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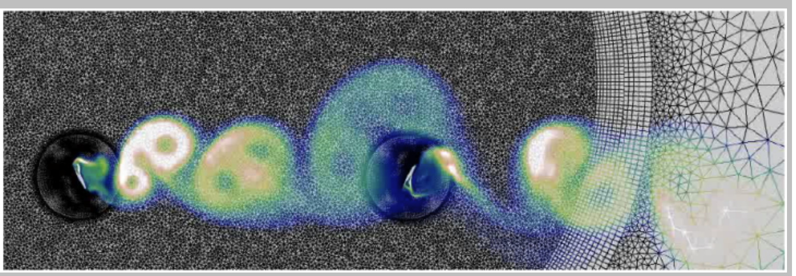

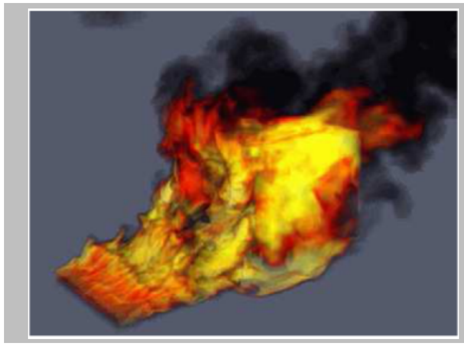

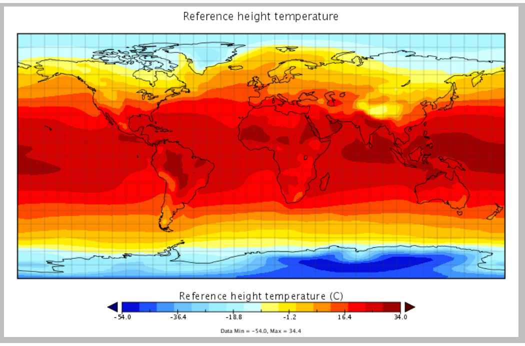

General Introduction: Optimization Under Uncertainty

Michael S. Eldred

Sandia National Laboratories, Albuquerque, NM

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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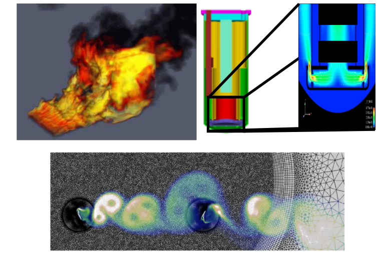
Emphasis on Scalable Methods for High-fidelity UQ on HPC

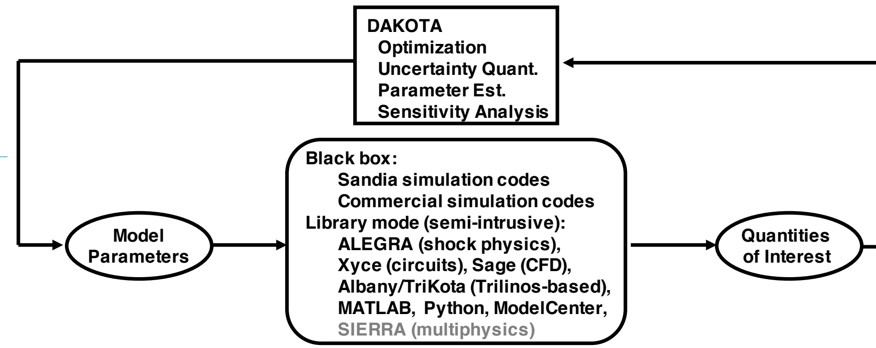


Common theme across DOE/DOD M&S:

High-fidelity simulations: push forward SOA in computational M&S w/ HPC
→ Severe simulation budget constraints (e.g., a handful of runs)
→ Significant dimensionality, driven by model complexity (multi-physics,scale)

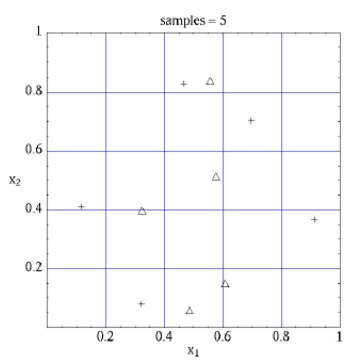
<u>Compounding effects:</u> mixed uncertainties, rare events, nonsmooth QoI

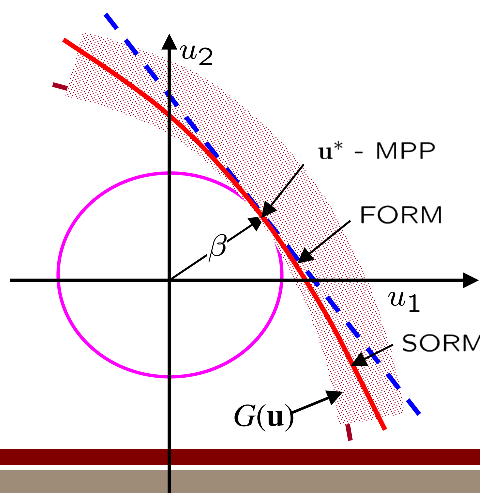
Steward Scalable Algorithms within DAKOTA

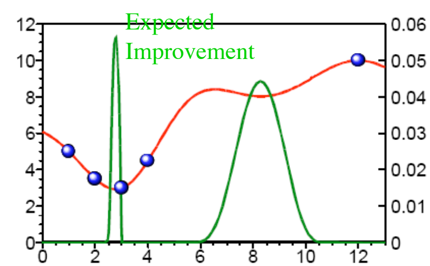


Core UQ Capabilities:

- Sampling methods: MC, LHS, QMC, et al.
- Reliability methods: local (MV, AMV+, FORM, …), global (EGRA, GPAIS, POFDarts)
- Stochastic expansion methods: PCE, SC, fn train
- Epistemic methods: interval est., Dempster-Shafer evidence

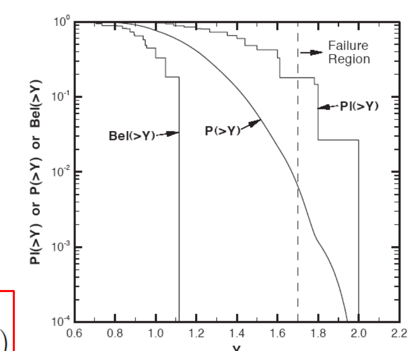






$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

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



Emphasis on Scalable Methods for High-fidelity UQ on HPC

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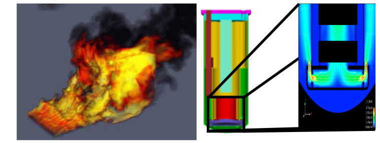

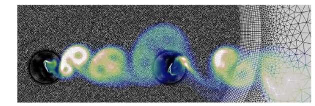

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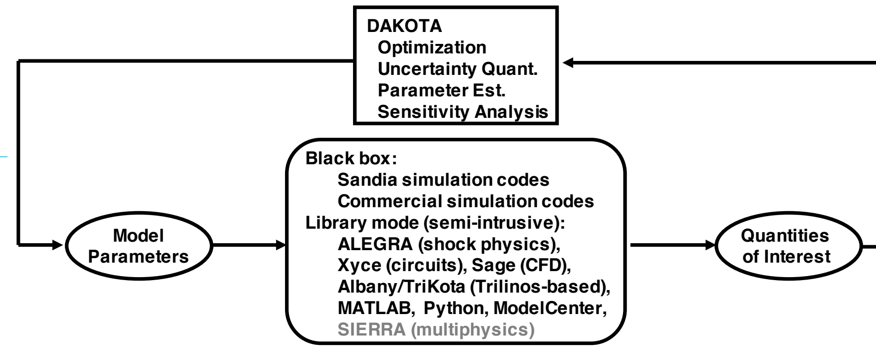
Steward Scalable Algorithms within

DAKOTA
Explore and predict with confidence



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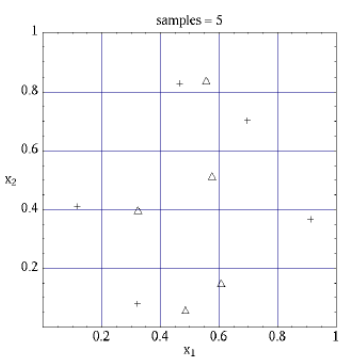

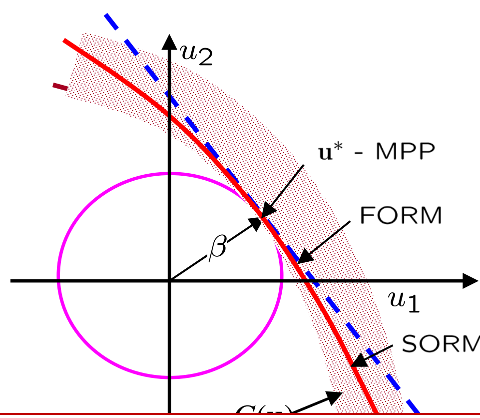

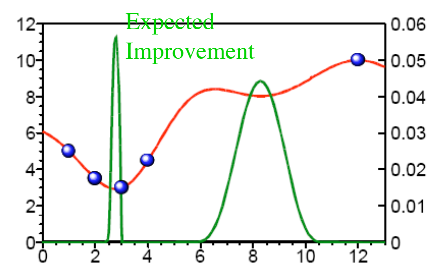

$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

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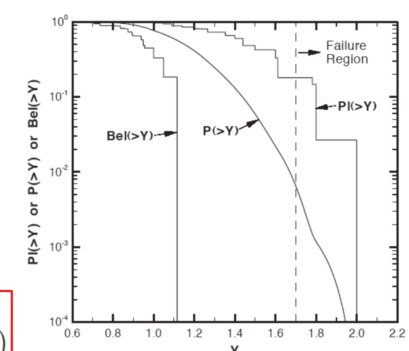


Tailor OUU approaches to exploit features of specific UQ algorithms

Optimization Under Uncertainty

Standard NLP

$$
\begin{aligned}
\min \quad & f(d) \\
\text{s.t.} \quad & g_l \le g(d) \le g_u \\
& h(d) = h_t \\
& d_l \le d \le d_u
\end{aligned}
$$

optimize, accounting for uncertainty metrics

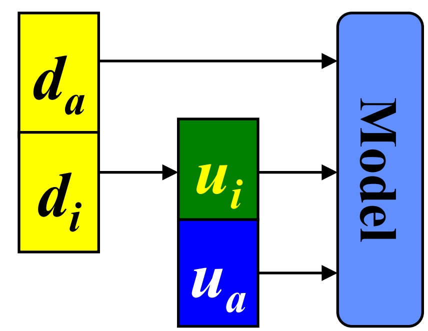
(using any UQ method)

Add resp stats s_u $(\mu, \sigma, z/\beta/p)$

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

Input design parameterization

- **Design vars may augment uncertain vars in simulation**
- **Inserted design vars: an optimization design var may be a parameter of an uncertain dist, e.g., the mean of a normal**



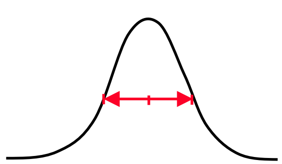
Control response statistics to design for…

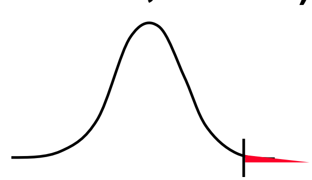
…robustness:
min/constrain moments μ, σ^2, or $z(\beta)$ range

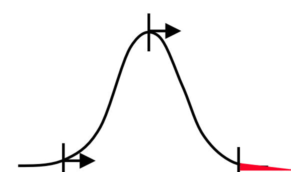
…reliability:
min/max/constrain p/β (tail stats, failure)

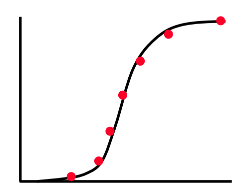
…combined/other:
Pareto, inversion/model calibration under uncertainty

Aleatory









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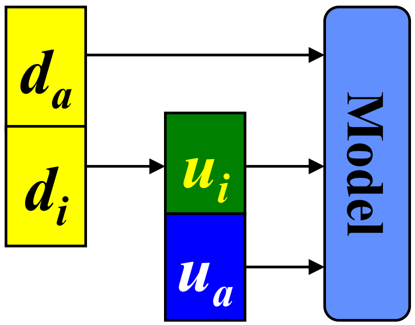

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Epistemic/Mixed

UQ with Reliability Methods

Mean Value Method

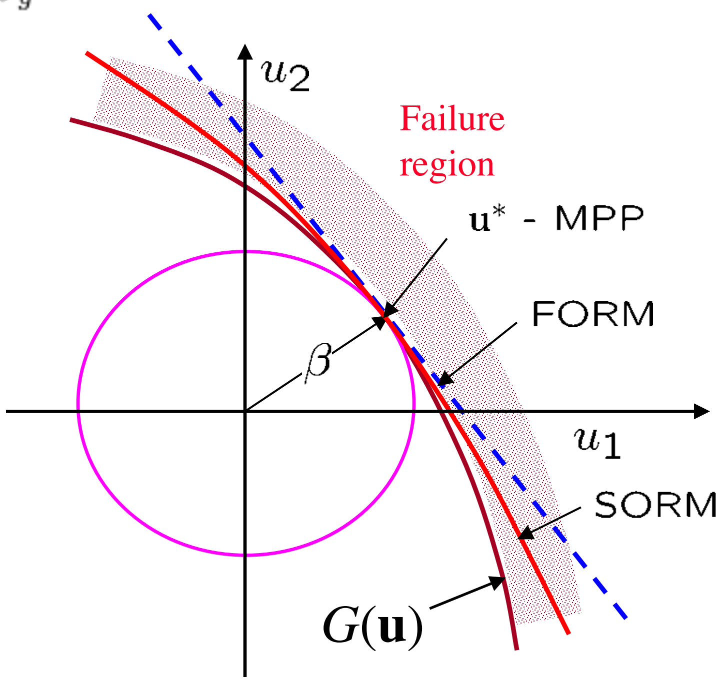
$$\mu_g = g(\mu_{\mathbf{x}})$$

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

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

Rough statistics

MPP search methods

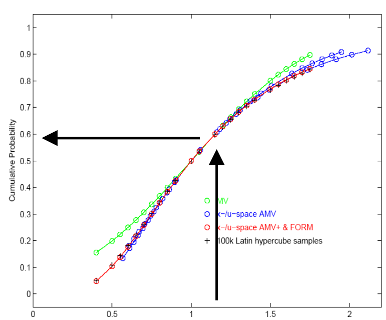


Reliability Index Approach (RIA)

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

Find min dist to *G* level curve

Used for fwd map *z* → *p*/*β*



Nataf x → u: $\Phi(z_i) = F(x_i)$

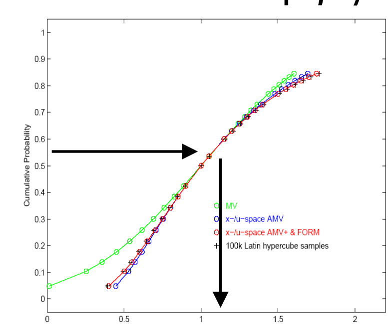
$\mathbf{z} = \mathbf{L}\mathbf{u}$

Performance Measure Approach (PMA)

$$\text{minimize} \quad \pm G(\mathbf{u})$$
$$\text{subject to} \quad \mathbf{u}^T\mathbf{u} = \bar{\beta}^2$$

Find min *G* at *β* radius

Used for inv map *p*/*β* → *z*



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RBDO Algorithms

Bi-level/Nested RBDO

- **Constrain RIA *z* → *p*/*β* result**
- **Constrain PMA *p*/*β* → *z* result**

RIA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \\ \text{or} & p \leq \bar{p} \end{cases}$$

