

$$\begin{array}{ll} \text{minimize} & \pm G(\mathbf{u}) \\ \text{subject to} & \mathbf{u}^T\mathbf{u} = \bar{\beta}^2 \end{array}$$

Find min G at β radius
Used for inv map $p/\beta \rightarrow z$

Nataf x → u:
$$\Phi(z_i) = F(x_i)$$
$$\mathbf{z} = \mathbf{L}\mathbf{u}$$

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Reliability Algorithm Variations

Limit state approximations

$$\begin{aligned}
\text{AMV:}\quad & g(\mathbf{x}) = g(\mu_{\mathbf{x}}) + \nabla_x g(\mu_{\mathbf{x}})^T (\mathbf{x} - \mu_{\mathbf{x}}) \\
\text{u-space AMV:}\quad & G(\mathbf{u}) = G(\mu_{\mathbf{u}}) + \nabla_u G(\mu_{\mathbf{u}})^T (\mathbf{u} - \mu_{\mathbf{u}}) \\
\text{AMV+:}\quad & g(\mathbf{x}) = g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T (\mathbf{x} - \mathbf{x}^*) \\
\text{u-space AMV+:}\quad & G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T (\mathbf{u} - \mathbf{u}^*) \\
\text{FORM:}\quad & \text{no linearization}
\end{aligned}$$

- **2nd-order local, e.g. x-space AMV^2+:**

$$g(\mathrm{x}) \cong g(\mathrm{x}^*) + \nabla_x g(\mathrm{x}^*)^T (\mathrm{x} - \mathrm{x}^*) + \frac{1}{2} (\mathrm{x} - \mathrm{x}^*)^T \nabla_x^2 g(\mathrm{x}^*) (\mathrm{x} - \mathrm{x}^*)$$

- **Hessians may be full/FD/Quasi**
- **Quasi-Newton Hessians may be BFGS or SR1**

Reliability Algorithm Variations

Limit state approximations

$$\text{AMV:} \quad g(\mathbf{x}) = g(\mu_{\mathbf{x}}) + \nabla_x g(\mu_{\mathbf{x}})^T(\mathbf{x} - \mu_{\mathbf{x}})$$

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

$$\text{AMV+:} \quad g(\mathbf{x}) = g(\mathbf{x}^*) + \nabla_x g$$

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

FORM: no linearization

- **Multipoint, e.g. TPEA, TANA:**

$$g(\mathbf{x}) \cong g(\mathbf{x}_2) + \sum_{i=1}^{n} \frac{\partial g}{\partial x_i}(\mathbf{x}_2) \frac{x_{i,2}^{1-p_i}}{p_i}(x_i^{p_i} - x_{i,2}^{p_i}) + \frac{1}{2}\epsilon(\mathbf{x}) \sum_{i=1}^{n} (x_i^{p_i} - x_{i,2}^{p_i})^2$$

$$p_i = 1 + \ln\left[\frac{\frac{\partial g}{\partial x_i}(\mathbf{x}_1)}{\frac{\partial g}{\partial x_i}(\mathbf{x}_2)}\right] \Big/ \ln\left[\frac{x_{i,1}}{x_{i,2}}\right]$$

$$\epsilon(\mathbf{x}) = \frac{H}{\sum_{i=1}^{n}(x_i^{p_i} - x_{i,1}^{p_i})^2 + \sum_{i=1}^{n}(x_i^{p_i} - x_{i,2}^{p_i})^2}$$

$$H = 2\left[g(\mathbf{x}_1) - g(\mathbf{x}_2) - \sum_{i=1}^{n} \frac{\partial g}{\partial x_i}(\mathbf{x}_2)\frac{x_{i,2}^{1-p_i}}{p_i}(x_{i,1}^{p_i} - x_{i,2}^{p_i})\right]$$

- **2nd-order local, e.g. x-space AM**

$$g(\mathbf{x}) \cong g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T(\mathbf{x} - \mathbf{x}^*) + \frac{1}{2}(\mathbf{x}$$

- **Hessians may be full/FD/Quasi**
- **Quasi-Newton Hessians may be BFGS or SR1**

Integrations

1st-order:
$$\begin{cases} p(g \le z) = \Phi(-\beta_{cdf}) \\ p(g > z) = \Phi(-\beta_{ccdf}) \end{cases}$$

2nd-order: Breit, Hohen-Rack, Hong

$$p = \Phi(-\beta) \prod_{i=1}^{n-1} \frac{1}{\sqrt{1 + \beta\kappa_i}}$$

curvature correction

Additional refinement:

IS, AIS, MMAIS

MPP search algorithm

[HL-RF], Sequential Quadratic Prog. (SQP), Nonlinear Interior Point (NIP)

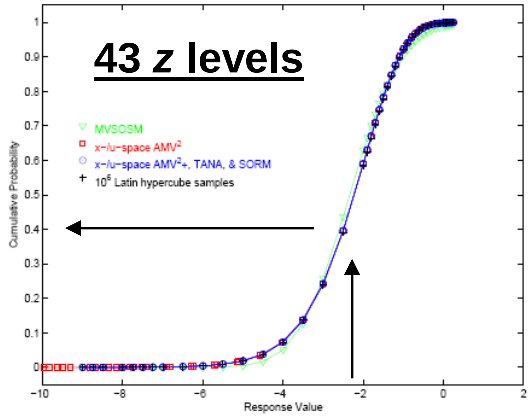
Warm starting (with projections)

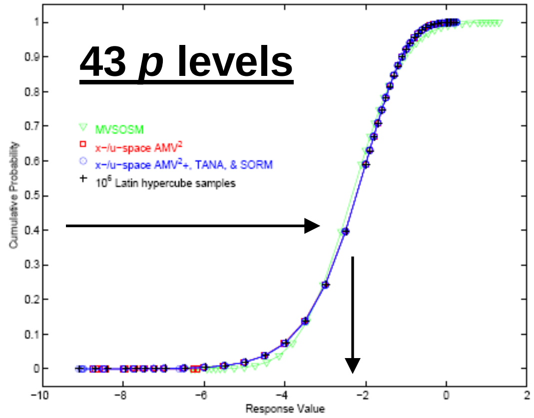
When: **AMV+ iteration increment, *z/p/β* level increment, or design variable change**

What: **linearization point & assoc. responses (AMV+), MPP search initial guess**

Reliability Algorithm Variations: Algorithm Performance Results

Analytic benchmark test problems: lognormal ratio, short column, cantilever





RIA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF p Error Norm	Target z Offset Norm
MVFOSM	1	1	0.1548	0.0
MVSOSM	1	1	0.1127	0.0
x-space AMV	45	45	0.009275	18.28
u-space AMV	45	45	0.006408	18.81
x-space AMV^2	45	45	0.002063	2.482
u-space AMV^2	45	45	0.001410	2.031
x-space AMV+	192	192	0.0	0.0
u-space AMV+	207	207	0.0	0.0
x-space AMV^2+	125	131	0.0	0.0
u-space AMV^2+	122	130	0.0	0.0
x-space TANA	245	246	0.0	0.0
u-space TANA	296*	278*	6.982e-5	0.08014
FORM	626	176	0.0	0.0
SORM	669	219	0.0	0.0

PMA Approach	SQP Function Evaluations	NIP Function Evaluations	CDF z Error Norm	Target p Offset Norm
MVFOSM	1	1	7.454	0.0
MVSOSM	1	1	6.823	0.0
x-space AMV	45	45	0.9420	0.0
u-space AMV	45	45	0.5828	0.0
x-space AMV^2	45	45	2.730	0.0
u-space AMV^2	45	45	2.828	0.0
x-space AMV+	171	179	0.0	0.0
u-space AMV+	205	205	0.0	0.0
x-space AMV^2+	135	142	0.0	0.0
u-space AMV^2+	132	139	0.0	0.0
x-space TANA	293*	272	0.04259	1.598e-4
u-space TANA	325*	311*	2.208	5.600e-4
FORM	720	192	0.0	0.0
SORM	535	191*	2.410	6.522e-4

Note: 2nd-order PMA with prescribed *p* level is harder problem → requires $\beta(p)$ update/inversion

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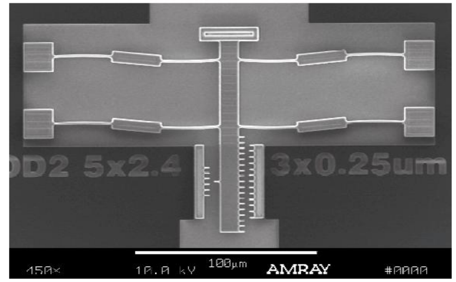
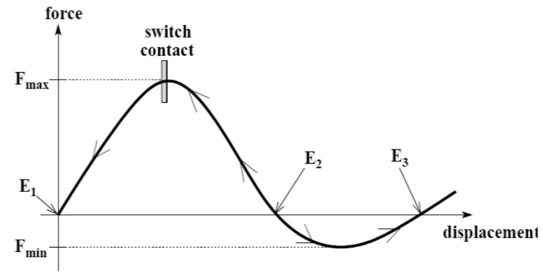
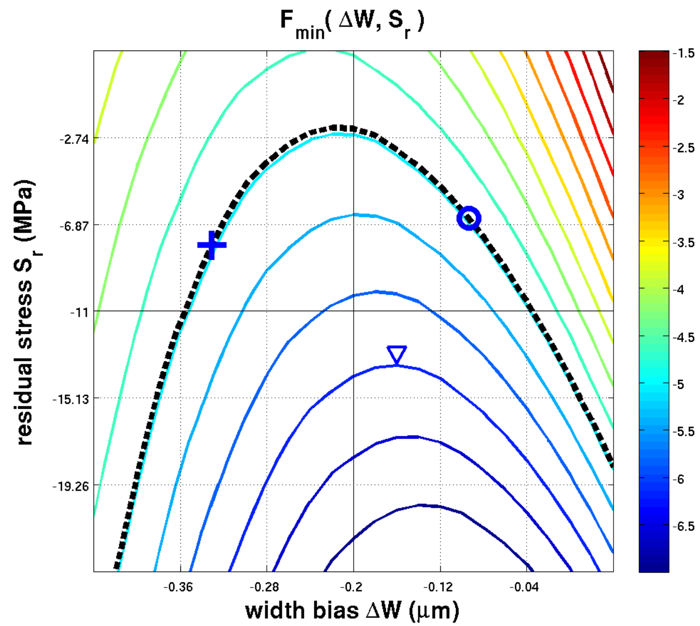
Solution-Verified Reliability Analysis and Design of MEMS

- **Problem:** MEMS subject to substantial variabilities
  - Material properties, manufactured geometry, residual stresses
  - Part yields can be low or have poor durability
  - Data can be obtained → aleatory UQ → probabilistic methods
- **Goal:** account for both uncertainties and errors in design
  - Integrate UQ/OUU (DAKOTA), ZZ/QOI error estimation (Encore), adaptivity (SIERRA), nonlin mech (Aria) → MESA application
  - Perform soln verification in automated, parameter-adaptive way
  - Generate fully converged UQ/OUU results at lower cost





- AMV^2+ and FORM converge to different MPPs (+ and O respectively)
- Issue: high nonlinearity leading to multiple legitimate MPP solns.
- Challenge: design optimization may tend to seek out regions encircled by the failure domain. 1st-order and even 2nd-order probability integrations can experience difficulty with this degree of nonlinearity. Optimizers can/will exploit this model weakness.