PMA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & z \geq \bar{z} \end{cases}$$

Analytic Bi-level RBDO

- **Analytic reliability sensitivities avoid numerical differencing at design level**

$$\begin{cases} \nabla_{\mathbf{d}} z = \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} \beta_{cdf} = \dfrac{1}{\| \nabla_{\mathbf{u}} G \|} \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} p_{cdf} = -\phi(-\beta_{cdf}) \nabla_{\mathbf{d}} \beta_{cdf} \end{cases}$$

(1st order)

If $\mathbf{d}$ = distr param, then expand

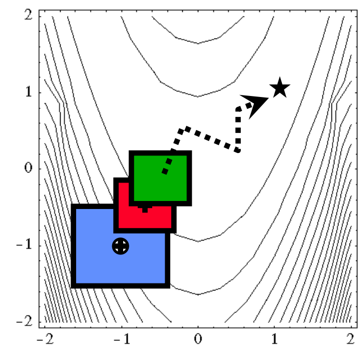
$$\nabla_{\mathbf{d}} g = \nabla_{\mathbf{d}} \mathbf{x} \nabla_{\mathbf{x}} g$$

Sequential/Surrogate-based RBDO:

- **Break nesting: iterate between opt & UQ until target is met. Trust-region surrogate-based approach is non-heuristic.**

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{d}_c) + \nabla_d f(\mathbf{d}_c)^T (\mathbf{d} - \mathbf{d}_c) \\ \text{subject to} \quad & \beta(\mathbf{d}_c) + \nabla_d \beta(\mathbf{d}_c)^T (\mathbf{d} - \mathbf{d}_c) \geq \bar{\beta} \\ \text{or} \quad & p(\mathbf{d}_c) + \nabla_d p(\mathbf{d}_c)^T (\mathbf{d} - \mathbf{d}_c) \leq \bar{p} \\ & \| \mathbf{d} - \mathbf{d}_c \|_\infty \leq \Delta^k \end{aligned}$$

1^{st}-order (also 2^{nd}-order w/ QN)



Unilevel RBDO:

- **All at once: apply KKT conditions of MPP search as equality constraints**
  - Opt. increases in scale (***d***,***u***)
  - Requires 2nd-order info for derivatives of 1st-order KKT

$$\begin{aligned} \min_{\mathbf{d}_{aug} = (\mathbf{d}, \mathbf{u}_1, .., \mathbf{u}_{N_{hard}})} \quad & : f(\mathbf{d}, \mathbf{p}, \mathbf{y}(\mathbf{d}, \mathbf{p})) \\ \text{s. t.} \quad & : G_i^R(\mathbf{u}_i, \eta) = 0 \\ & \beta_{allowed} - \beta_i \geq 0 \\ \|\mathbf{u}_i\| \, \|\nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i, \eta)\| + & \mathbf{u}_i^T \nabla_{\mathbf{u}} G_i^R(\mathbf{u}_i, \eta) = 0 \\ & \beta_i = \|\mathbf{u}_i\| \\ & \mathbf{d}^l \leq \mathbf{d} \leq \mathbf{d}^u \end{aligned}$$

KKT of MPP

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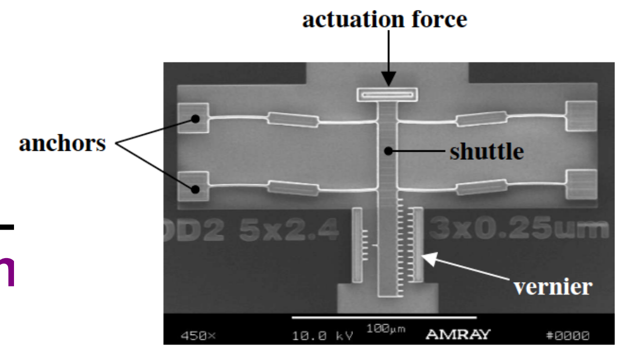
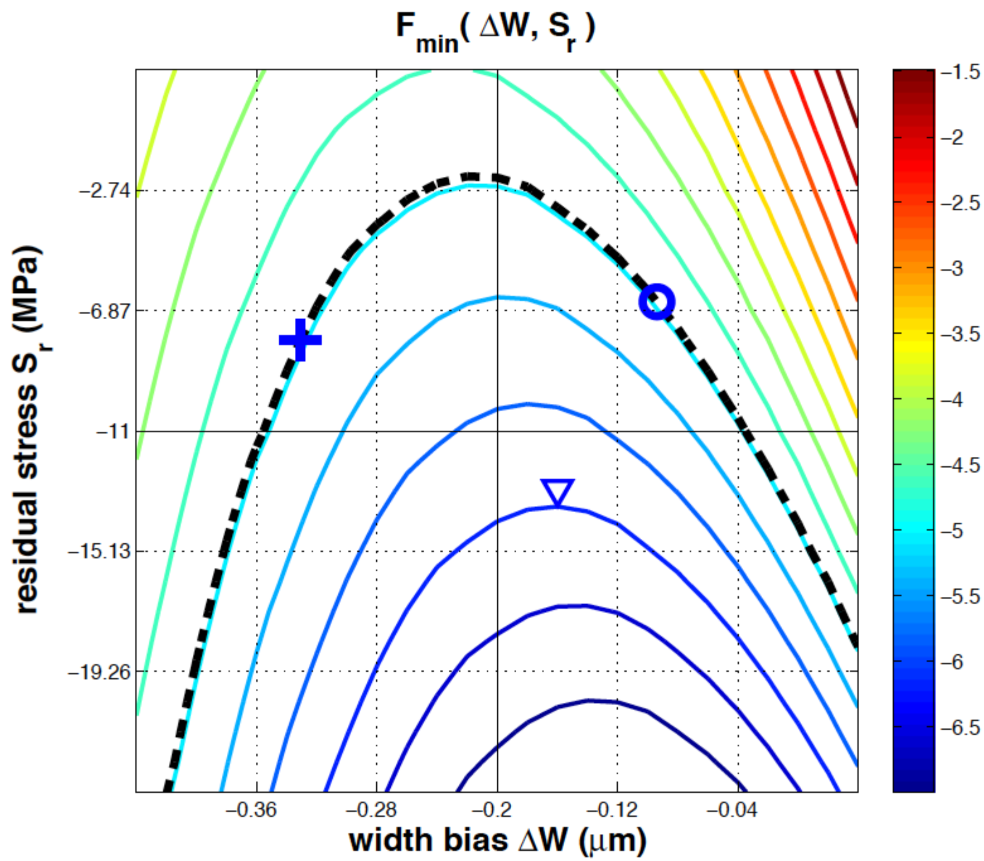
Issues with RBDO



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

- **AMV²+ 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.**



Stochastic Expansions: Polynomial Chaos & Stochastic Collocation

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Polynomial chaos: spectral projection using orthogonal polynomial basis fns

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

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

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

- Estimate α_j using regression or numerical integration: sampling, tensor quadrature, sparse grids, or cubature

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

Stochastic collocation: instead of estimating coefficients for known basis functions, form interpolants for known coefficients

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

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

$$L_j = \prod_{\substack{k=1\\k\neq j}}^{m} \frac{\xi - \xi_k}{\xi_j - \xi_k}$$

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

Sparse interpolants formed using Σ of tensor interpolants

- Tailor expansion form:
  - p-refinement: anisotropic tensor/sparse, generalized sparse
  - h-refinement: local bases with dimension & local refinement
- Method selection: requirements for fault tolerance, decay, sparsity, error estimation

Stochastic Sensitivity Analysis

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

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

- **PCE/SC have convenient analytic features**
  - Expansions readily differentiated w.r.t. ξ
  - Analytic moment expressions

$$\begin{cases} \mu_R = \alpha_0 \\ \sigma_R^2 = \sum_{j=1}^{P} \alpha_j^2 \langle \Psi_j^2 \rangle \end{cases} \qquad \begin{cases} \mu_R = \sum_{j=1}^{N_p} r_j w_j \\ \sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2 \end{cases}$$

- **Augment w/ nonprobabilistic dimensions *s***
  - Design, epistemic uncertain

- **Approach 1: PCE/SC over prob. vars for each set of nonprobabilistic vars**

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

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{k=1}^{N_p} r_k(\boldsymbol{s}) \boldsymbol{L}_k(\boldsymbol{\xi})$$

⇒ Moment sensitivity = expectation of response sensitivity

$$\begin{cases} \frac{d\mu}{ds} = \langle \frac{dR}{ds} \rangle \\ \frac{d\sigma^2}{ds} = 2 \sum_{k=1}^{P} \alpha_k \langle \frac{dR}{ds}, \Psi_k \rangle \end{cases} \qquad \begin{cases} \frac{d\mu}{ds} = \sum_{k=1}^{N_p} w_k \frac{dr_k}{ds} \\ \frac{d\sigma^2}{ds} = \sum_{k=1}^{N_p} 2 w_k (r_k - \mu) \frac{dr_k}{ds} \end{cases}$$

- **Approach 2: PCE/SC over all variables**

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

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

Moment sensitivity = expectations over ξ + differentiation of remaining polynomial in *s*

⇒

$$\begin{cases} \mu_R(\boldsymbol{s}) = \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \\ \sigma_R^2(\boldsymbol{s}) = \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \alpha_k \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \Psi_k(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} - \mu_R^2(\boldsymbol{s}) \end{cases}$$

$$\begin{cases} \mu_R(\boldsymbol{s}) = \sum_{j=1}^{N_p} r_j \langle \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \\ \sigma_R^2(\boldsymbol{s}) = \sum_{j=1}^{N_p} \sum_{k=1}^{N_p} r_j r_k \langle \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \boldsymbol{L}_k(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} - \mu_R^2(\boldsymbol{s}) \end{cases}$$

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$$\begin{cases} \mu_R = \alpha_0 \\ \sigma_R^2 = \sum_{j=1}^{P} \alpha_j^2 \langle \Psi_j^2 \rangle \end{cases} \qquad \begin{cases} \mu_R = \sum_{j=1}^{N_p} r_j w_j \\ \sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2 \end{cases}$$

- **Approach 1: PCE/SC over prob. vars for each set of nonprobabilistic vars**

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

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{k=1}^{N_p} r_k(\boldsymbol{s}) \boldsymbol{L}_k(\boldsymbol{\xi})$$

Moment sensitivity = expectation of response sensitivity

$$\Rightarrow \begin{cases} \frac{d\mu}{ds} = \langle \frac{dR}{ds} \rangle \\ \frac{d\sigma^2}{ds} = 2 \sum_{k=1}^{P} \alpha_k \langle \frac{dR}{ds}, \Psi_k \rangle \end{cases} \qquad \begin{cases} \frac{d\mu}{ds} = \sum_{k=1}^{N_p} w_k \frac{dr_k}{ds} \\ \frac{d\sigma^2}{ds} = \sum_{k=1}^{N_p} 2 w_k (r_k - \mu) \frac{dr_k}{ds} \end{cases}$$

→Additional data requirements (*dR/ds*), but no additional dimensions

- **Approach 2: PCE/SC over all variables**

$$R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=0}^{P} \alpha_j \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \qquad R(\boldsymbol{\xi}, \boldsymbol{s}) \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s})$$

Moment sensitivity = expectations over ξ + differentiation of remaining polynomial in *s*

$$\Rightarrow \begin{cases} \mu_R(\boldsymbol{s}) = \sum_{j=0}^{P} \alpha_j \langle \Psi_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \\ \sigma_R^2(\boldsymbol{s}) = \sum_{j=0}^{P} \sum_{k=0}^{P} \ldots \end{cases} \qquad \begin{cases} \mu_R(\boldsymbol{s}) = \sum_{j=1}^{N_p} r_j \langle \boldsymbol{L}_j(\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} \\ \sigma_R^2(\boldsymbol{s}) = \sum_{j=1}^{N_p} \sum_{k=1}^{N_p} \ldots (\boldsymbol{\xi}, \boldsymbol{s}) \rangle_{\boldsymbol{\xi}} - \mu_R^2(\boldsymbol{s}) \end{cases}$$

→ Additional dimensions, but no additional data requirements

PCE-based and SC-based OUU

Analytic Bi-level:

- Analytic moment/reliability sensitivities *(*avoid numerical derivs. at design level)
- Uncertain or Combined expansions

Reliability:

$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \end{cases}$$

(β initially based on moment proj)

Robustness:

$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \sigma^2 \leq \bar{\sigma}^2 \end{cases}$$

Sequential/Surrogate-based:

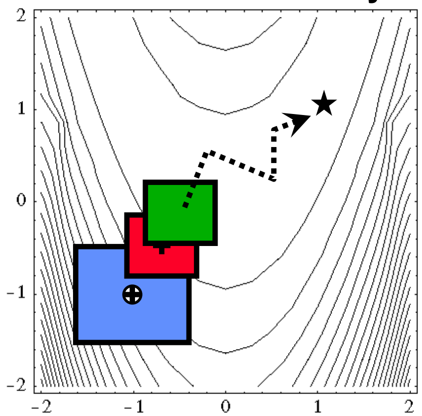
- Break nesting: iterate between opt & UQ w/ (surrogate) linkage
- Uncertain expansions

$$\begin{cases} \text{minimize} & f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \\ \text{subject to} & \beta(\mathbf{s}_c) + \nabla_s \beta(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \geq \bar{\beta} \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

$$\begin{cases} \text{minimize} & f(\mathbf{s}_c) + \nabla_s f(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \\ \text{subject to} & \sigma^2(\mathbf{s}_c) + \nabla_s \sigma^2(\mathbf{s}_c)^T(\mathbf{s} - \mathbf{s}_c) \leq \bar{\sigma}^2 \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

- 1^{st}-order
- Also QN 2^{nd}-order

TR-SBO with local data fit & multifidelity



Multifidelity (focused on UQ fidelity):

- Optimize corrected LF UQ model over TR
  - LF = Combined expansion (over *s*), MVFOSM
  - HF = Uncertain expansion (at single design pt)
- Additive corrections enforce LF/HF consistency
  - 1^{st} order & QN 2^{nd}-order

$$\hat{\beta_{hi}}(\mathbf{s}) = \beta_{lo}(\mathbf{s}) + \alpha_\beta(\mathbf{s})$$
$$\hat{\sigma_{hi}}^2(\mathbf{s}) = \sigma_{lo}^2(\mathbf{s}) + \alpha_{\sigma^2}(\mathbf{s})$$

$$\begin{cases} \text{minimize} & f(\mathbf{s}) \\ \text{subject to} & \hat{\beta_{hi}}(\mathbf{s}) \geq \bar{\beta} \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

$$\begin{cases} \text{minimize} & f(\mathbf{s}) \\ \text{subject to} & \hat{\sigma_{hi}}^2(\mathbf{s}) \leq \bar{\sigma}^2 \\ & \parallel \mathbf{s} - \mathbf{s}_c \parallel_\infty \leq \Delta^k \end{cases}$$