Parameter study over 3σ uncertain variable range for fixed design variables d_M*. ***Dashed black line denotes $g(x) = F_{min}(x) = -5.0$.***

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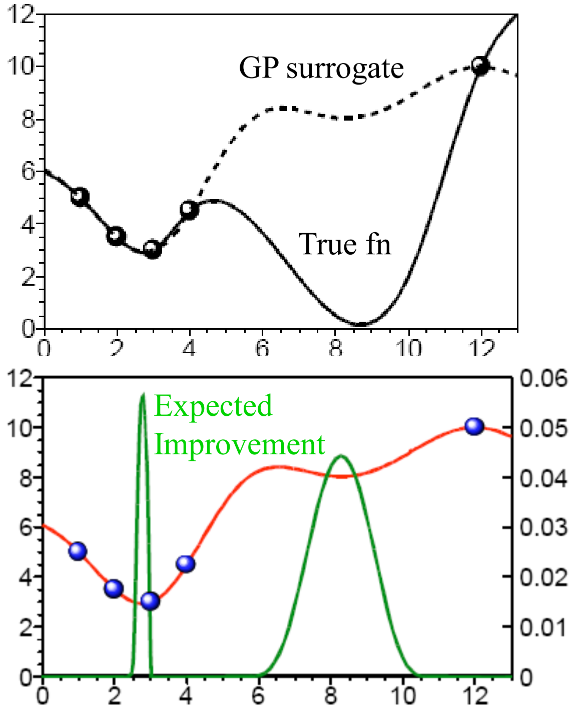
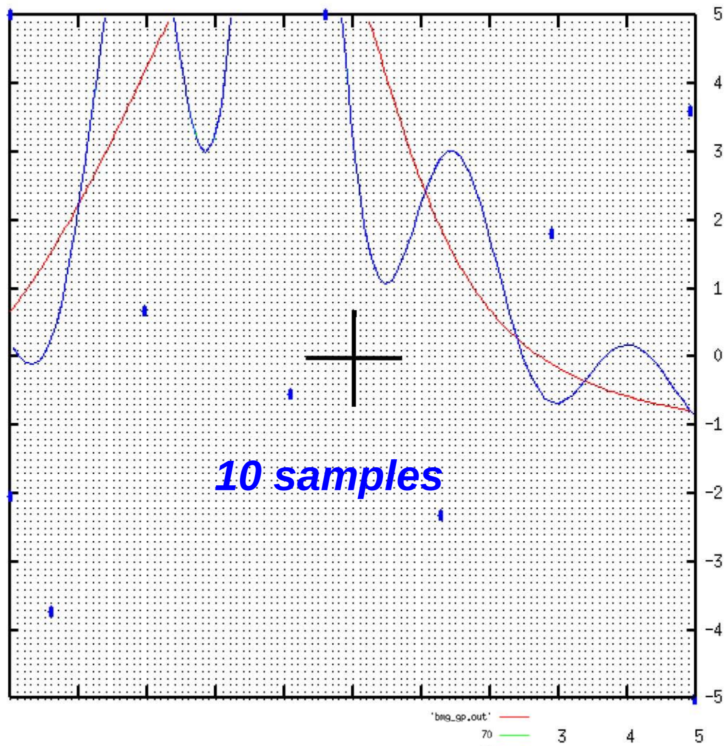
Efficient Global Reliability Analysis (EGRA)

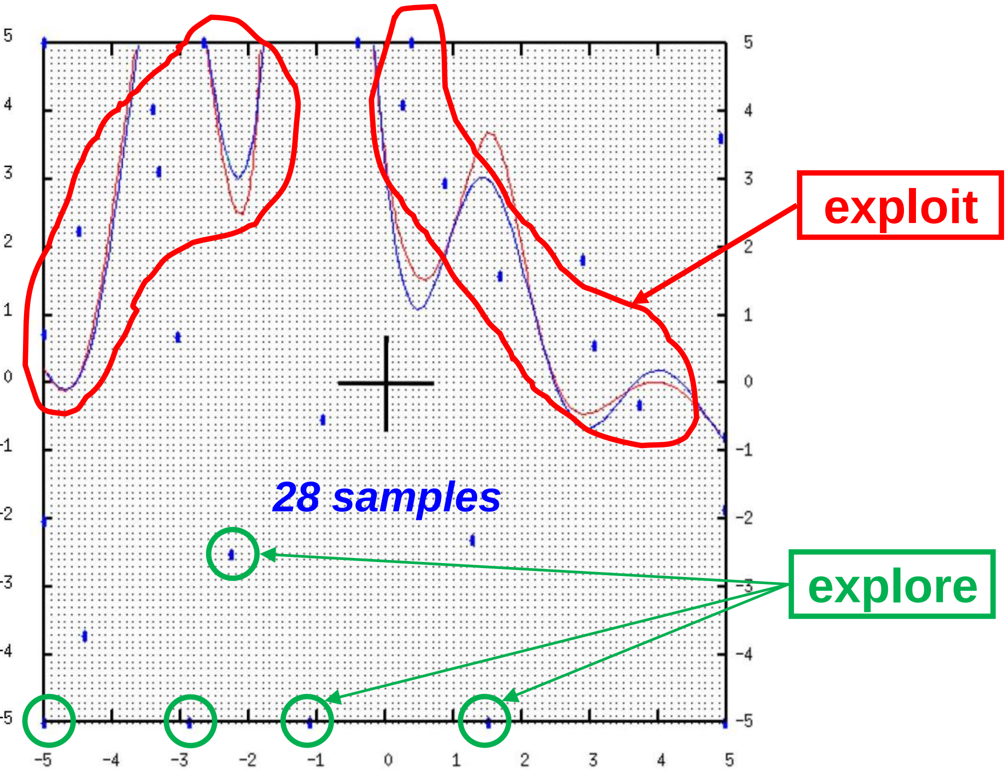
- **Address known failure modes of local reliability methods:**
  - Nonsmooth: fail to converge to an MPP
  - Multimodal: only locate one of several MPPs
  - Highly nonlinear: low order limit state approxs. fail to accurately estimate probability at MPP
- **Based on EGO (surrogate-based global opt.), 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)

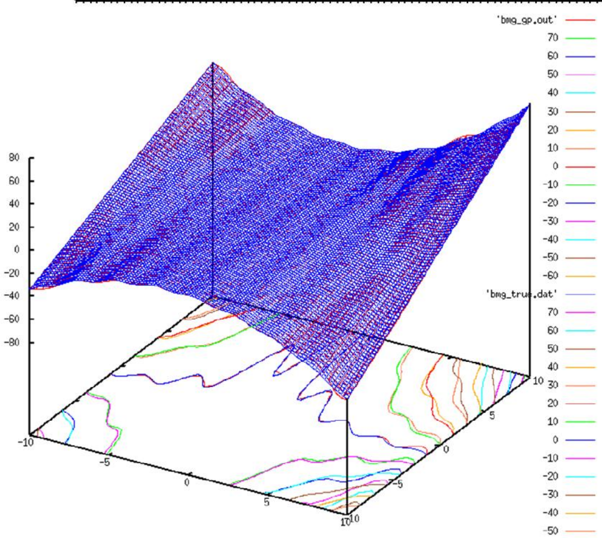


From Jones, Schonlau, Welch, 1998

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%)

Stochastic Expansion Methods for UQ

Polynomial Chaos Expansions (PCE)

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

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

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

- Nonintrusive: estimate α_j using sampling, regression, tensor-product quadrature, sparse grids, or cubature

$$\boxed{\alpha_j \;=\; \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} \;=\; \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R \, \Psi_j \, \varrho(\boldsymbol{\xi}) \, d\boldsymbol{\xi}}$$

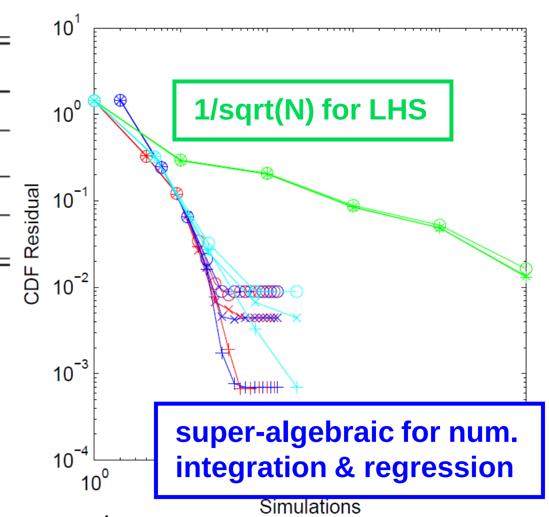
$$\boxed{\langle \Psi_j^2 \rangle \;=\; \prod_{i=1}^{n} \langle \psi_{m_i^j}^2 \rangle}$$

Generalized PCE (Wiener-Askey + numerically-generated)

- Tailor basis: selection of basis orthogonal to input PDF avoids additional nonlinearity

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

Additional bases generated numerically (discretized Stieltjes + Golub-Welsch)



- Tailor expansion form:
  - Dimension p-refinement: anisotropic TPQ/SSG, generalized SSG
  - Dimension & region h-refinement: local bases with global & local refinement

Stochastic Collocation
(based on interpolation polynomials)

Instead of estimating coefficients for known basis functions, form <u>interpolants</u> for known coefficients

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

- ***Global:*** Lagrange (values) or Hermite (values+derivatives)
- ***Local:*** linear (values) or cubic (values+gradients) splines

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

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

Sparse interpolants formed using Σ of tensor interpolants

Advantages relative to PCE:

- Somewhat simpler (no expansion order to manage separately)
- Often less expensive (no integration for coefficients)
- Expansion only formed for sampling → probabilities (estimating moments of any order is straightforward)
- Adaptive h-refinement with hierarchical surpluses; explicit gradient-enhancement

Disadvantages relative to PCE:

- Less flexible/fault tolerant → structured data sets (tensor/sparse grids)
- Expansion variance not guaranteed positive (important in opt./interval est.)
- No direct inference of spectral decay rates

With sufficient care on PCE form, PCE/SC performance is essentially identical for many cases of interest (tensor/sparse grids with standard Gauss rules)

Approaches for forming PCE/SC Expansions

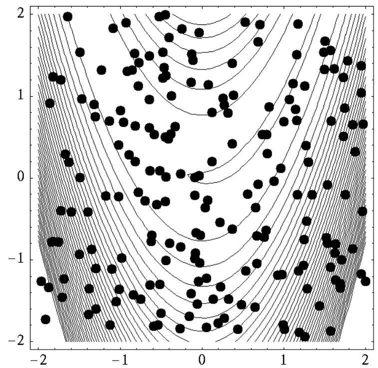
Random sampling: PCE

Expectation (sampling):

- Sample w/i distribution of ξ
- Compute expected value of product of $\boldsymbol{R}$ and each Ψ_j

Linear regression ("point collocation"):

- Sample w/i distribution of ξ
- Solves least squares data fit for all coefficients at once:



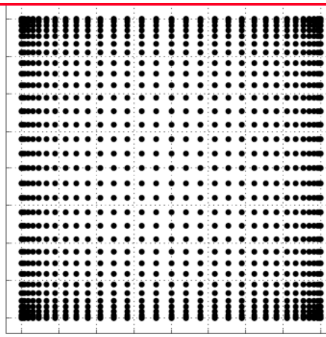
$$\boxed{\Psi\alpha = R}$$

Tensor-product quadrature: PCE/SC

$$\boxed{\mathscr{U}^i(f)(\xi) = \sum_{j=1}^{m_i} f(\xi_j^i)\, w_j^i}$$

$$\boxed{\mathcal{Q}_{\mathbf{i}}^n f(\xi) = \left(\mathscr{U}^{i_1}\otimes\cdots\otimes\mathscr{U}^{i_n}\right)(f)(\xi) = \sum_{j_1=1}^{m_{i_1}}\cdots\sum_{j_n=1}^{m_{i_n}} f\left(\xi_{j_1}^{i_1},\dots,\xi_{j_n}^{i_n}\right)\left(w_{j_1}^{i_1}\otimes\cdots\otimes w_{j_n}^{i_n}\right)}$$

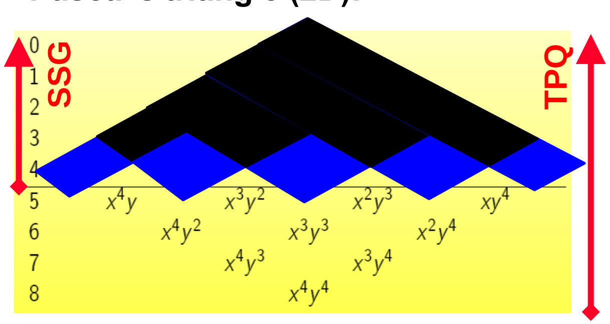
- **Every combination of 1-D rules**
- **Scales as m^n**
- **1-D Gaussian rule of order m → integrands to order $2m-1$**
- **Assuming $R\,\Psi_j$ of order $2p$, select $m = p + 1$**

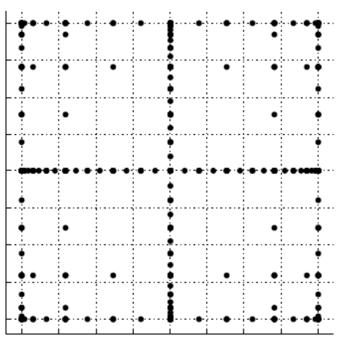


Smolyak Sparse Grid: PCE/SC

$$\mathscr{A}(\mathrm{w},n) = \sum_{\mathrm{w}+1\le|\mathbf{i}|\le\mathrm{w}+n} (-1)^{\mathrm{w}+n-|\mathbf{i}|}\binom{n-1}{\mathrm{w}+n-|\mathbf{i}|}\cdot\left(\mathscr{U}^{i_1}\otimes\cdots\otimes\mathscr{U}^{i_n}\right)$$

Pascal's triangle (2D):



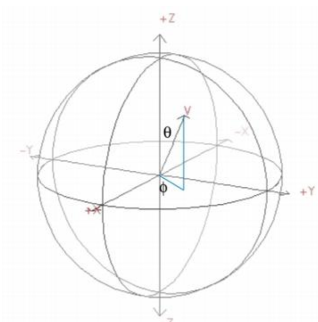


Cubature: PCE

Stroud and extensions (Xiu, Cools)

→ Low order PCE

→ global SA, anisotropy detection



Gaussian $i = 2$ → $p = 1$

$$\boxed{x_{k,2r-1} = \sqrt{2}\cos\frac{2rk\pi}{n+1}, \qquad x_{k,2r} = \sqrt{2}\sin\frac{2rk\pi}{n+1}}$$

Arbitrary PDF $\boxed{t^{(k)} = \frac{1}{\gamma}\left[\sqrt{\gamma c_1}\,x^{(k)} - \delta\right]}$

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Adaptive Collocation Methods

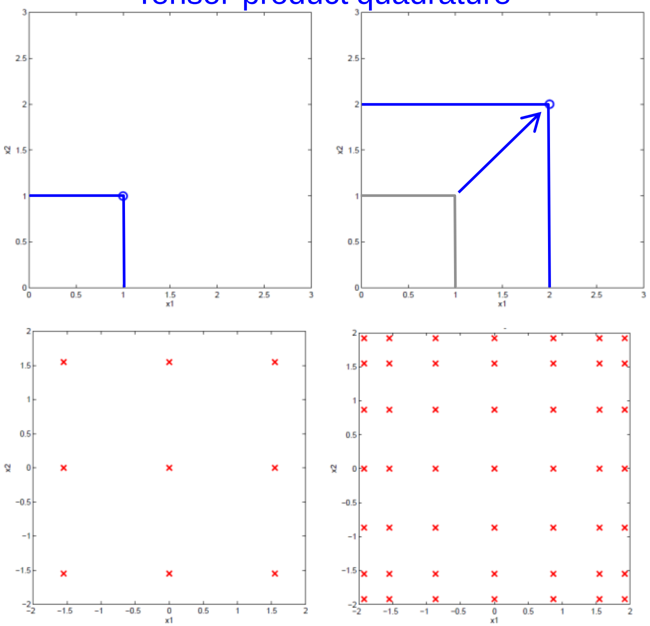
Drivers: Efficiency, robustness, *scalability* → adaptive methods, adjoint enhancement

Polynomial order (p-) refinement approaches:

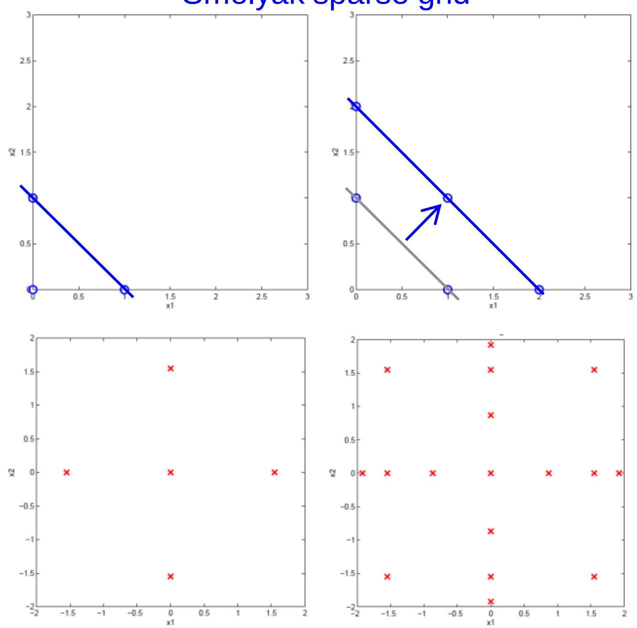
- **Uniform:** *isotropic* tensor/sparse grids
  - *Increment grid:* increase order/level, ensure change (restricted growth in nested rules)
  - *Assess convergence:* L^2 change in response covariance