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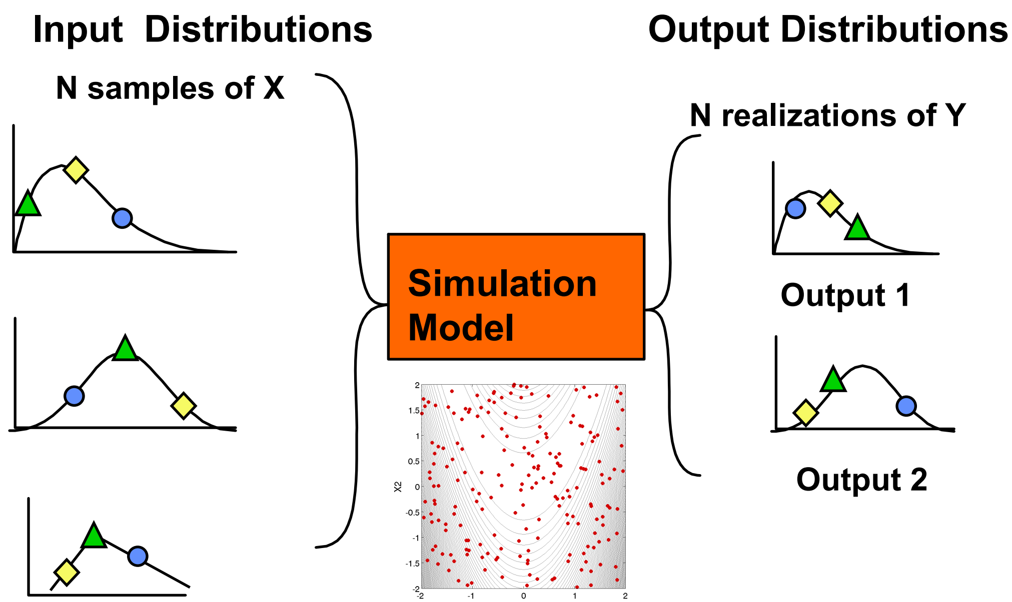
UQ with Sampling Methods

Starting from distributions on the uncertain input values, draw observations from each distribution, pair samples, and execute the model for each pairing
→ ensemble of results yields distributions of the outputs

- Monte Carlo: **basic random sampling**
- Pseudo Monte Carlo: **Latin Hypercube Sampling (LHS)**
- Quasi Monte Carlo: **Halton, Hammersley, Sobol sequences**
- Orthogonal arrays, Centroidal Voronoi Tesselation (CVT), Importance Sampling

<u>Advantage:</u> **Sampling is easy to implement, robust, and transparent.**

<u>Disadvantage:</u> **$N^{-1/2}$ convergence, often impractical for p_{fail}, stats nonsmooth over d**

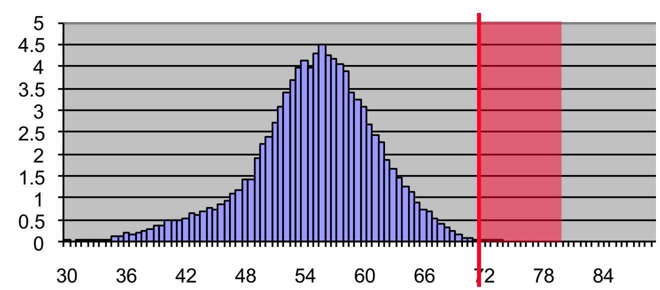


- **sample mean and variance**

$$\bar{T} = \frac{1}{N}\sum_{i=1}^{N} T(u^i)$$

$$T_{\sigma^2} = \frac{1}{N-1}\sum_{i=1}^{N}\left[T(u^i) - \bar{T}\right]^2$$

- **full PDF(probabilities)**



OUU with Sampling

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Employ ***surrogate models*** for interpolation of noisy data due to under-resolved sampling

- Dakota TRMM using smoothing data fits at design level
- SNOWPAC internally uses trust region management on low-order surrogates, integrating estimates of noise

Stochastic DSA

- Independent design vars: Derivative of expectation = expectation of derivative

$$\frac{d\mu}{ds} = \frac{1}{N}\sum_{i=1}^{N}\frac{dQ}{ds}$$

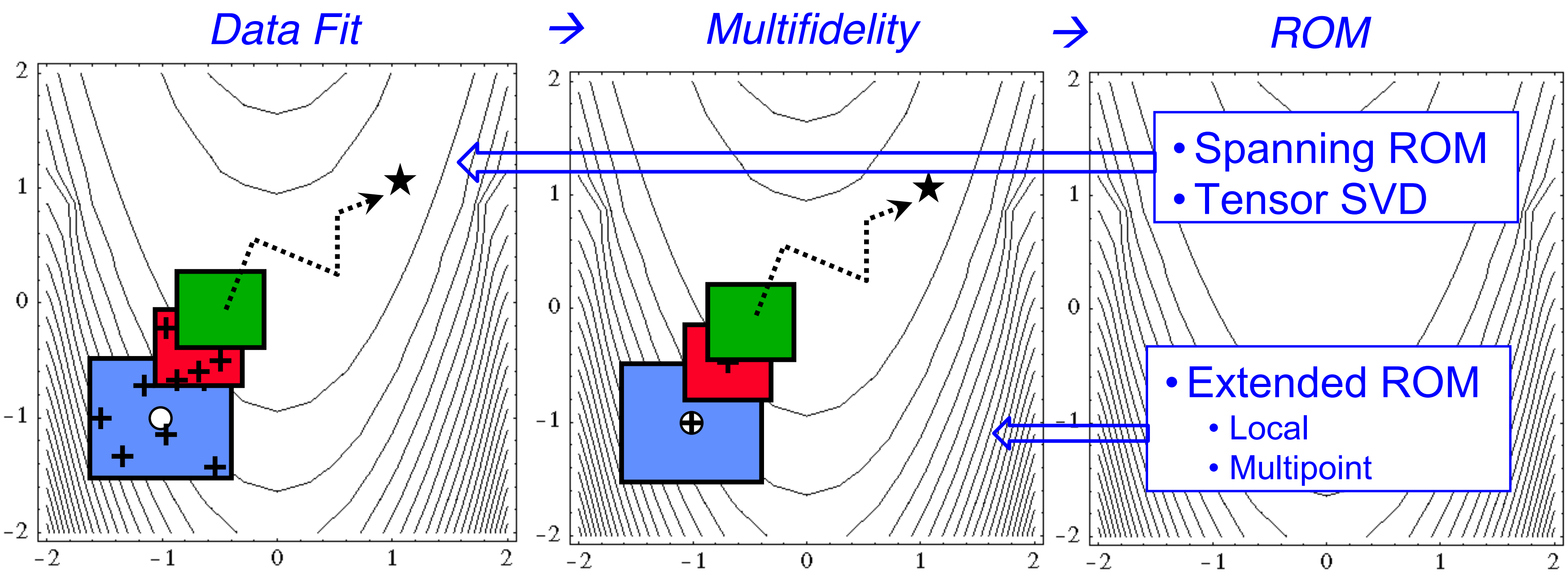
$$\frac{d\sigma}{ds} = \left[\sum_{i=1}^{N}(Q\frac{dQ}{ds}) - N\mu\frac{d\mu}{ds}\right] / (\sigma(N-1))$$

Gradient-based OUU can again be employed: analytic bi-level, 1st-order TRMM, etc.

For Scramjet OUU, multilevel and multilevel-multifidelity Monte Carlo extensions are used

Time Permitting

Trust-Region Model Management



Data fit surrogates:

- Global: polynomial regress., splines, neural net, kriging/GP, radial basis fn
- Local: 1st/2nd-order Taylor
- Multipoint: TPEA, TANA, …

Data fits in SBO

- Smoothing: extract global trend
- DACE: number of des. vars. limited
- Local consistency should be balanced with global accuracy

Multifidelity surrogates:

- Coarser discretizations, looser conv. tols., reduced element order
- Omitted physics: e.g., Euler CFD, panel methods

Multifidelity SBO

- HF evals scale better w/ des. vars.
- Requires smooth LF model
- May require design vect. mapping
- Correction quality is crucial

ROM surrogates:

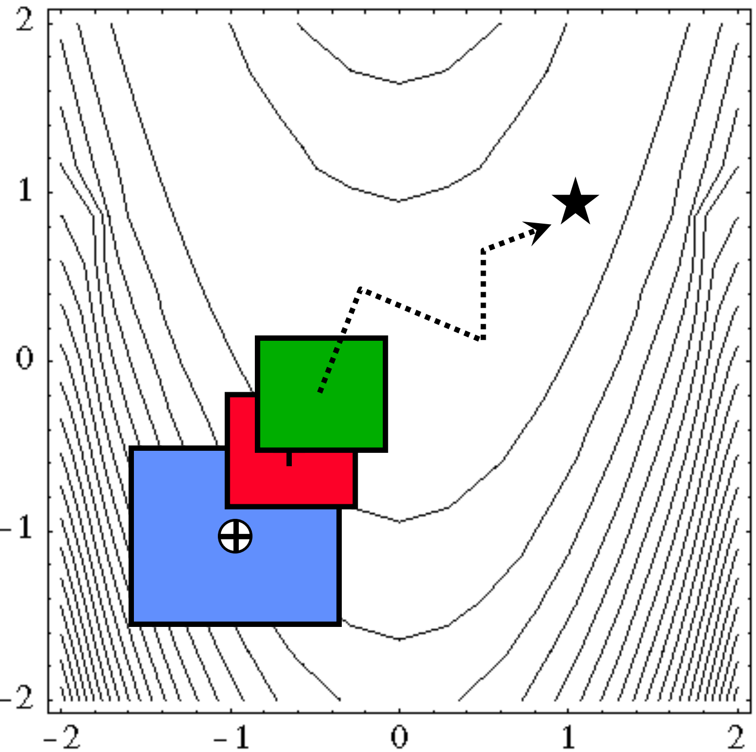
- Spectral decomposition (str. dynamics)
- POD/PCA w/ SVD (CFD, image analysis)

ROMs in SBO

- Key issue: *parametric* ROM
  - E- ROM, S-ROM, tensor SVD
- Some simulation intrusion to re-project
- TR progressions resemble local, multipoint, or global

TRMM – Multifidelity Case

Sequence of trust regions



Algorithm 2 Compute correction

procedure COMPUTE_CORRECTION(x_c, R, $f_{HI}(x)$, $f_{LO}(x)$)

$A_0, A_1, A_2, B_0, B_1, B_2 = 0$

if (correction order ≥ 0) **then**

$A_0 = f_{hi}(x_c) - f_{lo}(Rx_c)$, $\quad B_0 = \frac{f_{hi}(x_c)}{f_{lo}(Rx_c)}$

end if

if (correction order ≥ 1) **then**

$A_1 = R\left[\nabla f_{hi}(x_c)\right] - \nabla f_{lo}(Rx_c)$, $\quad B_1 = \frac{1}{f_{lo}(Rx_c)} R\left[\nabla f_{hi}(x_c)\right] - \frac{f_{hi}(x_c)}{f_{lo}^2(Rx_c)} \nabla f_{lo}(Rx_c)$

end if

if (correction order ≥ 2) **then**

$A_2 = R\left[\nabla^2 f_{hi}(x_c)\right] R^T - \nabla^2 f_{lo}(Rx_c)$

$B_2 = \frac{1}{f_{lo}(Rx_c)} R\left[\nabla^2 f_{hi}(x_c)\right] R^T - \frac{f_{hi}(x_c)}{f_{lo}^2(Rx_c)} \nabla^2$

$- \frac{1}{f_{lo}^2(Rx_c)} \left[\nabla f_{lo}(Rx_c)\left(R \nabla f_{hi}(x_c)\right)^T\right.$

end if

end procedure

Algorithm 3 Apply correction

procedure APPLY_CORRECTION($\tilde{x}$, R, $f_{HI}(x)$, $f_{LO}(x)$)

$\alpha(\tilde{x}) = A_0 + A_1^T (\tilde{x} - Rx_c) + \frac{1}{2} (\tilde{x} - Rx_c)^T A_2 (\tilde{x} - Rx_c)$

$\beta(\tilde{x}) = B_0 + B_1^T (\tilde{x} - Rx_c) + \frac{1}{2} (\tilde{x} - Rx_c)^T B_2 (\tilde{x} - Rx_c)$

if additive correction **then**

$\gamma = 1$

else if multiplicative correction **then**

$\gamma = 0$

else if combined correction **then**

x_p is from a previous iterate

)) + $(1 - \gamma) f_{lo}(\tilde{x}) \beta(\tilde{x})$

Algorithm 4 Compute trust region updates

procedure TR($\mathbf{x}_c^k$, $\mathbf{x}_*^k$, $\mathbf{f}(\mathbf{x})$, $\hat{\mathbf{f}}_{CORR}(\mathbf{x})$)

$\rho^k = \frac{\Phi(\mathbf{x}_c^k) - \Phi(\mathbf{x}_*^k)}{\hat{\Phi}(\mathbf{x}_c^k) - \hat{\Phi}(\mathbf{x}_*^k)}$ where $\Phi(\mathbf{x}^k) = \text{MeritFn}(\mathbf{f}(\mathbf{x}^k))$ and $\hat{\Phi}(\mathbf{x}^k) = \text{MeritFn}(\hat{\mathbf{f}}_{corr}(\mathbf{x}^k))$

if $\rho^k \leq 0$ **then**

Reject step: $\mathbf{x}_c^{k+1} = \mathbf{x}_c^k$

$\Delta^{k+1} = \Delta^k \nu_{contract}$

else

Accept step: $\mathbf{x}_c^{k+1} = \mathbf{x}_*^k$

if $\rho^k \leq \eta_{contract}$ **then**

$\Delta^{k+1} = \Delta^k \nu_{contract}$

else if $\eta_{expand} \leq \rho^k \leq 2 - \eta_{expand}$ **then**

$\Delta^{k+1} = \Delta^k \nu_{expand}$

else

$\Delta^{k+1} = \Delta^k$

end if

end if

Apply Δ^{k+1} factor to global bounds to compute new TR bounds

If nested trust regions, truncate new TR bounds to parent bounds

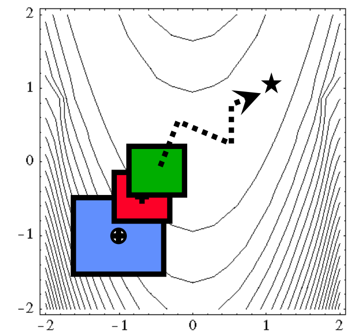
end procedure

Algorithm R&D: Multilevel-Multifidelity OUU

Hybrid MG/Opt with recursive TRMM (w/ Monschke)

Trust-region model management

- targets *hierarchy of model forms* (now an arbitrary number)
- each opt cycle performed on corrected LF model



Multigrid optimization (MG/Opt)

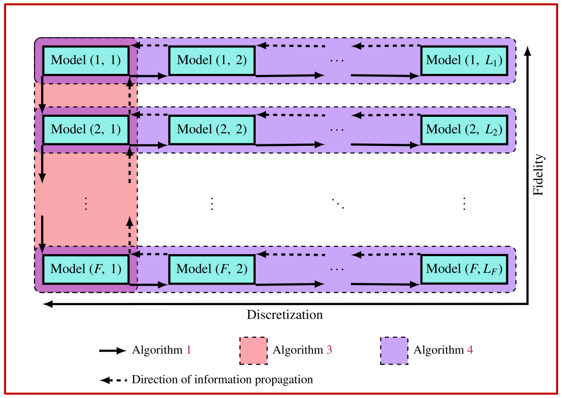
- targets *hierarchy of discretization levels*
- multigrid V cycle to hierarchy of *optimization solves*
- coarse optim. generates search direction for fine optim.
  - corrections + line search globalization → provable convergence

Algorithm 1 Multigrid Optimization

procedure MGOPT(k, $x_0^{(k)}$, $f^{(k)}(x)$, $v^{(k)}$)
  if $k = 0$ **then**
    $x_1^{(k)} = \arg\min_x \; f^{(k)}(x) - \left[v^{(k)}\right]^T x$
    return $x_1^{(k)}$
  else
    Partially solve: $x_1^{(k)} = \arg\min_x \; f^{(k)}(x) - \left[v^{(k)}\right]^T x$
    $x_1^{(k-1)} = R\left[x_1^{(k)}\right]$
    $v^{(k-1)} = \nabla f^{(k-1)}(x_1^{(k-1)}) - R\left[\nabla f^{(k)}(x_1^{(k)})\right]$
    $x_2^{(k-1)} =$ MGOPT($k-1$, $x_1^{(k-1)}$, $f^{(k-1)}(x)$, $v^{(k-1)}$)
    $e = P\left[x_2^{(k-1)} - x_1^{(k-1)}\right]$
    $x_2^{(k)} = x_1^{(k)} + \alpha e$
    return $x_2^{(k)}$
  end if
end procedure

Towards MLMF using MG/Opt with recursive TRMM

- both model forms & discretization levels



a) 1 fidelity and 1 level

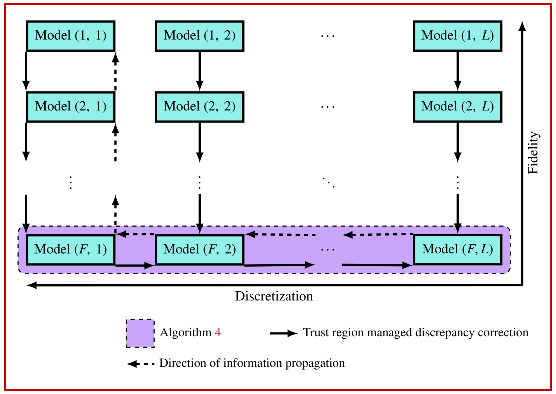
	Fine
High-Fidelity	229

b) 1 fidelity and 2 levels

	Fine	Coarse
High-Fidelity	112	146

c) 2 fidelities and 2 levels

	Fine	Coarse
High-Fidelity	65	82
Low-Fidelity	26	29



Monschke, J. and E., "Multilevel-Multifidelity Acceleration of PDE-Constrained Optimization." *AIAA SciTech 2017* (accepted).