$$\boxed{\mathrm{w}+1 \leq |\mathbf{i}| \leq \mathrm{w}+n}$$

Tensor-product quadrature



Smolyak sparse grid



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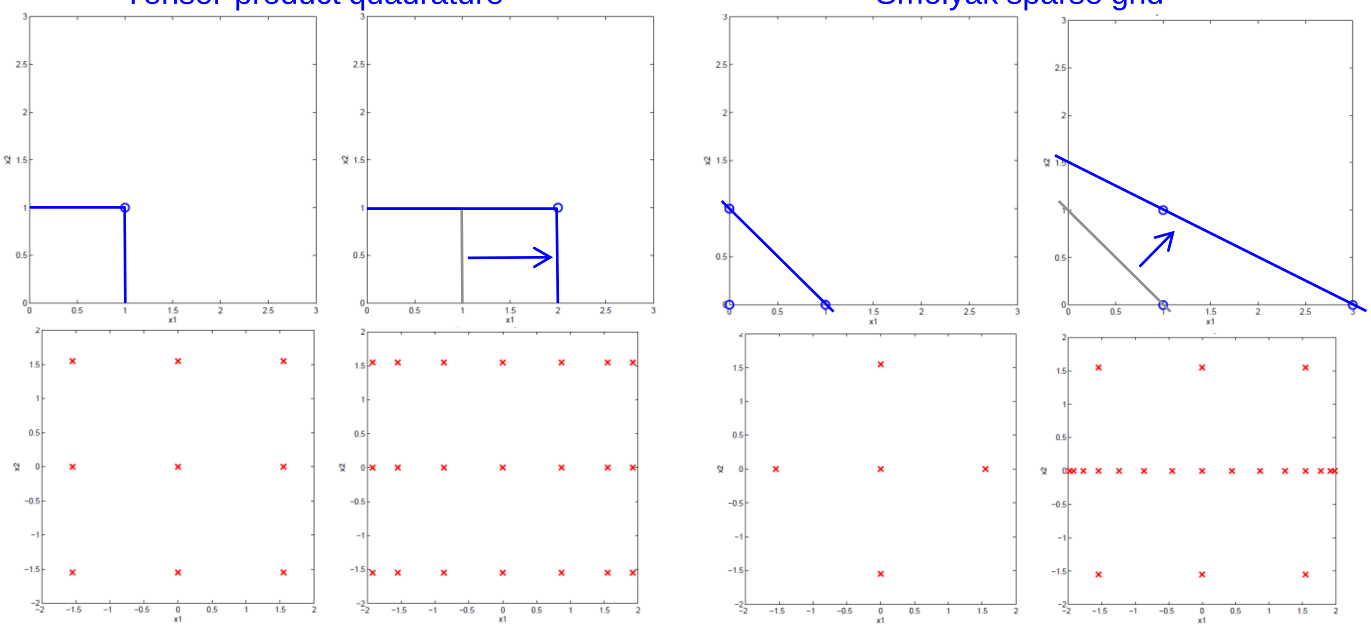
  - *Assess convergence:* L^2 change in response covariance
- **Dimension-adaptive:** *anisotropic* tensor/sparse grids
  - **PCE/SC:** variance-based decomp. → total Sobol' indices → anisotropy (dimension preference)
  - **PCE:** spectral coefficient decay rates → anisotropy (index set weights)

$$\boxed{\mathrm{w}\underline{\gamma} < \mathbf{i}\cdot\gamma \le \mathrm{w}\underline{\gamma} + |\gamma|}$$

Tensor-product quadrature

Smolyak sparse grid



Adaptive Collocation Methods

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- **Dimension-adaptive:** *anisotropic* tensor/sparse grids $\boxed{w\underline{\gamma} < \mathbf{i}\cdot\gamma \leq w\underline{\gamma} + |\gamma|}$
  - **PCE/SC:** variance-based decomp. → total Sobol' indices → anisotropy
  - **PCE:** spectral coefficient decay rates → anisotropy
- **Goal-oriented dimension-adaptive:** *generalized* sparse grids
  - **PCE/SC:** change in QOI induced by trial index sets on active front

1. ***Initialization:*** Starting from reference grid (often w = 0 grid), define active index sets using admissible forward neighbors of all old index sets.

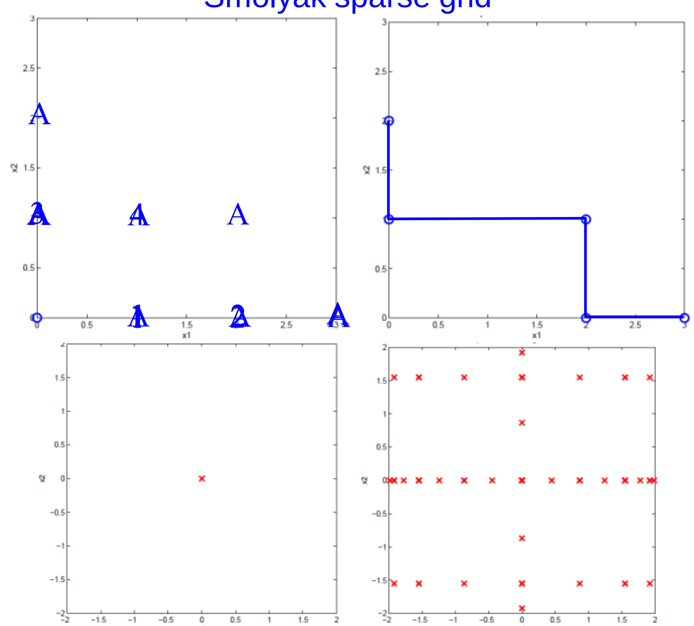
2. ***Trial set evaluation:*** For each trial index set, evaluate tensor grid, form tensor expansion, update combinatorial coefficients, and combine with reference expansion. Perform necessary bookkeeping to allow efficient restoration.

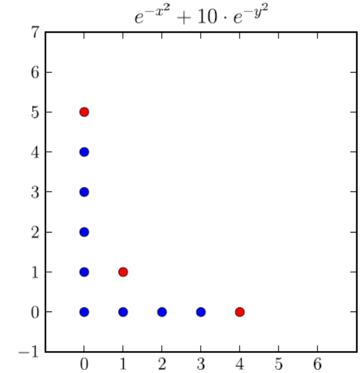
3. ***Trial set selection:*** Select trial index set that induces largest change in statistical QOI.

4. ***Update sets:*** If largest change > tolerance, then promote selected trial set from active to old and compute new admissible active sets; return to 2. If tolerance is satisfied, advance to step 5.

5. ***Finalization:*** Promote all remaining active sets to old set, update combinatorial coefficients, and perform final combination of tensor expansions to arrive at final result for statistical QOI.

Smolyak sparse grid





(Gerstner, 2003)

Fine-grained control: frontier not limited by prescribed shape of index set constraint

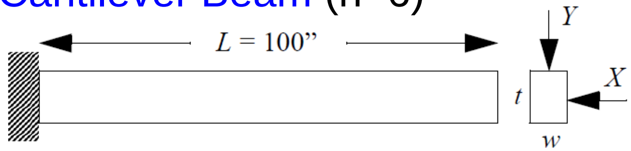
Numerical Experiments

Short Column (n=5)

$$g(\mathbf{x}) = 1 - \frac{4M}{bh^2Y} - \frac{P^2}{b^2h^2Y^2}$$

$b = U[5,15]$, $h = U[15,25]$,
$P = N(500, 100)$, $M = N(2000, 400)$,
$\rho_{P,M} = 0.5$, $Y = logN(5, 0.5)$

Cantilever Beam (n=6)



$$\begin{aligned} S &= \frac{600}{wt^2}Y + \frac{600}{w^2t}X &\leq R \\ D &= \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} &\leq D_0 \end{aligned}$$

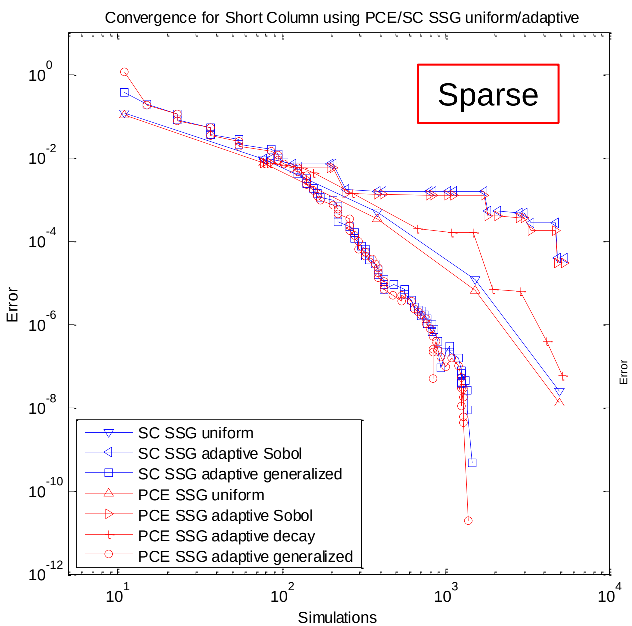
w, t, R, E, X, Y: $U[1,10]$, $U[1,10]$,
$N(4E4, 2E3)$, $N(2.9E7, 1.45E6)$,
$N(500, 100)$, $N(1E3, 100)$; $D_0 = 2.2535$”

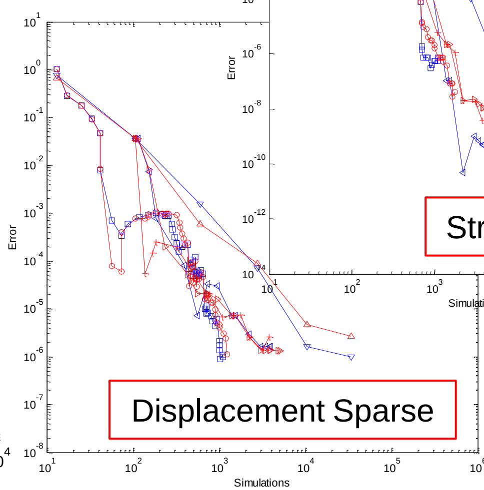
Ishigami (n=3)

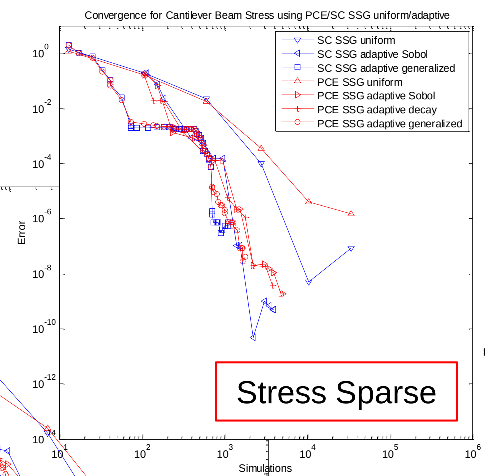
$$\begin{aligned} f(\mathbf{x}) &= \sin(2\pi x_1 - \pi) \\ &+ 7\sin^2(2\pi x_2 - \pi) \\ &+ 0.1(2\pi x_3 - \pi)^4 \sin(2\pi x_1 - \pi) \end{aligned}$$

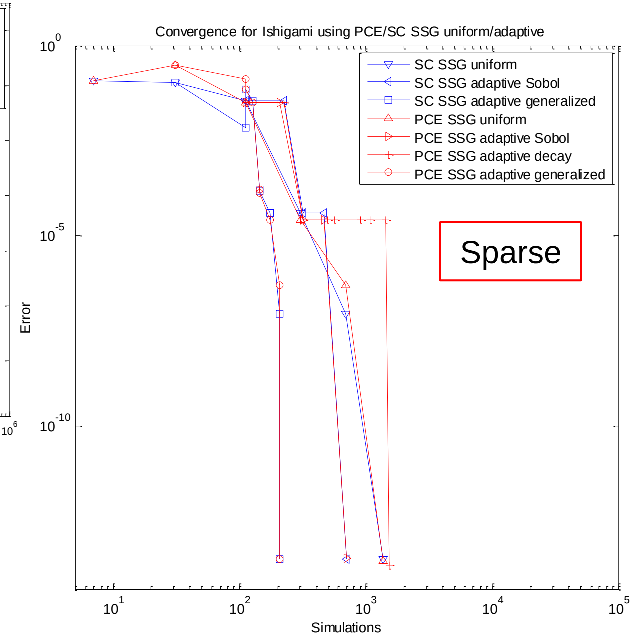
x_1, x_2, x_3: *iid* $U[0, 1]$

- Designed to be challenging for global SA: term cancellations at mid-point & bounds
- Premature convergence in adaptive methods → start from higher-order grid









Extend Scalability through Adjoint Derivative-Enhancement

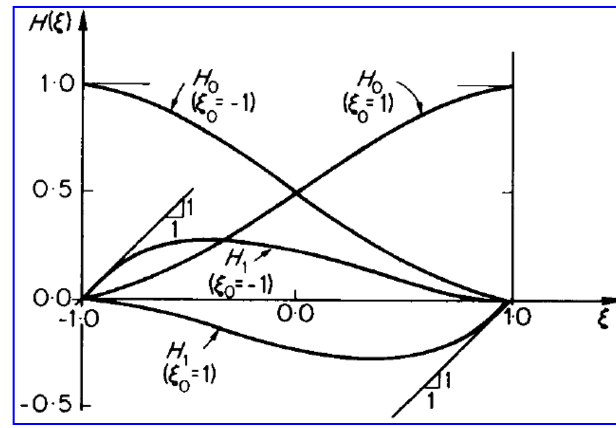
PCE:

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

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

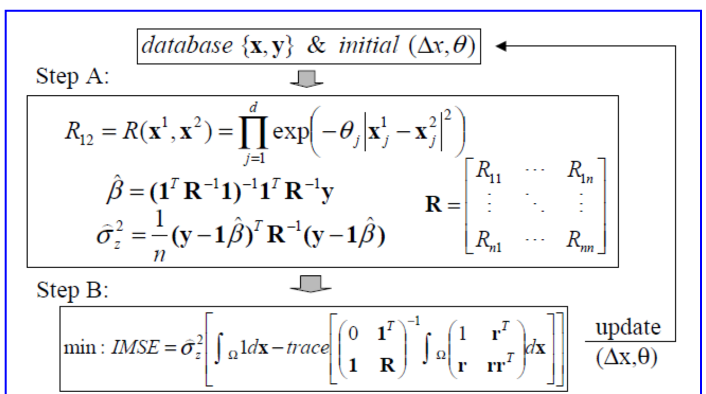
SC:

- Gradient-enhanced interpolants
  - Local: cubic Hermite splines
  - Global: Hermite interpolation polynomials



EGRA:

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



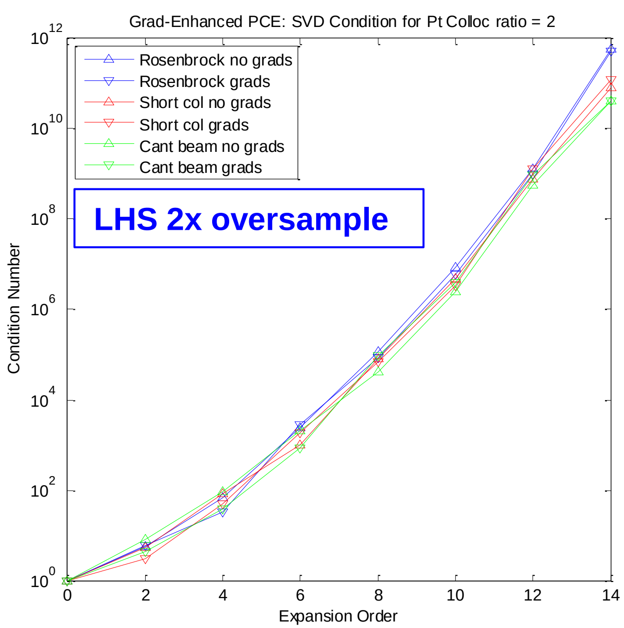
Gradient-Enhanced PCE

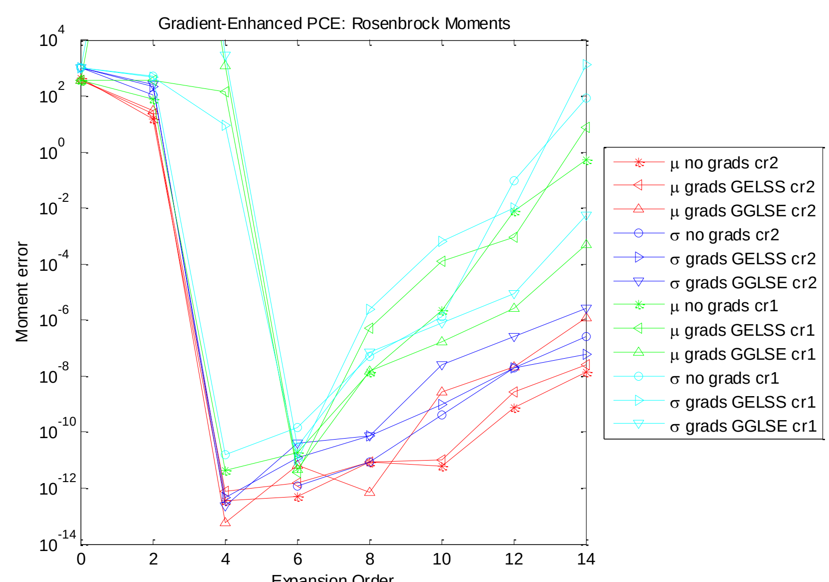
Straightforward regression approach:

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

- unweighted LLS by SVD (LAPACK GELSS)
- equality constrained LLS by QR (LAPACK GGLSE) when under-determined by values alone

Vandermonde-like systems known to suffer from ill-conditioning





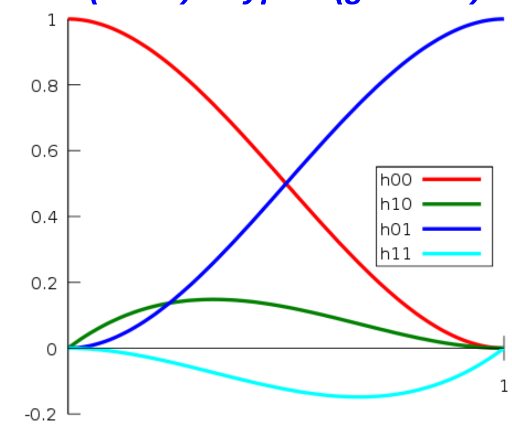
Error growth as we over-resolve exact solutions

Dimension-adaptive h-refinement with gradient-enhanced interpolants

Dimension-adaptive h-refinement for SC:

- *Local spline interpolants:* linear Lagrange (value-based), cubic Hermite (gradient-enhanced)
- *Global grids:* iso/aniso tensor, iso/aniso/generalized sparse
- *h-refinement:* uniform, adaptive, goal-oriented adaptive
- *Basis formulations:* nodal, hierarchical

Cubic shape fns: type 1 (value) & type 2 (gradient)



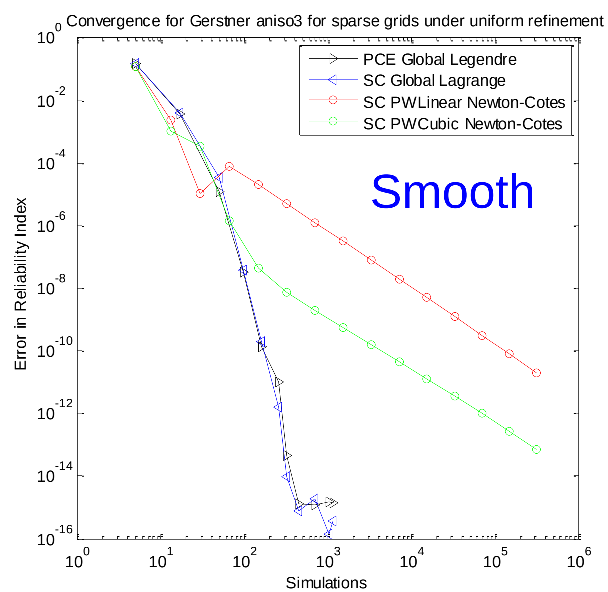
Multivariate tensor product to arbitrary derivative order (Lalescu):