Exceptional service in the national interest

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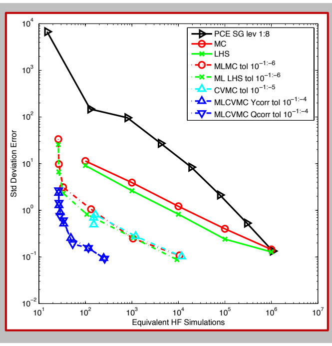
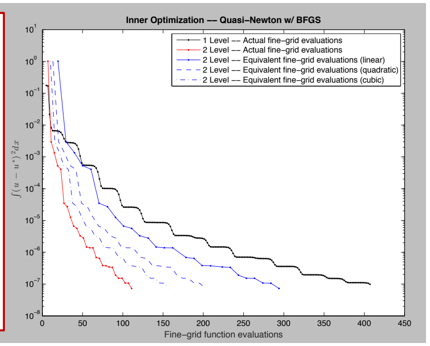
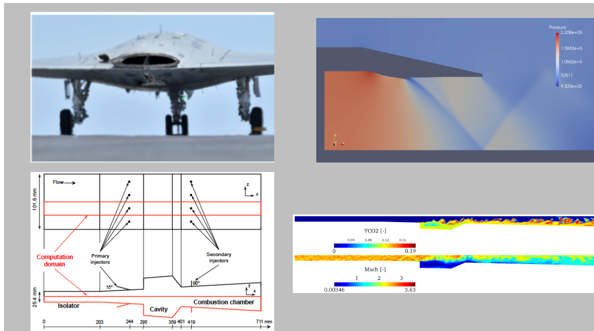




DAKOTA

Explore and predict with confidence



Scramjet OUU

Michael S. Eldred, Gianluca Geraci, Friedrich Menhorn, Youssef Marzouk

DARPA EQUiPS Livermore site visit, November 2017

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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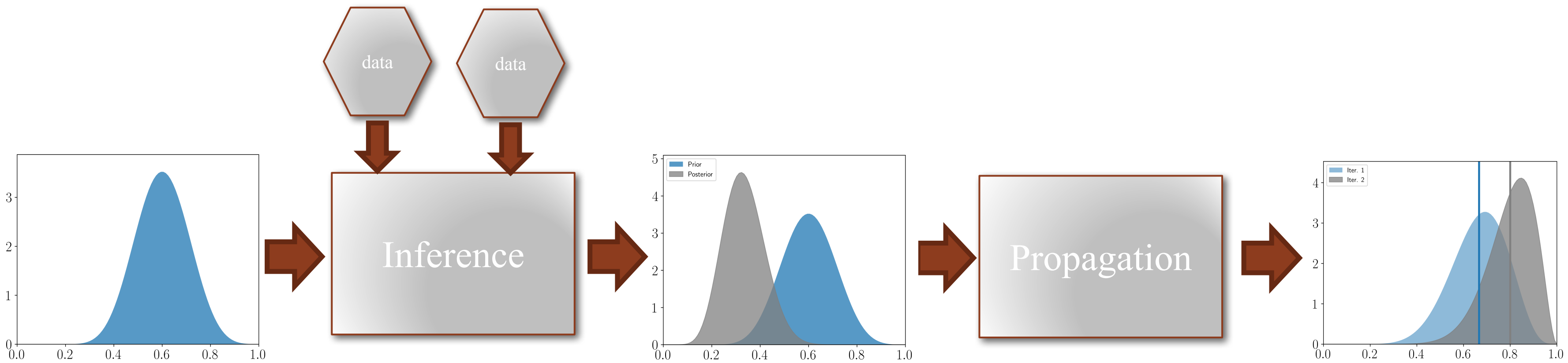
Integration of TAs 1, 2: Uncertainty Quantification Workflow

Characterization of input uncertainties through assimilation of data

- Prior distributions based on *a priori* knowledge
- Observational data (experiments, reference solns.) → infer posterior distributions via Bayes rule
  - Use of data can significantly reduce uncertainty in obj./constraints (priors are constrained)
  - Design using prior uncertainties can be overly conservative
  - Reduced uncertainty of data-informed UQ can produce designs with greater performance



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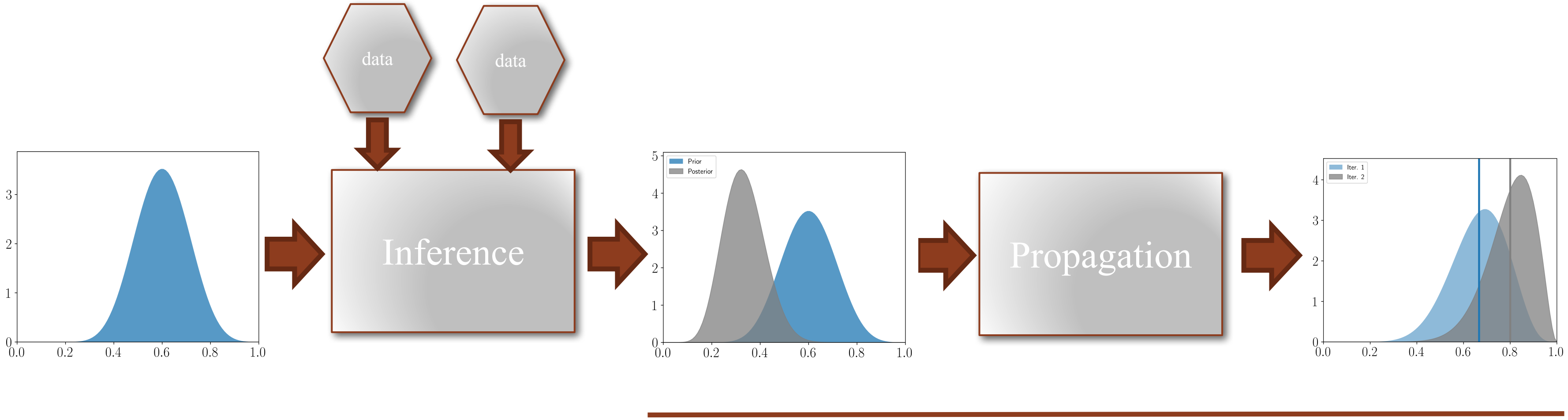


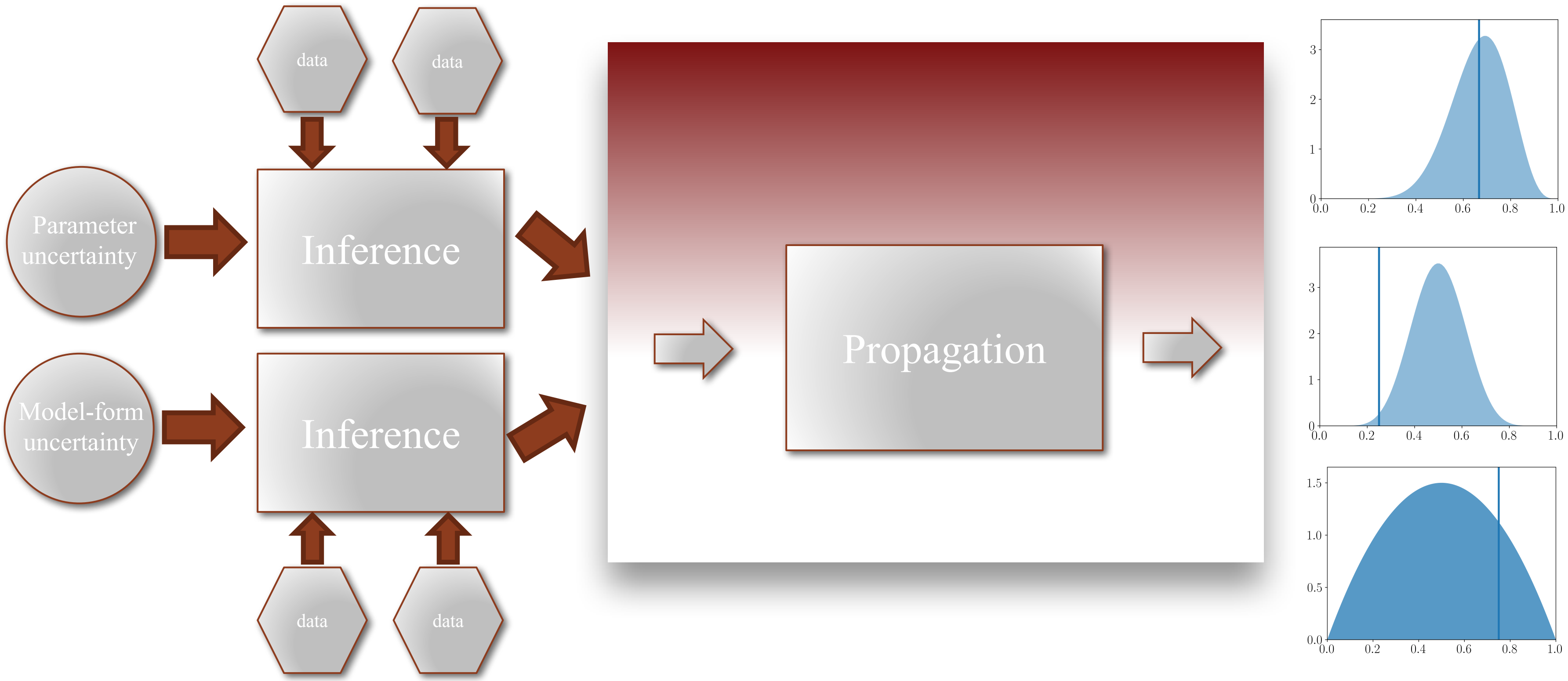
Propagation of input uncertainties to response QoI

- Push forward of posterior distributions
- Compute statistics that reflect goals of DUU process (i.e., moments, failure probabilities)

Integration of TA3: Generic OUU Workflow

Roll up of capabilities

- Inference
- Scalable forward propagation
- Surrogates



Integration of TA3: Generic OUU Workflow

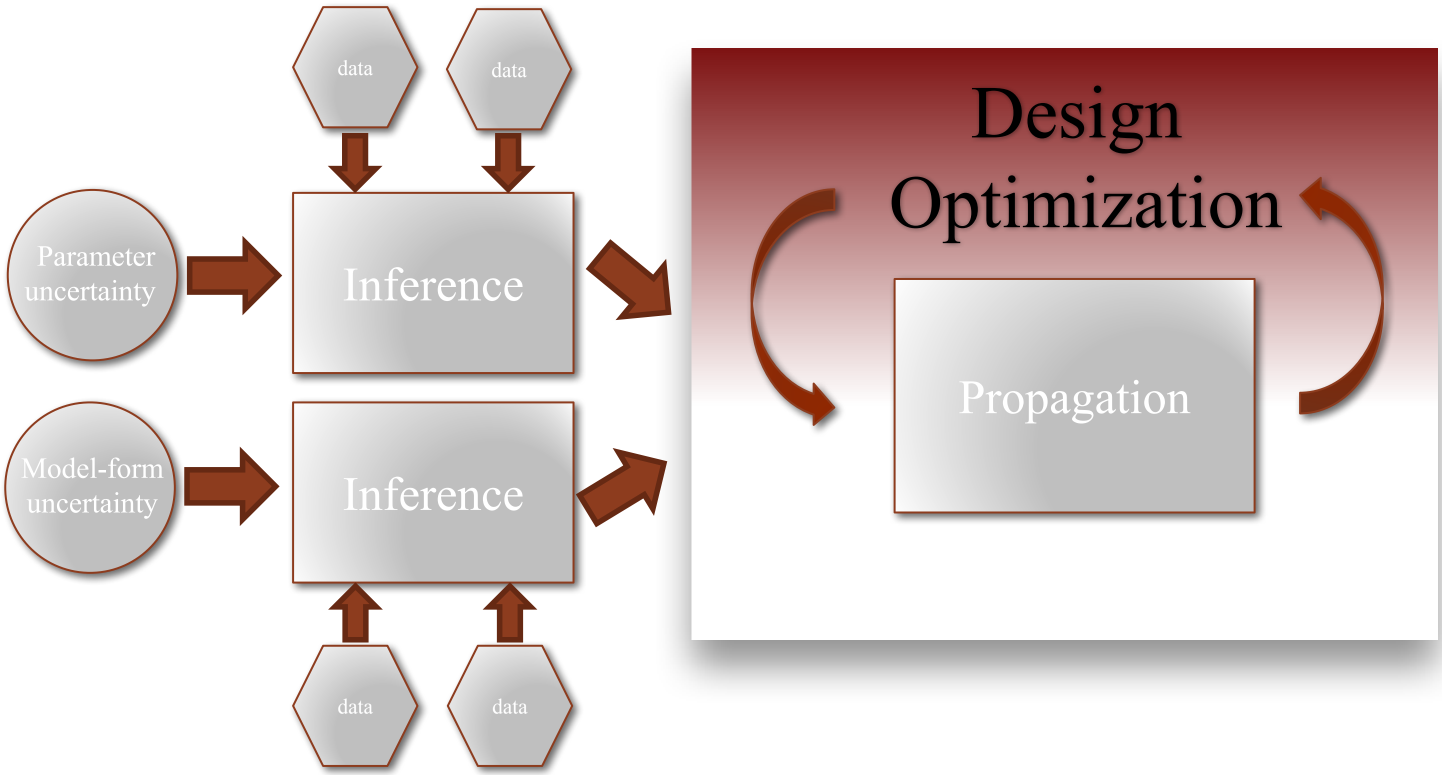
Sandia National Laboratories

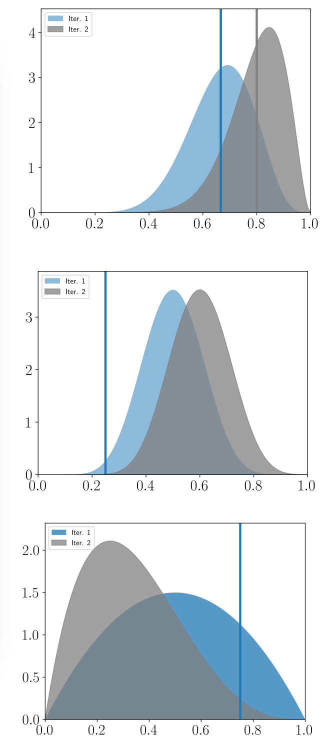
Roll up of capabilities

- Inference
- Scalable forward propagation
- Surrogates

Achieve desired statistical performance

- Common DUU goals:
  - Robustness → minimize QoI variance
  - Reliability → constrain failure probability