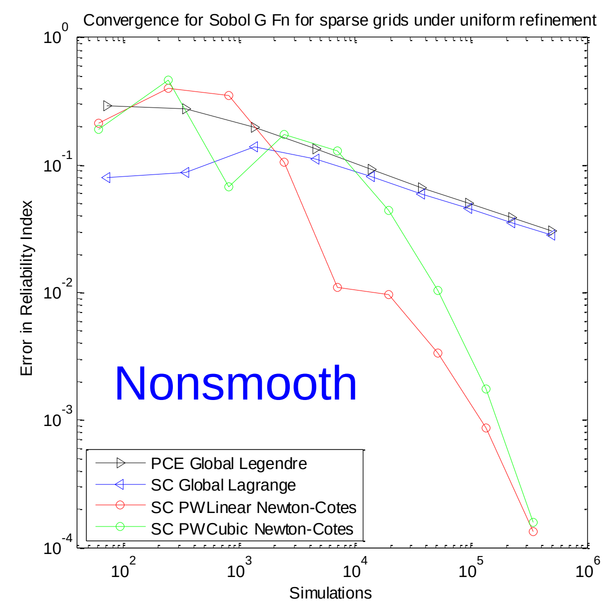
$$s^{(n)}(x_1, x_2, \ldots, x_D) = \sum_{l_1,\ldots,l_D=0}^{m} \sum_{i_1,\ldots,i_D=0,1} f^{(l_1,\ldots,l_D)}(i_1,\ldots,i_D) \prod_{k=1}^{D} \alpha_{i_k}^{(n,l_k)}(x_k)$$

$$\begin{aligned} f = &\sum_{i=1}^{N} f_i H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \\ &\sum_{i=1}^{N} \frac{df_i}{dx_1} H_i^{(2)}(x_1) H_i^{(1)}(x_2) H_i^{(1)}(x_3) + \\ &\sum_{i=1}^{N} \frac{df_i}{dx_2} H_i^{(1)}(x_1) H_i^{(2)}(x_2) H_i^{(1)}(x_3) + \\ &\sum_{i=1}^{N} \frac{df_i}{dx_3} H_i^{(1)}(x_1) H_i^{(1)}(x_2) H_i^{(2)}(x_3) \end{aligned}$$

$$\begin{aligned} \mu = &\sum_{i=1}^{N} f_i w_i^{(1)} w_i^{(1)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_1} w_i^{(2)} w_i^{(1)} w_i^{(1)} + \\ &\sum_{i=1}^{N} \frac{df_i}{dx_2} w_i^{(1)} w_i^{(2)} w_i^{(1)} + \sum_{i=1}^{N} \frac{df_i}{dx_3} w_i^{(1)} w_i^{(1)} w_i^{(2)} \end{aligned}$$

and similar for higher-order moments





Build on efficient/scalable UQ core

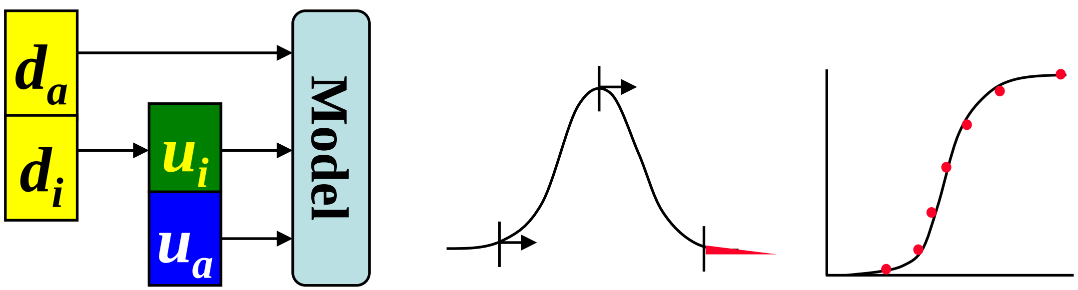
Stochastic sensitivity analysis

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

$$\boxed{R(\boldsymbol{\xi}, \boldsymbol{s}) = \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}, \boldsymbol{s})} \quad \left\{ \begin{array}{rcl} \frac{d\mu_R}{ds} & = & \langle \frac{dR}{ds} \rangle \\ \frac{d\sigma_R^2}{ds} & = & 2 \sum_{j=1}^{P} \alpha_j \langle \frac{dR}{ds}, \Psi_j \rangle \end{array} \right.$$

$$\boxed{R(\boldsymbol{\xi}, \boldsymbol{s}) = \sum_{j=0}^{P} \alpha_j(\boldsymbol{s}) \Psi_j(\boldsymbol{\xi})} \quad \left\{ \begin{array}{rcl} \mu_R(\boldsymbol{s}) & = & \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \\ \sigma_R^2(\boldsymbol{s}) & = & \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \alpha_k \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \Psi_k(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \; - \; \mu_R^2(\boldsymbol{s}) \end{array} \right.$$

Design and Model Calibration Under Uncertainty



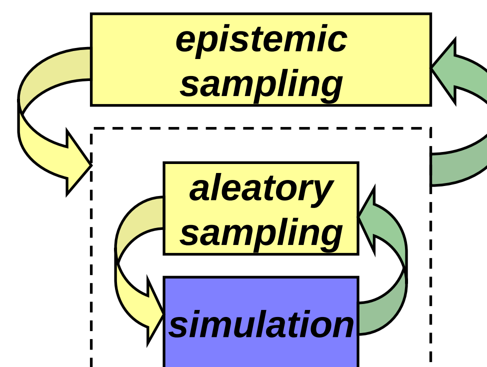
Add resp stats s_u *(μ, σ, $z/\beta/p$)*

$$\begin{array}{ll} \min & f(d) + W s_u(d) \\ \text{s.t.} & g_l \le g(d) \le g_u \\ & h(d) = h_t \\ & d_l \le d \le d_u \\ & a_l \le A_i\, s_u(d) \le a_u \\ & A_e\, s_u(d) = a_t \end{array}$$

Mixed Aleatory-Epistemic UQ

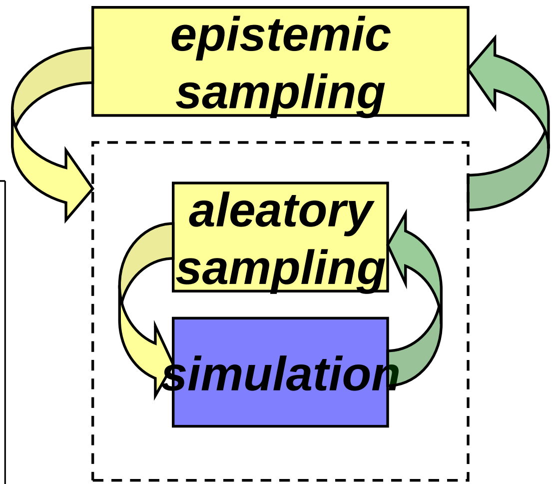
- Approaches that are more accurate/efficient than nested sampling
  - Interval-valued probability (IVP), *aka* PBA
  - Dempster-Shafer theory of evidence (DSTE)
  - Second-order probability (SOP), *aka* PoF

Increasing epistemic structure (stronger assumptions)



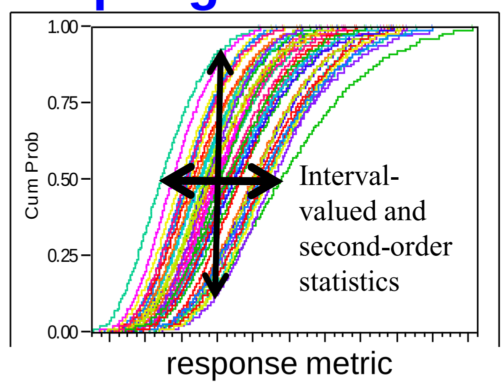
Mixed Aleatory-Epistemic UQ: IVP, DSTE, and SOP

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)

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

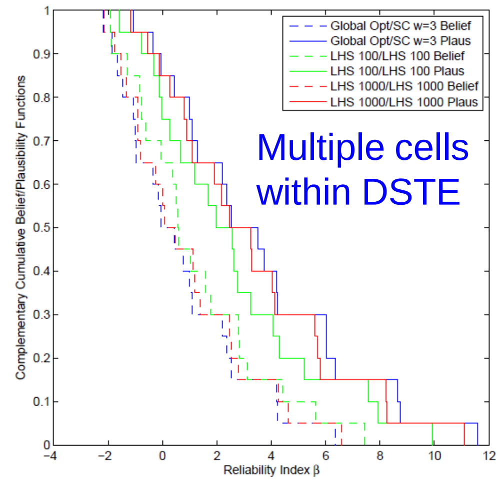
$$\begin{array}{ll} \text{maximize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \end{array}$$

Mixed Aleatory-Epistemic UQ:

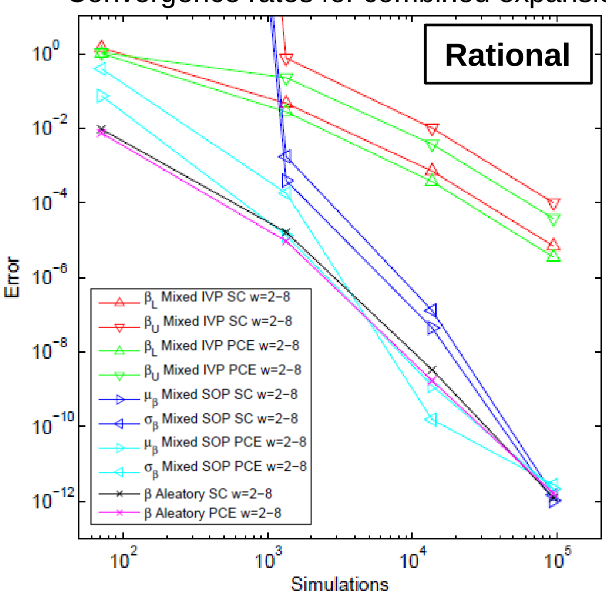
IVP, SOP, and DSTE based on Stochastic Expansions

Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals					
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]