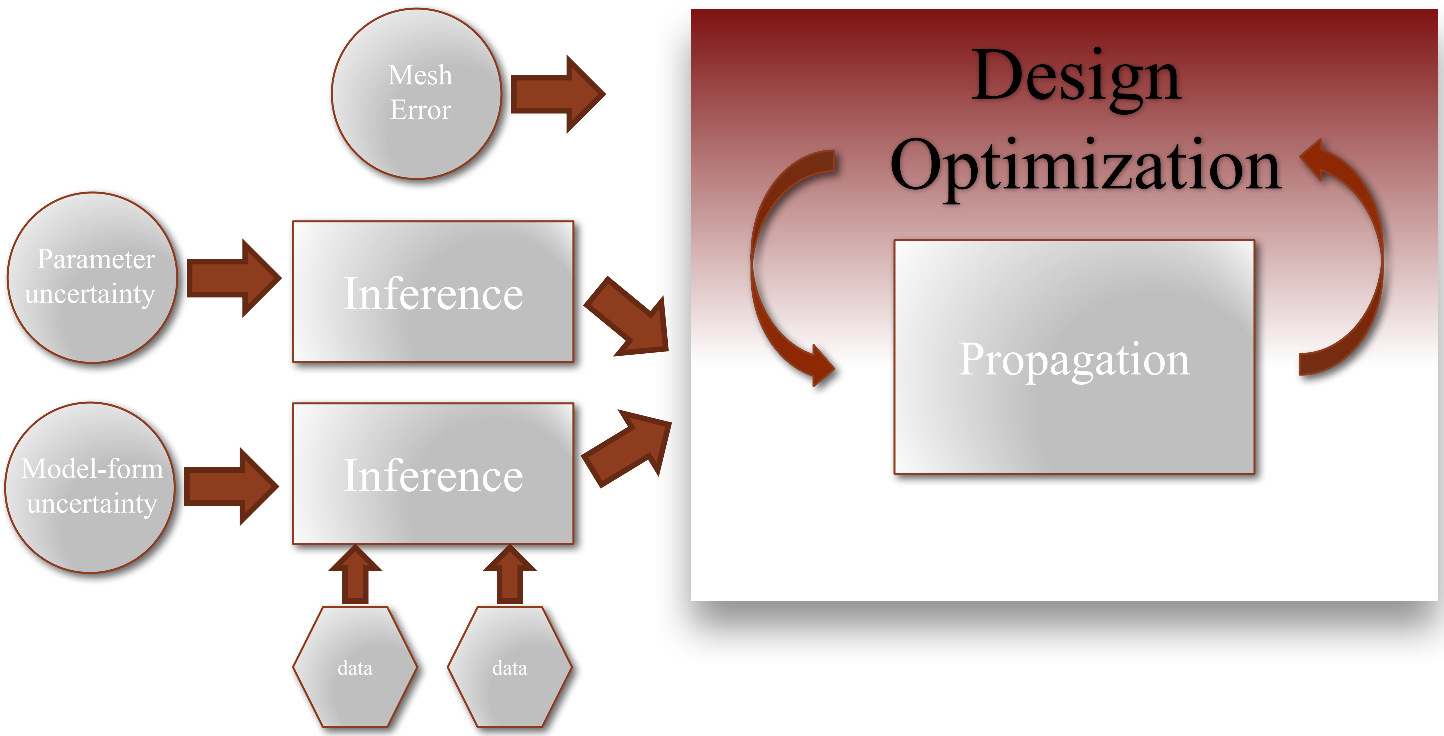


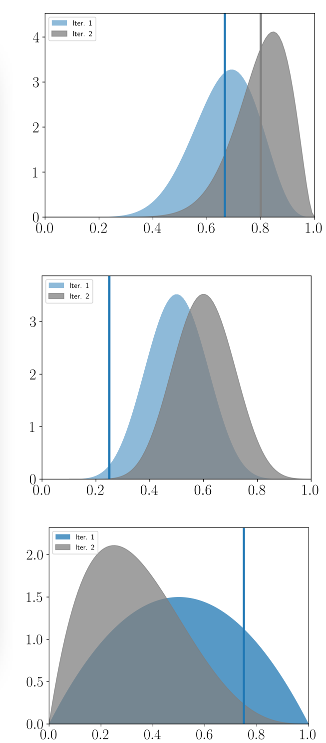
Integration of TA3: Scramjet OUU Workflow

Offline:
- Inference for parametric + model form
- GSA with ML-MF Adapt sparse quad

Online:
- ML-MF parametric
- Mesh error, Model error

Formulation: gradient-free opt & UQ
- SNOWPAC (error aware, error controlled)
- MLMC UQ for 2D {d/8,d/16} + error estimates
- Error balance: mesh error ~ ML estimator variance





Review (FY16-FY17)

OUU Algorithms – Phase 1

Algorithms & infrastructure:

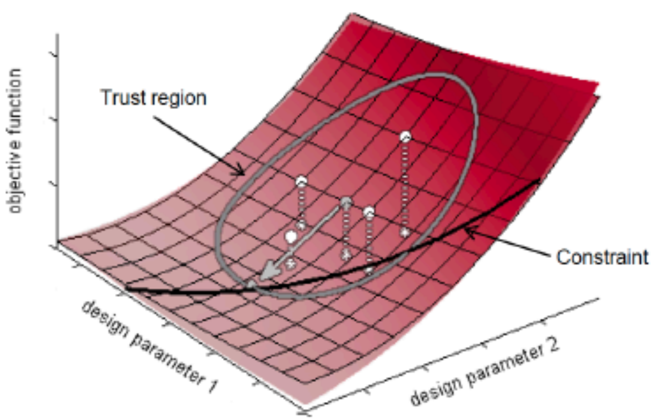
- Dakota trust region model management (TRMM):
  - TRMM incorporates multilevel-multifidelity in simulation, UQ, both
  - Leverage RAPTOR model forms {2D, 3D} + discretizations {d/8, d/16}
  - Recursions for deep hierarchies (beyond bi-fidelity)
- (S)NOWPAC derivative-free opt: deterministic/stochastic solvers
  - NOWPAC $\rightarrow$ SNOWPAC: adapt TR to noise, GP's to mitigate noise, efficient GP regression via low rank approx (SoR, DTC, FITC)
  - Performance eval against other common DFO solvers
- Integration of (S)NOWPAC + Dakota
  - `NOWPACOptimizer`: solver spec, input var transforms, constraint mappings, final result logging, parallel config
  - Abstract error est. in `Iterator`, `Model`: std errors in MC, MLMC stats
  - Phase II target for P2 OUU: SNOWPAC + MLMC

NOWPAC/ SNOWPAC

No adjoints → optim must be derivative-free or derivative-inferred

Nonlinear Optimization with Path-Augmented Constraints (NOWPAC)

- TR approach for nonlinear constrained DFO
- Non-intrusive optimization framework
- New way of handling constraints using an inner boundary path
- Provable convergence to a first order local optimal design



NOWPAC framework

- Build fully linear surrogate models of objective and constraints
- Find improved designs by minimizing surrogate models

SNOWPAC introduces statistical error estimates + GP smoothing

Multilevel Standard Error estimation

- MC std errors are well developed
- Multilevel std errors are more involved (e.g., std error of variance)

$$\begin{aligned}
\text{Var}(\hat{\sigma}^2_L) &= \sum_{\ell=0}^{L} \text{Var}(\hat{P}^2_\ell) - \text{Var}(\hat{P}^2_{\ell-1}) - 2\text{Cov}(\hat{P}^2_\ell, \hat{P}^2_{\ell-1}) \\
\text{Var}(\hat{P}^2_\ell) &= \frac{1}{N_\ell}\left(\mu_{4,\ell} - \text{Var}^2(Q_\ell)\right) + \frac{2}{N_\ell(N_\ell - 1)}\text{Var}^2(Q_\ell) \\
\text{Cov}(\hat{P}^2_\ell, \hat{P}^2_{\ell-1}) &= \frac{1}{N_\ell}\left(\mathbb{E}\left[P^2_\ell P^2_{\ell-1}\right] - \text{Var}(Q_\ell)\text{Var}(Q_{\ell-1})\right) + \frac{1}{N_\ell(N_\ell-1)}\left(\mathbb{E}\left[Q_\ell Q_{\ell-1}\right] - \mathbb{E}\left[Q_\ell\right]\mathbb{E}\left[Q_{\ell-1}\right]\right)^2 \\
\mathbb{E}\left[P^2_\ell P^2_{\ell-1}\right] &= \mathbb{E}\left[Q^2_\ell Q^2_{\ell-1}\right] - 2\mathbb{E}\left[Q_{\ell-1}\right]\mathbb{E}\left[Q^2_\ell Q_{\ell-1}\right] + \mathbb{E}^2\left[Q_{\ell-1}\right]\mathbb{E}\left[Q^2_\ell\right] - 2\mathbb{E}\left[Q_\ell\right]\mathbb{E}\left[Q_\ell Q^2_{\ell-1}\right] \\
&+ 4\mathbb{E}\left[Q_\ell\right]\mathbb{E}\left[Q_{\ell-1}\right]\mathbb{E}\left[Q_\ell Q_{\ell-1}\right] + \mathbb{E}^2\left[Q_\ell\right]\mathbb{E}\left[Q^2_{\ell-1}\right] - 3\mathbb{E}^2\left[Q_\ell\right]\mathbb{E}^2\left[Q_{\ell-1}\right]
\end{aligned}$$

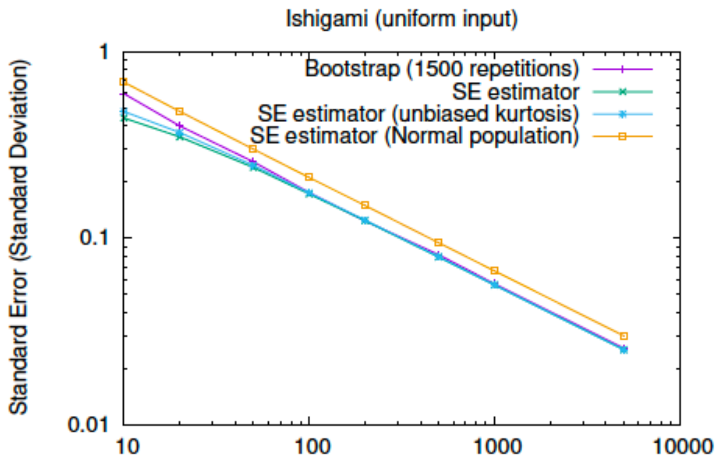
- Multilevel std error for std deviation (no closed form for single level)
  - Normally-distributed *population*

$$SE(\hat{\sigma}) = \frac{\hat{\sigma}}{\sqrt{2(N-1)}}$$

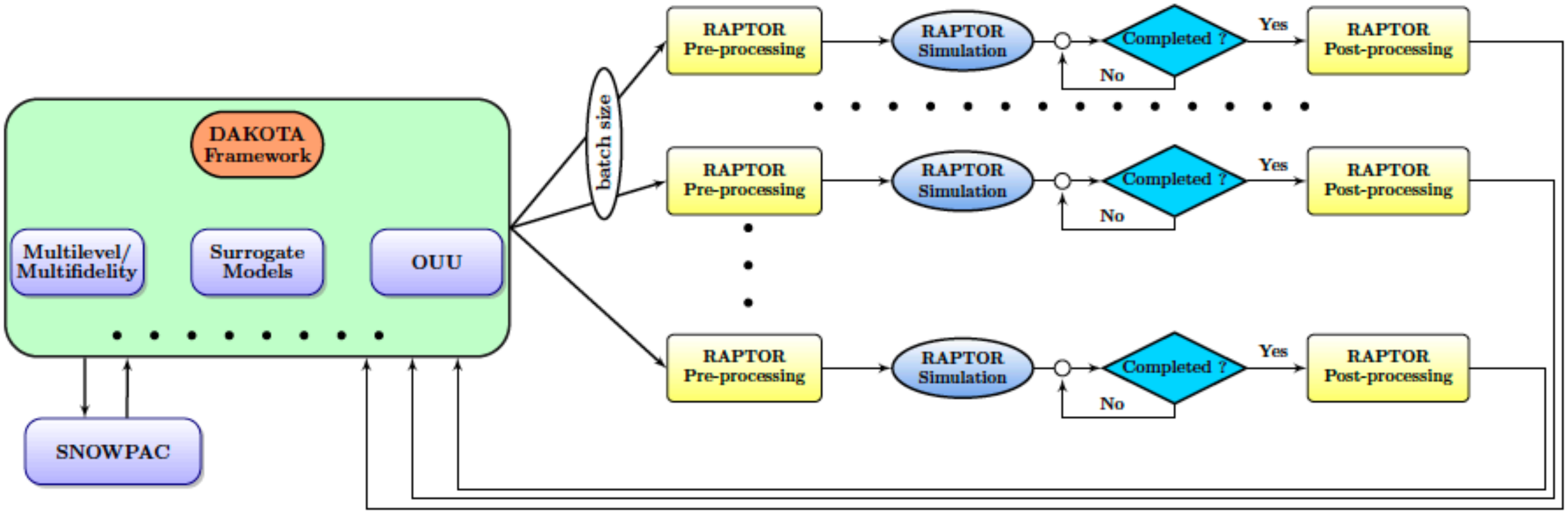
  - Function of a normally-distributed *estimator* (Delta Method)

$$SE(\hat{\sigma}) = \frac{1}{2\hat{\sigma}}\sqrt{\frac{1}{N}\left(\mu_4 + \frac{3-N}{N-1}(\sigma^2)^2\right)}$$

- Additional need for unbiased multilevel (4^{th}) central moments
- Harden for small sample sizes (e.g., 5 - 2 fail)



OUU Software Framework – Phase 1



(DAKOTA+SNOWPAC) – RAPTOR Interface

- RAPTOR black box driver based on system/fork + file I/O
- Asynchronous local concurrency with work directories
- Detection and mitigation of failed simulations (e.g., residual divergence, node failure)
- Up to 3 levels of parallelism: optimizer, UQ, RAPTOR

OUU Demo – Phase 1

P1 (jet-in-crossflow) deployments:

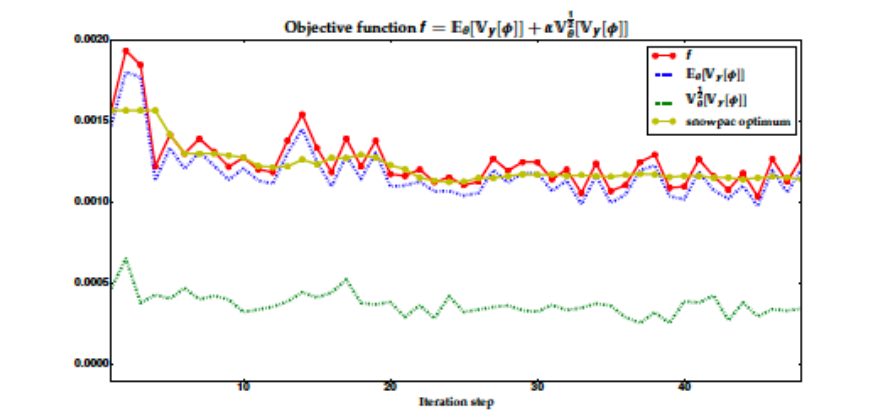
- PCBDO w/ combined exp: reuse of 2D/3D GSA data sets