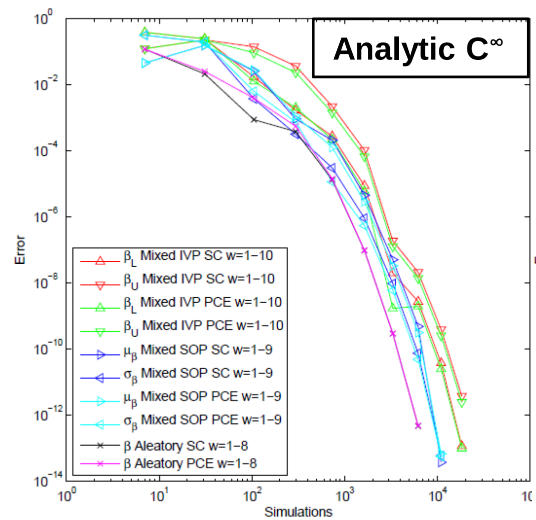


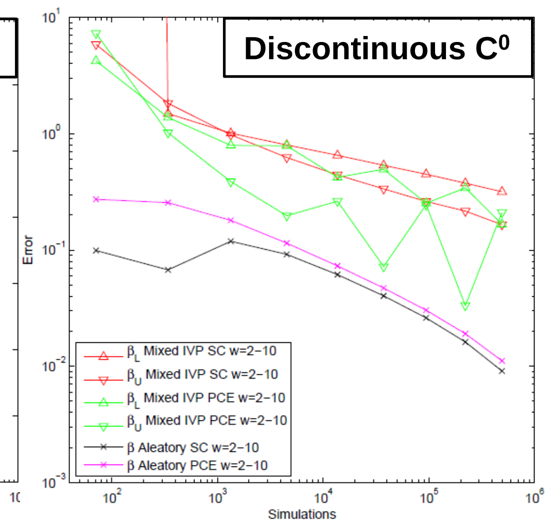
Convergence rates for combined expansions



L^∞ metrics: IVP mixed, DSTE mixed

L^2 metrics: Aleatory, SOP mixed





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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
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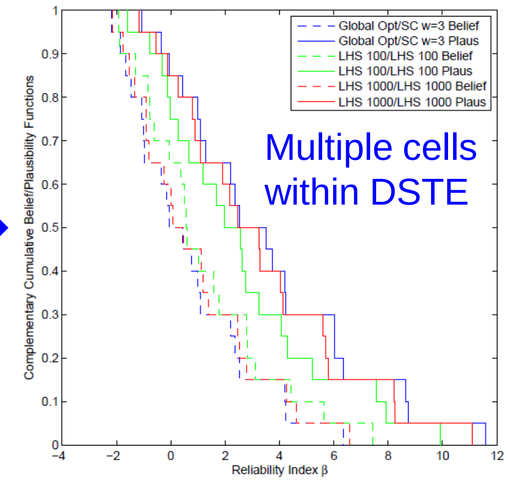
EGO	SC SSG w = 3	Aleatory	(1260/1365, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
EGO	SC SSG w = 4	Aleatory	(3564/3861, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 1	Aleatory	(21/77, 21/77)	[75.0000, 375.000]	[-2.26264, 11.8623]
NPSOL	SC SSG w = 2	Aleatory	(93/341, 93/341)	[75.0000, 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

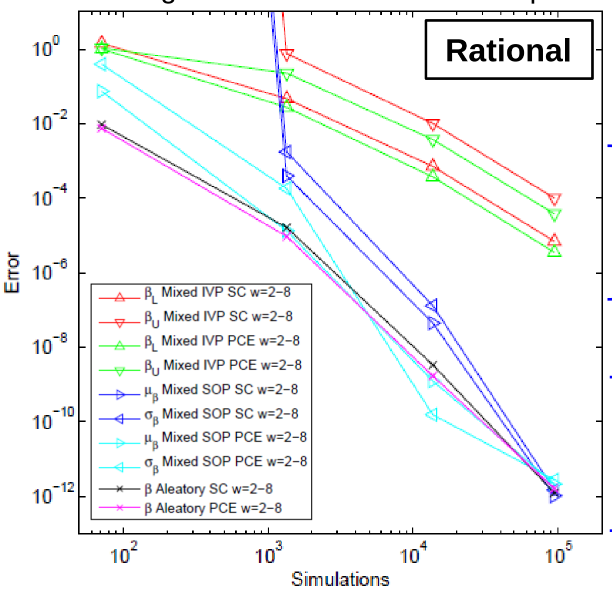
LHS 100	LHS 100	N/A	$(10^4/10^4, 0/0)$	[80.5075, 338.607]	[-2.14505, 8.64891]
LHS 1000	LHS 1000	N/A	$(10^6/10^6, 0/0)$	[76.5939, 368.225]	[-2.19883, 11.2353]
LHS 10^4	LHS 10^4	N/A	$(10^8/10^8, 0/0)$	[76.4755, 373.935]	[-2.16323, 11.5593]

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



Multiple cells within DSTE

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

Concluding Remarks

R&D Drivers: **efficient/robust/scalable core, complex random environments**

Survey of core UQ algorithms: **strengths, weaknesses, research needs**

Sampling (nongradient-based)

- ***Strengths:*** **Simple and reliable, convergence rate is dimension-independent**
- ***Weaknesses:*** **1/sqrt(N) convergence → expensive for accurate tail statistics**

Local reliability (gradient-based)

- ***Strengths:*** **computationally efficient, widely used, scalable to large *n* (w/ efficient derivs.)**
- ***Weaknesses:*** **algorithmic failures for limit states with following features**
  - **Nonsmooth: fail to converge to an MPP**
  - **Multimodal: only locate one of several MPPs**
  - **Highly nonlinear: low order limit state approxs. insufficient to resolve probability at MPP**

Global reliability (typically nongradient-based)

- ***Strengths:*** **handles multimodal and/or highly nonlinear limit states**
- ***Weaknesses:***
  - **Conditioning, nonsmoothness → ensemble emulation (recursion, discretization)**
  - **Scaling to large *n* → adjoints, additional refinement bias**

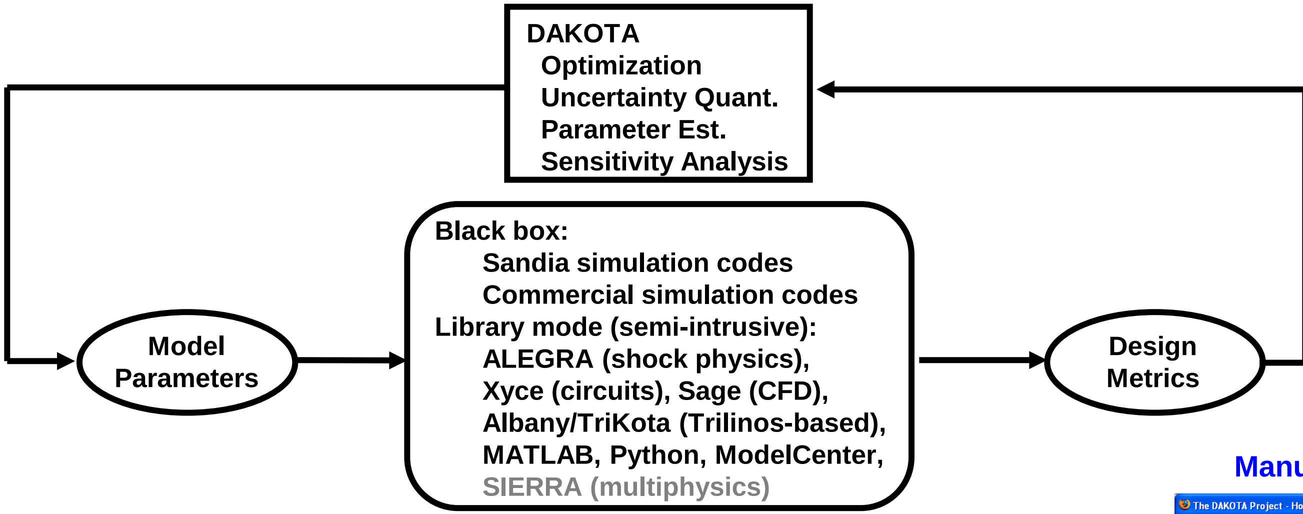
Stochastic expansions (typically nongradient-based)

- ***Strengths:*** **functional representation, exponential convergence rates for smooth problems**
- ***Weaknesses:***
  - **Nonsmoothness → basis enrichment, h-refinement, Pade approx.**
  - **Scaling to large *n* → adaptive refinement, adjoints**