Model	$\hat{\phi}$	Initial $\mathbb{E}[\chi]$	Initial $\mathbb{E}[\phi]$	Final $\mathbb{E}[\chi]$	Final $\mathbb{E}[\phi]$	Iter
2D	.06	3.480e-1	6.356e-2	3.229e-1	6.000e-2	3
3D	.013	1.377e-3	1.392e-2	1.212e-3	1.300e-2	2

- Multifidelity TRMM with UQ/simulation resolutions

Iteration	$\mathbb{E}[\phi]$	$\mathbb{V}^{\frac{1}{2}}[\phi]$	$\mathbb{E}[\chi]$	Trust region ratio
0	1.142e-01	5.800e-03	9.848e-02	N/A
1	1.074e-01	5.646e-03	8.832e-02	1.443
2	1.003e-01	5.390e-03	7.790e-02	1.497

- SNOWPAC closed-loop coupling with RAPTOR P1 code



OUU Demo – Phase 1

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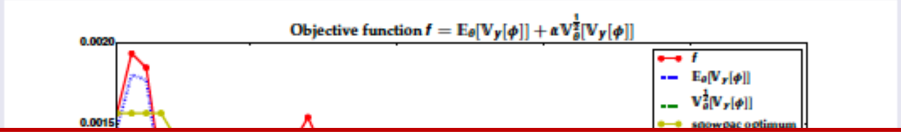

P1 (jet-in-crossflow) deployments:

- QoI trends for {2D,3D} {d/8,d/16} are well correlated
  $\rightarrow$ MLMF is effective
  $\rightarrow$ High turbulence levels will likely require {d/32,d/64}
- Deployments are promising, but interesting design trade-offs are lacking $\rightarrow$ move on to P2 with combustion

P2 Stochastic Optimization, SNOWPAC/MLMC/RAPTOR Case 1
Minimal / insufficient time windowing, Unknown combustion behavior

AFRL WPAFB site visit → finalize OUU formulation:

$$\begin{aligned} \max \quad & \mathbb{E}[\eta_{\text{thermal}}] \\ s.t. \quad & p[\phi_{\text{burn}} \leq 0.7] \leq .01 \\ & p[x_{\text{shocktrain}} \leq 4\, in] \leq .01 \\ & p[\Delta_{\text{press}} \geq .05 * \mu_{\text{press}}] \leq .01 \end{aligned}$$

P2 OUU demo in progress: MLMC analyses at initial design points

	$\mathbb{E}[\eta_{\text{thermal}}]$	$\mathbb{E}[\phi_{\text{burn}}]$	$\mathbb{E}[x_{\text{shocktrain}}]$
Nominal	$0.018494 \pm 3.7542e{-}08$	$0.10151 \pm 1.1309e{-}06$	$74.744 \pm 0.$
Δd_1	$0.018804 \pm 5.6828e{-}08$	$0.098653 \pm 1.5642e{-}06$	$74.744 \pm 0.$
Δd_2	$0.018682 \pm 6.1177e{-}08$	$0.10254 \pm 1.8430e{-}06$	$74.744 \pm 0.$
Δd_3	$0.018739 \pm 1.2493e{-}07$	$0.10285 \pm 3.7635e{-}06$	26.033 ± 133.06
Δd_4	$0.018434 \pm 2.2739e{-}08$	$0.10117 \pm 6.8503e{-}07$	$74.744 \pm 0.$
Δd_5	$0.019003 \pm 2.8257e{-}08$	$0.10430 \pm 8.5124e{-}07$	21.637 ± 95.363
Step 1	pending	pending	pending

Table: History to date for statistical QoIs from MLMC analyses in P2 OUU for design variables d = { global equiv ratio, fuel ratio$_{1:2}$, inj locn$_1$, inj locn$_2$, inj angle$_1$ }.

P2 Stochastic Optimization, SNOWPAC/MLMC/RAPTOR Case 1
Minimal / insufficient time windowing, Unknown combustion behavior

AFRL WPAFB site visit → finalize OUU formulation:

$$\begin{aligned} \max \quad & \mathbb{E}[\eta_{\text{thermal}}] \\ s.t. \quad & p[\phi_{\text{burn}} \leq 0.7] \leq .01 \\ & p[x_{\text{shocktrain}} \leq 4\, in] \leq .01 \\ & p[\Delta_{\text{press}} \geq .05 * \mu_{\text{press}}] \leq .01 \end{aligned}$$

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Step 1	pending	pending	pending

Table: History to d
design variables d

Phase II planned work:

- Increase resolution as enabled by large-scale HPC: include 3D, increase FTTs, tighten ML tolerances, include chance constraints, etc.
- Integrate emerging capabilities from TAs 1,2 → comprehensive OUU

FY18Q1: RAPTOR

Deterministic Optimization for P2, RAPTOR Case 2
Tuned time windows, insufficient combustion → maximize ϕ_{burn}

Motivation:

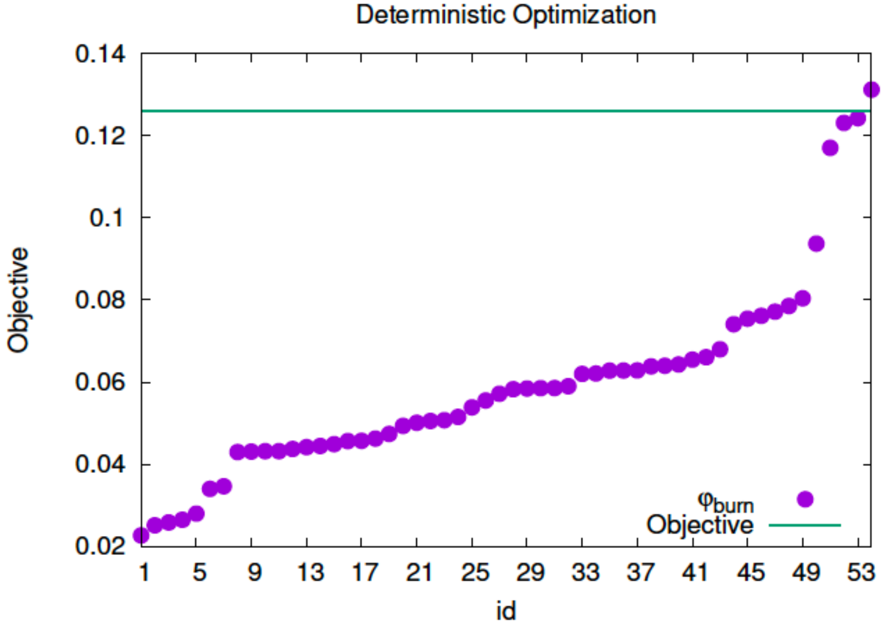
- For the initial configuration of the 2D d/8 code some of the realizations failed to ignite
- We performed a deterministic optimization in order to find an initial design for which the combustion was attained

Optimization features:

- Deterministic design in a 5 dimensional space

Design parameter	Range
Global Eqv ratio	[0.5-0.8]
Primary-Secondary ratio	[0.25-0.35]
Primary inj loc	[0.231-0.2564]
Secondary inj loc	[0.40755-0.43295]
Primary inj angle	[5-25]

- Optimization at nominal (stochastic) conditions
- 54 total 2D d/8 evaluations: 32 corners + 22 internal points
- Surrogate-based optimization: Gaussian Process (`Surfpack`) + linear trend (in order to capture large-scale variations)



- Final design point $[\phi_{burn} = 0.126079]$

Design parameter	Range
Global Eqv ratio	0.5
Primary-Secondary ratio	0.25308
Primary inj loc	0.231
Secondary inj loc	0.40755
Primary inj angle	15.0005

Deterministic Optimization for P2, RAPTOR Case 3
Tuned time windows, repaired combustion → max η_{comb} s.t. ϕ_{burn} >= .19

Sandia National Laboratories

Motivation:

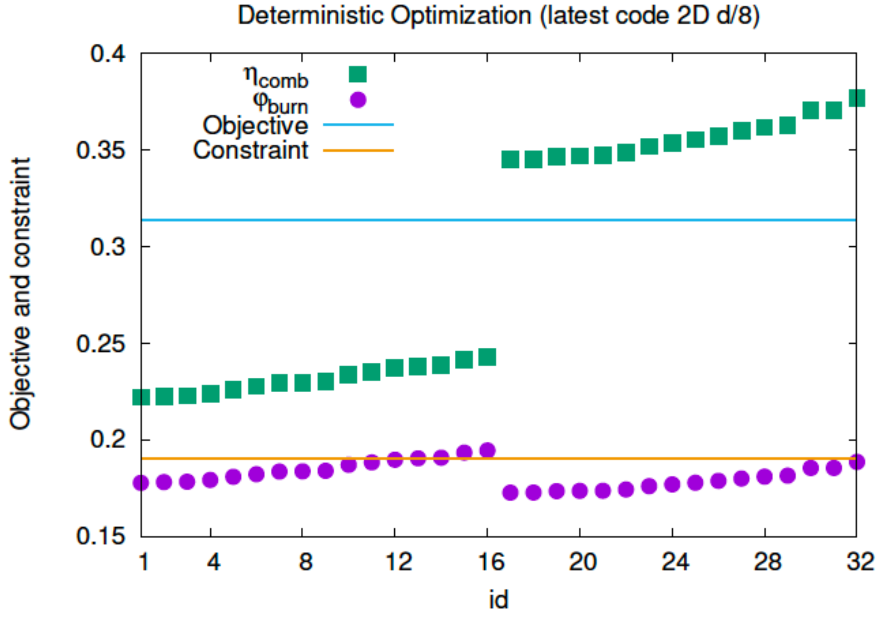
- For the latest version of the 2D d/8 code we wanted to obtain an initial design for the constrained optimization problem
- Constraint allowable $\phi_{burn} \geq 0.19$

Optimization features:

- Deterministic design in a 5 dimensional space

Design parameter	Range
Global Eqv ratio	[0.5-0.8]
Primary-Secondary ratio	[0.25-0.35]
Primary inj loc	[0.231-0.2564]
Secondary inj loc	[0.40755-0.43295]
Primary inj angle	[5-25]

- Optimization at nominal (stochastic) conditions
- 32 total 2D d/8 evaluations (corners)
- Surrogate-based optimization: Gaussian Process (`Surfpack`) + linear trend (in order to capture large-scale variations)



- Final design point $[\eta_{comb} = 0.313936, \phi_{burn} = 0.19]$

Design parameter	Range
Global Eqv ratio	0.63645
Primary-Secondary ratio	0.35
Primary inj loc	0.231
Secondary inj loc	0.424862
Primary inj angle	25

FY18Q1: Model problem

Supersonic Duct

Case configuration and features

- Geometry parametrization (HiFIRE inspired) in `gmsh` to add a wedge before the cavity – 5 parameters
- Inflow conditions subject to uncertainty (same scramjet inlet conditions) – 3 parameters (P_0, T_0 and M)
- 2 Geometrical parametrization in order to obtain 2 resolutions: COARSE and MEDIUM
- Number of points: 2800 COARSE Vs 9600 MEDIUM
- Execution time: 30 s COARSE Vs 300 s MEDIUM

- **Objective:** Pressure loss (inlet outlet)

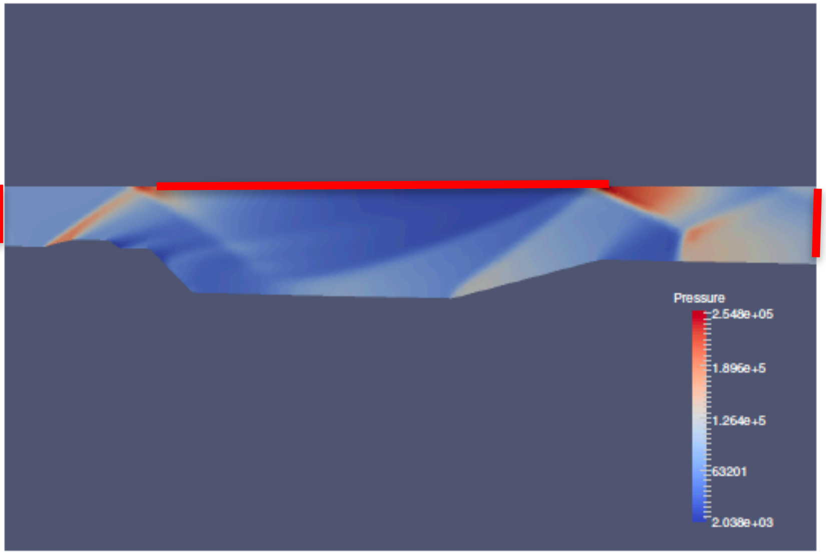
$$P_{loss} = \left(P_0^{in} - \frac{1}{L_y} \int_{out} P_0(y) \mathrm{d}y \right) / P_0^{in}$$

- **Constraint:** Average temperature along the cavity centerline

$$T_c = \frac{1}{L_x} \int_{L_c} T(x) \mathrm{d}x$$

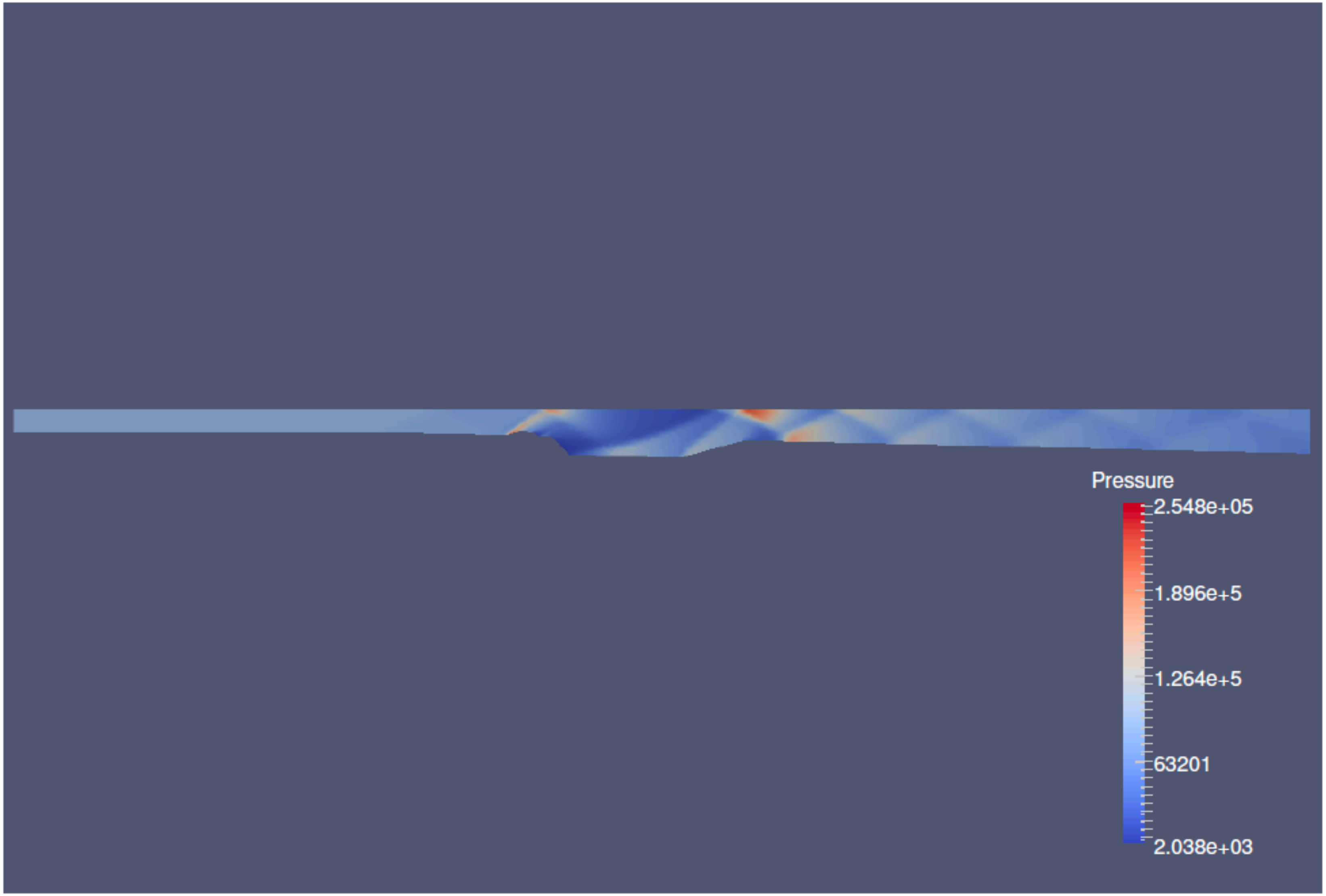
CFD settings (SU2)