Build on algorithmic foundations

Design under uncertainty, Mixed UQ with IVP/SOP/DSTE

DAKOTA Software



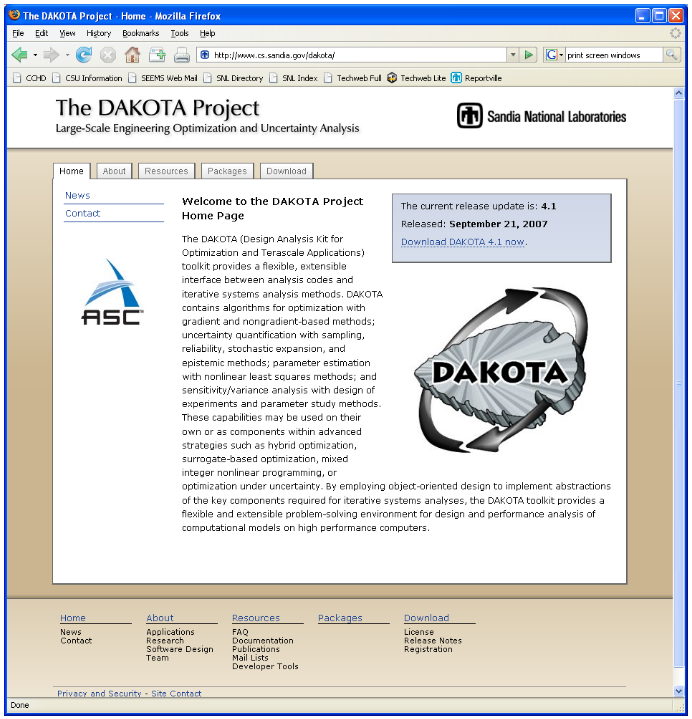
Iterative systems analysis

Multilevel parallel computing

Simulation management

http://dakota.sandia.gov

Manuals, Publications, Training matls. online



Releases: **Major/Interim, Stable/VOTD; *5.1 released 12/10***

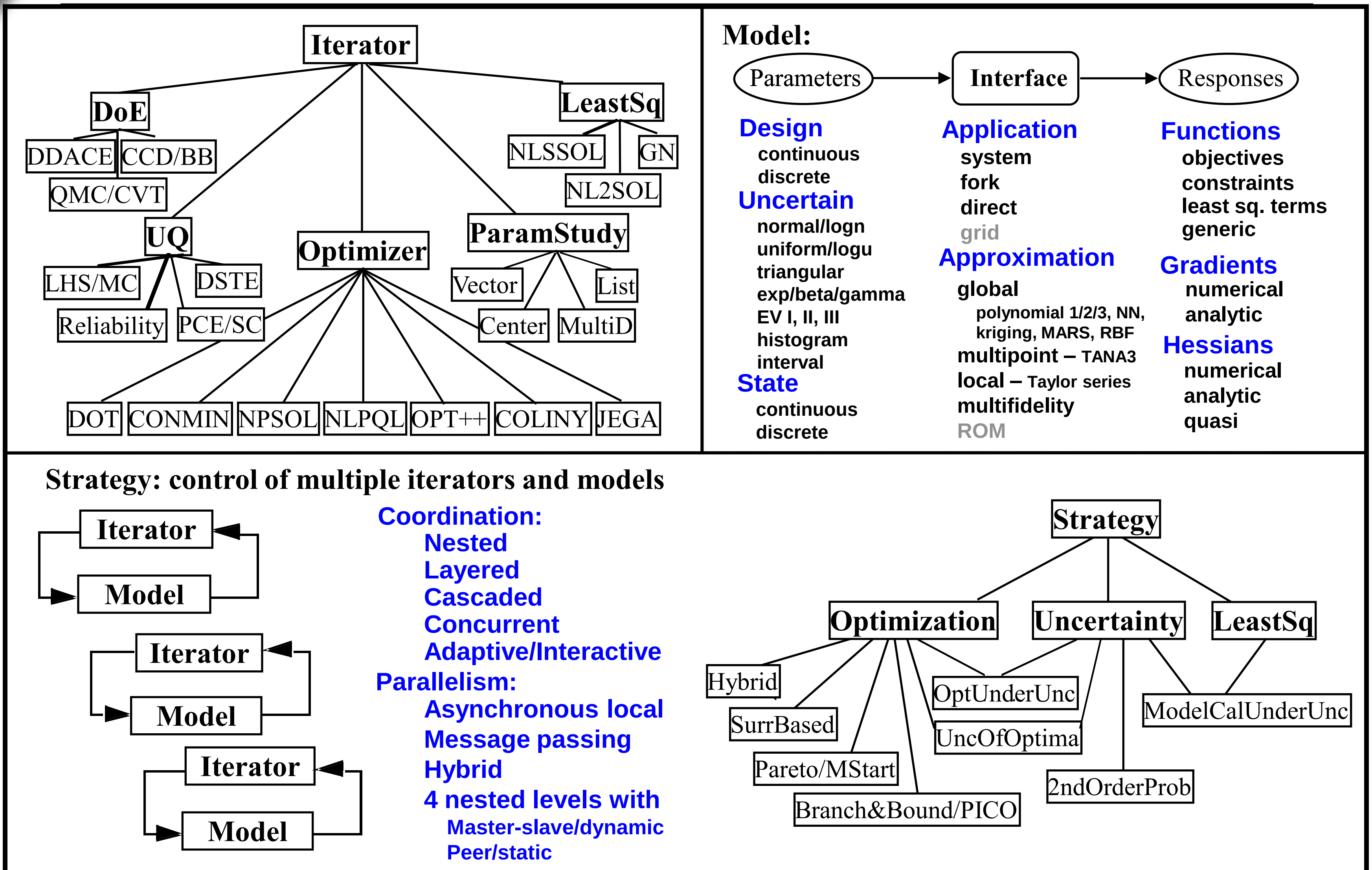
Modern SQE: **Linux/Unix, Mac, Windows; Nightly builds/testing; subversion, TRAC, autotools/Cmake**

GNU LGPL: **free downloads worldwide (>7000 total ext. registrations, ~3500 distributions last yr.)**

Community development: **open checkouts now available**

Community support: **dakota-users, dakota-help**

DAKOTA Framework

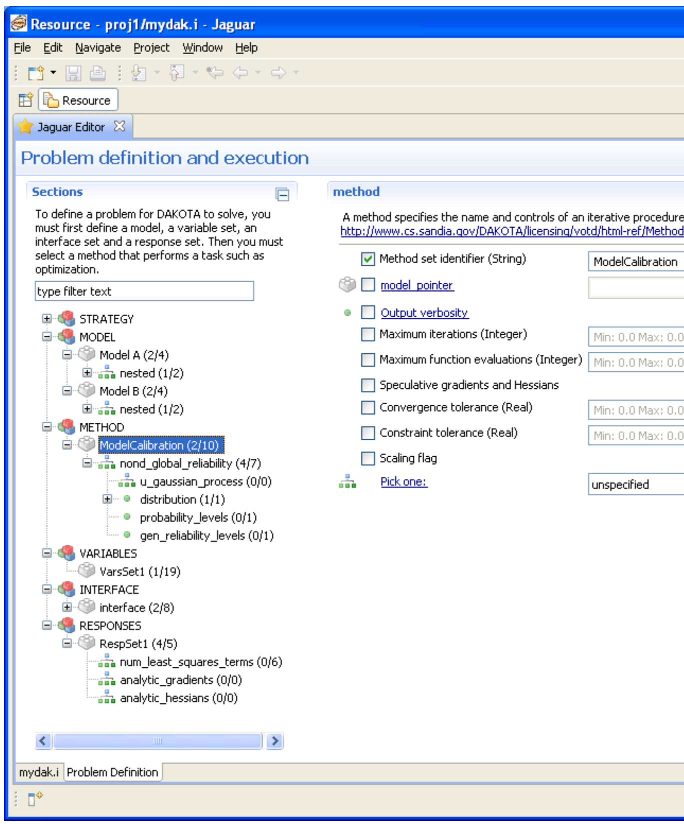


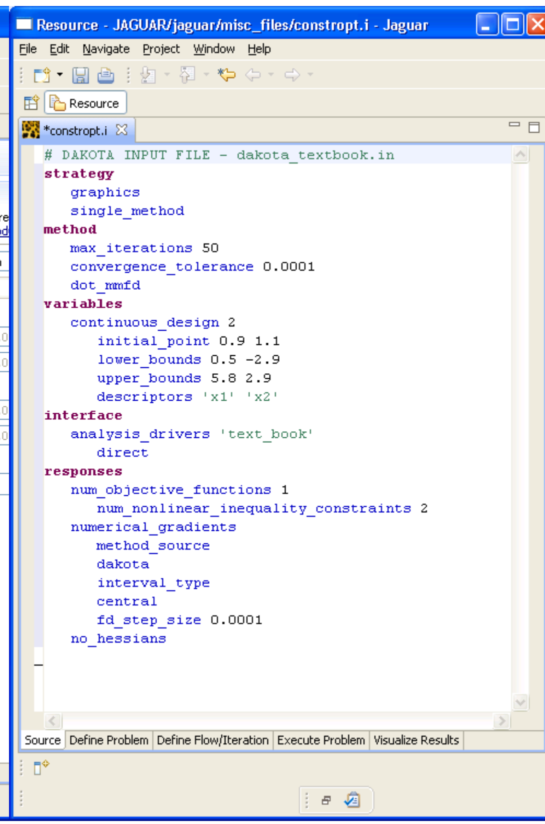
Deployment Initiative: JAGUAR User Interface

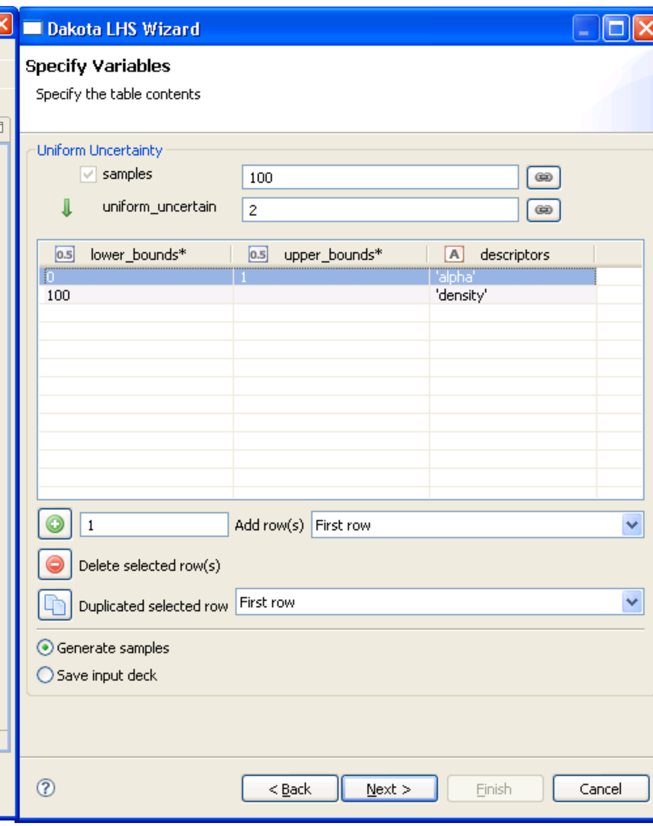
- Eclipse-based rendering of full DAKOTA input spec.
- Automatic syntax updates
- Tool tips, Web links, help
- Symbolics, sim. interfacing

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

- Simplified views for high-use applications (“Wizards”)







Deployment Initiative: 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 algorithm intrusion

SNL Embedding

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

External Embedding

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

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`

- No residuals eliminated
- MOOCHO opt., Stokhos UQ, NOX, LOCA