- Multigrid solver: 4 levels – V cycle
- Convective numerical method: Jameson-Turkel-Schmidt (JST)
- Spatial discretization: 2nd order with Venkatakrishnan limiter



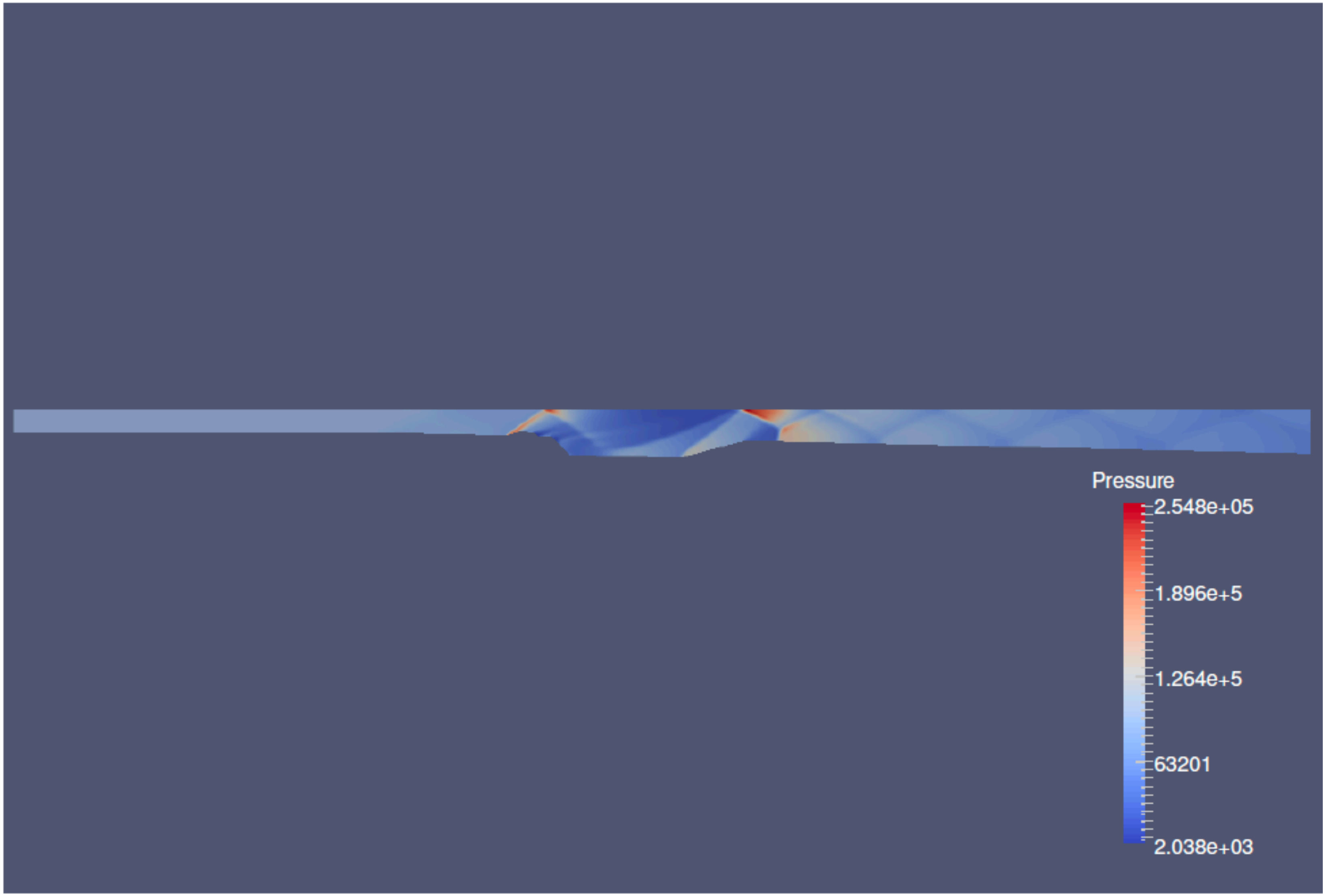
Supersonic Duct

Coarse solution – Execution time 30 s



Supersonic Duct

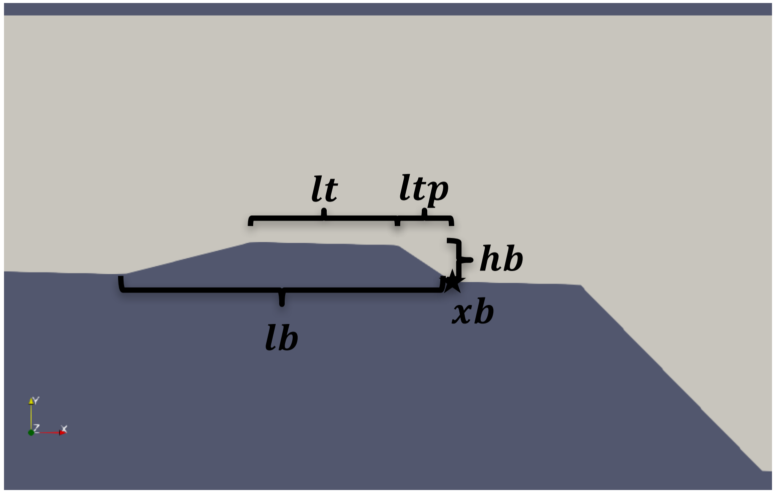
Medium solution – Execution time 300 s



OUU OPTIMIZATION - SETUP

Design: $\vec{x} = [hb, lt, ltp, lb, xb]^T$

$$
\begin{gathered}
0.5 \leq hb \leq 2.5 \\
7.5 \leq lt \leq 11.5 \\
2.5 \leq ltp \leq 4.5 \\
17.5 \leq lb \leq 20.5 \\
79.5 \leq xb \leq 85.5
\end{gathered}
$$



Uncertain: $\vec{q} = \left[p_{o,in}, T_{0,in}, M_{in}\right]^T$

$$
\begin{gathered}
p_{o,in} \sim \mathcal{N}(1.48e6, (7.4e3)^2) \\
T_{0,in} \sim \mathcal{N}(1550, 7.75^2) \\
M_{in} \sim \mathcal{N}(2.51, 0.01255^2)
\end{gathered}
$$

Deterministic:

$$
\begin{gathered}
p^*_{loss}(\vec{x}^*, \vec{q}) = \min p_{loss}(\vec{x}, \vec{q}) \\
s.t. 593 \leq T_{cav}(\vec{x}, \vec{q}) \leq 605
\end{gathered}
$$

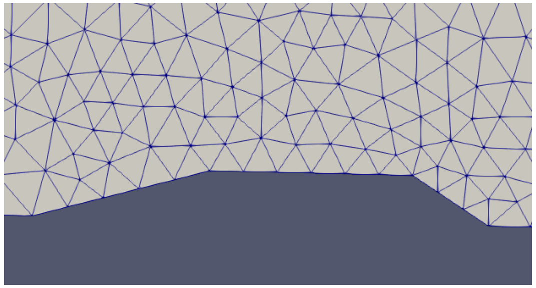
Stochastic:

$$
\begin{gathered}
\tilde{p}^*_{loss}(\vec{x}^*, \vec{q}) = \min \mathbb{E}[p_{loss}(\vec{x}, \vec{q})] \\
s.t. 593 \leq \mathbb{E}[T_{cav}(\vec{x}, \vec{q})] \leq 605
\end{gathered}
$$

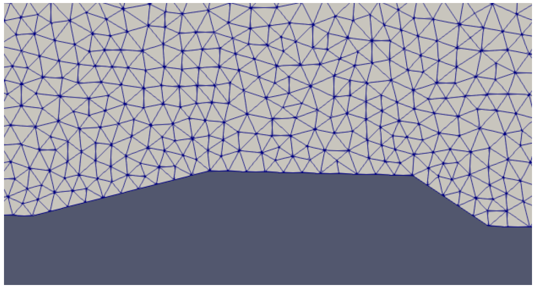
OUU OPTIMIZATION - SETUP

Problems and solution methods:

- Deterministic:
  - Dakota + NOWPAC
  - Medium grid
- Stochastic:
  - Dakota + SNOWPAC+ MC Estimator
    - 20 samples
    - Medium grid
  - Dakota + SNOWPAC + MLMC Estimator
    - 25 + 5 samples coarse grid
    - 5 samples medium grid



coarse



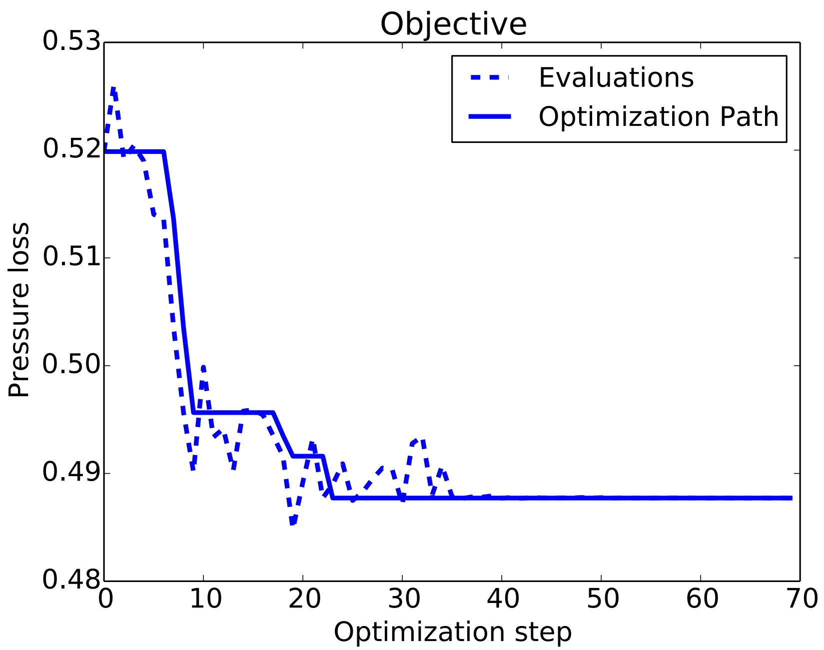
medium

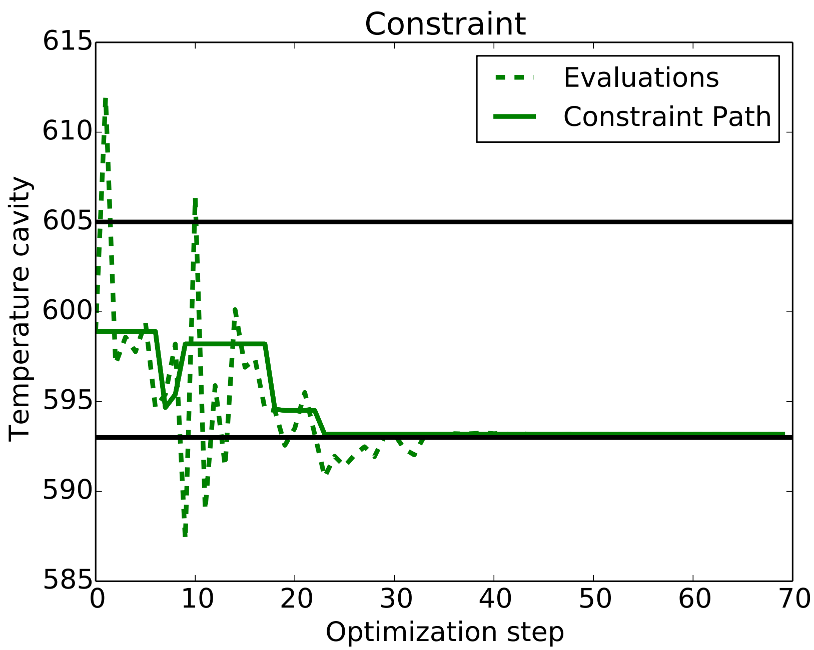
Same initial design: $\vec{x} = [2., 11., 3., 18., 85]^T$

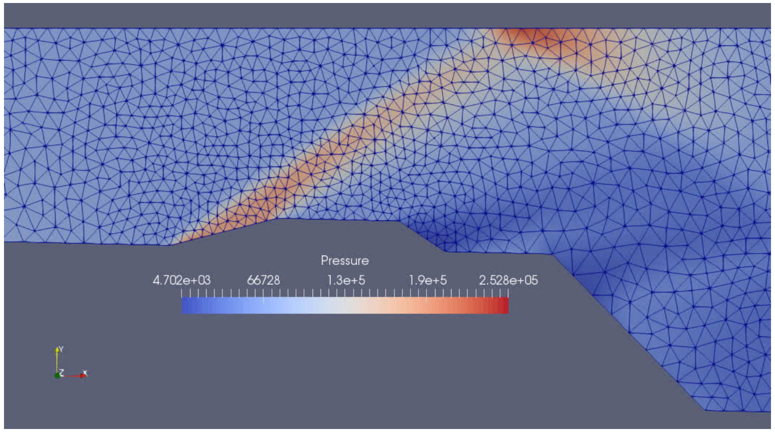
Computational cost:

- Coarse grid: ~ 30s/evaluation
- Medium grid: ~ 4min/evaluation

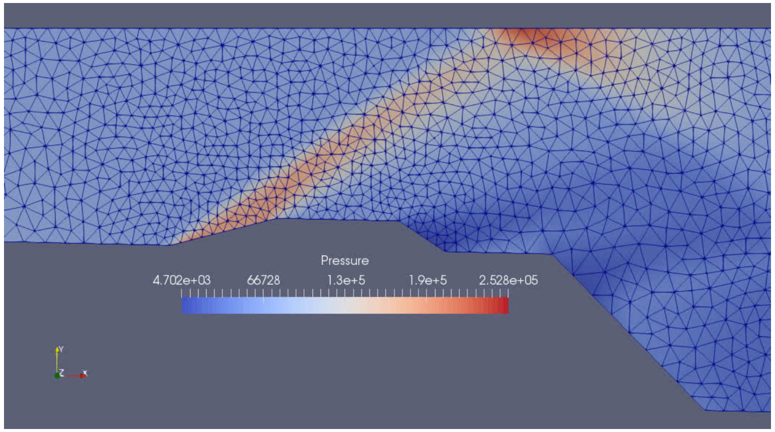
Deterministic OPTIMIZATION - Results





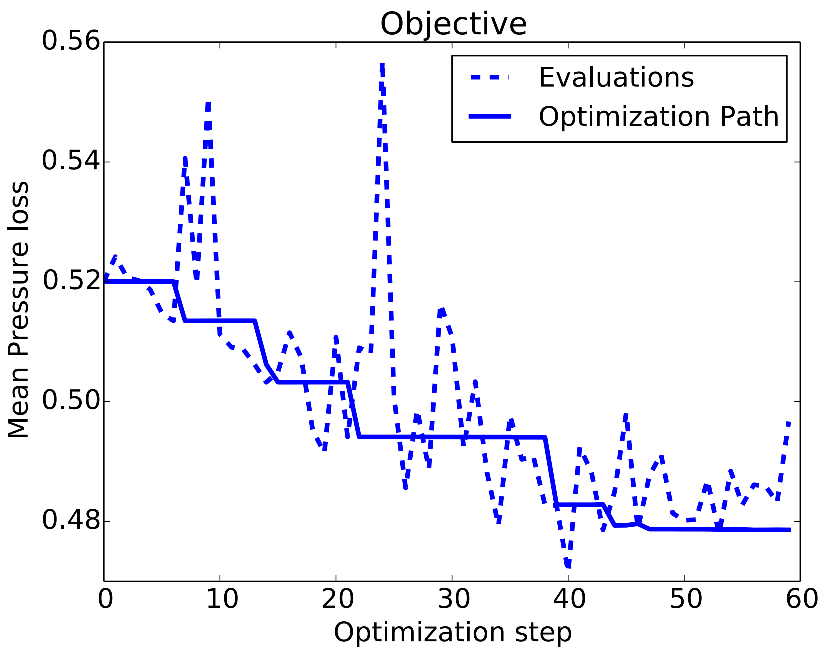


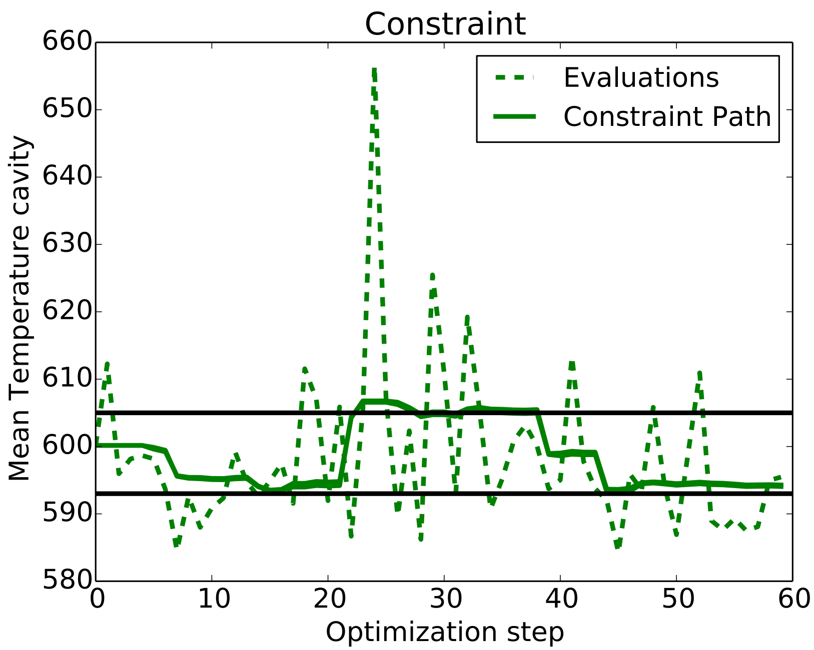
Optimization Path

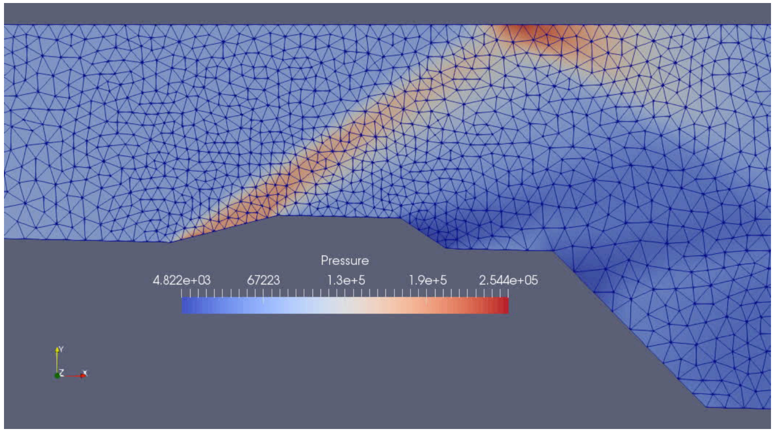


Evaluations

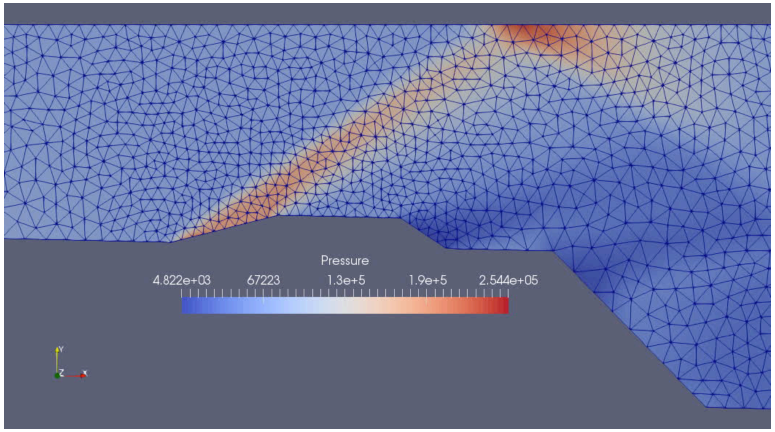
Stochastic MC OPTIMIZATION - Results





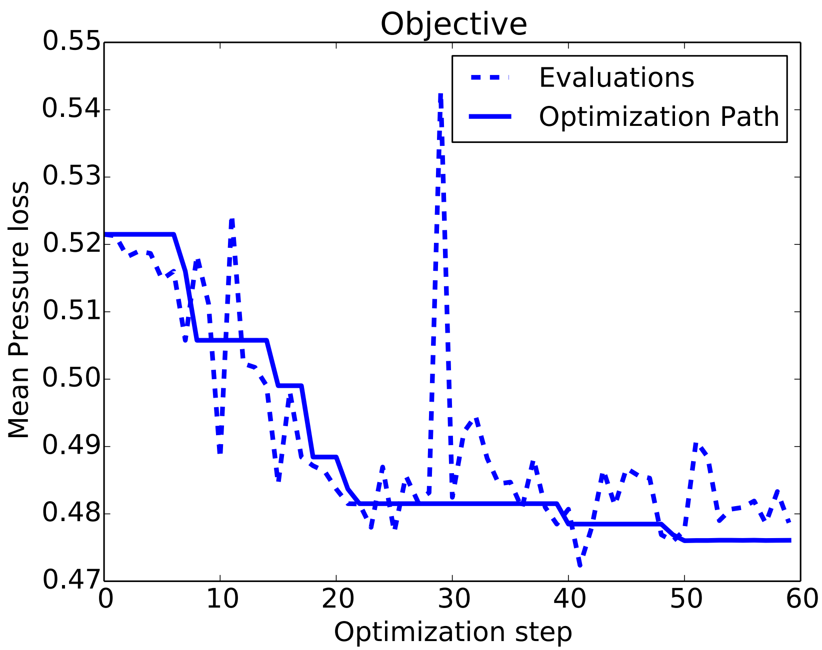


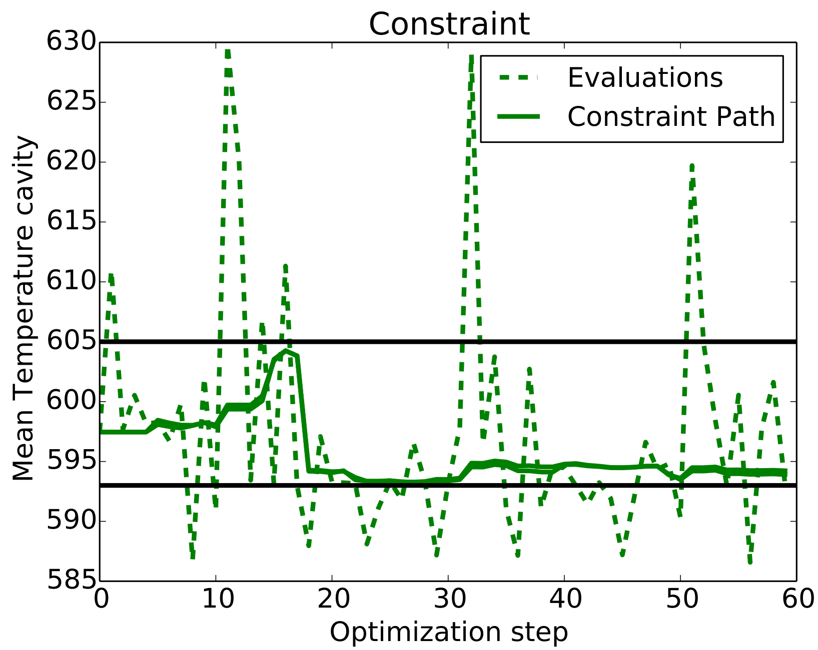
Optimization Path

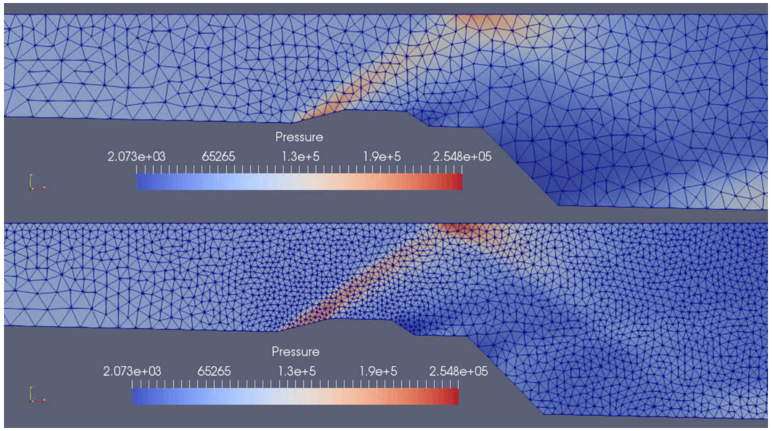


Evaluations

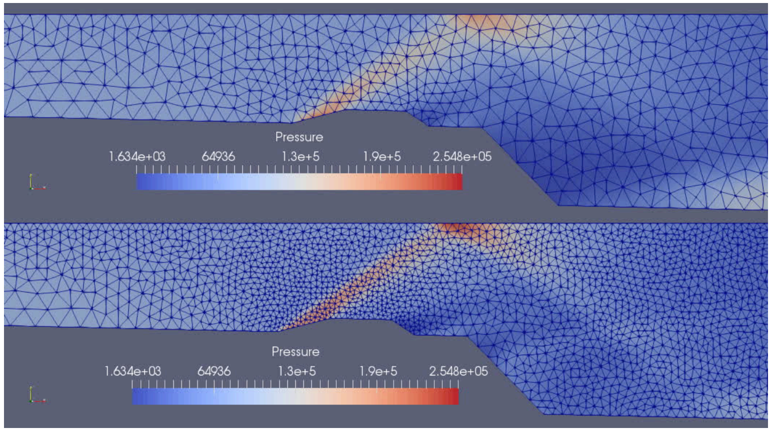
Stochastic MLMC OPTIMIZATION - Results







Optimization Path



Evaluations

OUU OPTIMIZATION – Results Summary

Reminder:

- Initial design: $\vec{x} = [2., 11., 3., 18., 85]^T$
- Constraint: $s.t. 593 \leq T_{cav}/\mathbb{E}[T_{cav}] \leq 605$

$0.5 \leq hb \leq 2.5$ $\quad 17.5 \leq lb \leq 20.5$

$7.5 \leq lt \leq 11.5$ $\quad 79.5 \leq xb \leq 85.5$

$2.5 \leq ltp \leq 4.5$

Problem	Final Design x^*	Final Objective $p^*_{loss}/\tilde{p}^*_{loss}$	Final Constraint	~ Runtime/ Total Evaluations
Deterministic	[1.72, 10.5, 2.79, 18.12, 80.26]	0.48771833	593.18	18h 70 Medium, serial
Stochastic MC	[2.07, 9.28, 2.5, 20.5, 79.5]	0.478597896	595.03	24h 1200 Medium, 4 parallel
Stochastic MLMC	[2.09, 7.5, 3.67, 18.35, 79.5]	0.47607471	594.23	15h 1800 Coarse, 4 parallel 300 Medium, 4 parallel

- Different final designs } Multimodal objective
- Similar final objectives } Multimodal objective
- Feasibility restoration visible in stochastic optimization
- Slower convergence for stochastic optimization

- Lower bound constraint active
- Box constraints active
- Computational speed up due to asynchronous evaluations in MC and MLMC

From here, move towards robust/reliable designs

Dakota Workflow Details (time permitting)

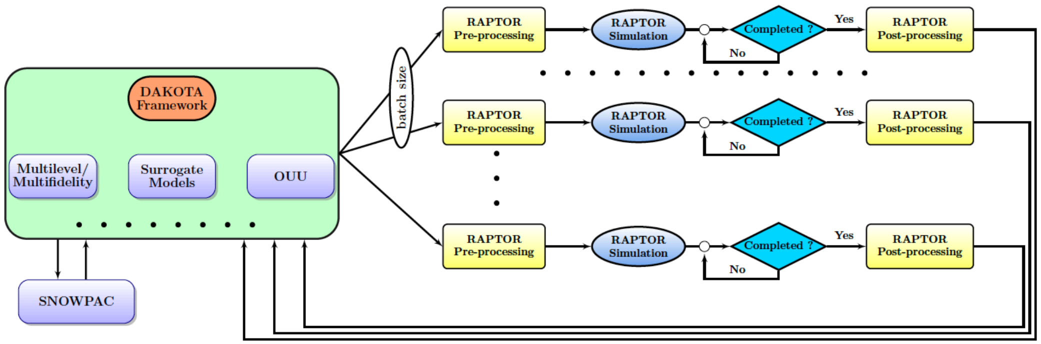
dakota_su2_mlmc.out

```
environment,
#       graphics
        tabular_data
        method_pointer = 'OPTIM'

###########################
# begin opt specification #
###########################
method,
        id_method = 'OPTIM'
        model_pointer = 'OPTIM_M'
        snowpac
          seed = 25041981
          max_iterations = 100
#         max_function_evaluations = 1000
#         convergence_tolerance = 1e-4
          trust_region
            initial_size = 0.15
            minimum_size = 1.0e-6
            contract_threshold = 0.25
            expand_threshold   = 0.75
            contraction_factor = 0.50
            expansion_factor   = 1.50
#         output debug

model,
        id_model = 'OPTIM_M'
        nested
          variables_pointer  = 'OPTIM_V'
          sub_method_pointer = 'UQ'
          responses_pointer  = 'OPTIM_R'
          primary_response_mapping   = 1. 0. 0. 0.
          secondary_response_mapping = 0. 0. 1. 0.

variables,
        id_variables = 'OPTIM_V'
        continuous_design = 5
          initial_point      2.   11.   3.   18.  85
          upper_bounds    2.5    11.5    4.5    20.5    85.5
          lower_bounds     0.5  7.5     2.5     17.5    79.5
          descriptors      'hb'    'lt' 'ltp'   'lb'    'xb'
          #scale_types     'none'
          #scales          0.1

responses,
# minimize mean Weight
# s.t.     mean_S <= 0
#          mean_D <= 0
        id_responses = 'OPTIM_R'
        objective_functions = 1
        nonlinear_inequality_constraints = 1 # default upper bounds < 0.0
        nonlinear_inequality_lower_bounds = 593
        nonlinear_inequality_upper_bounds = 605
        no_gradients
        no_hessians
        #primary_scale_types = 'none'
        #primary_scales = 0.1

##########################
# begin UQ specification #
##########################
-:**-  dakota_su2_mlmc.out    1% L42    SVN:2974  (Fundamental)
```

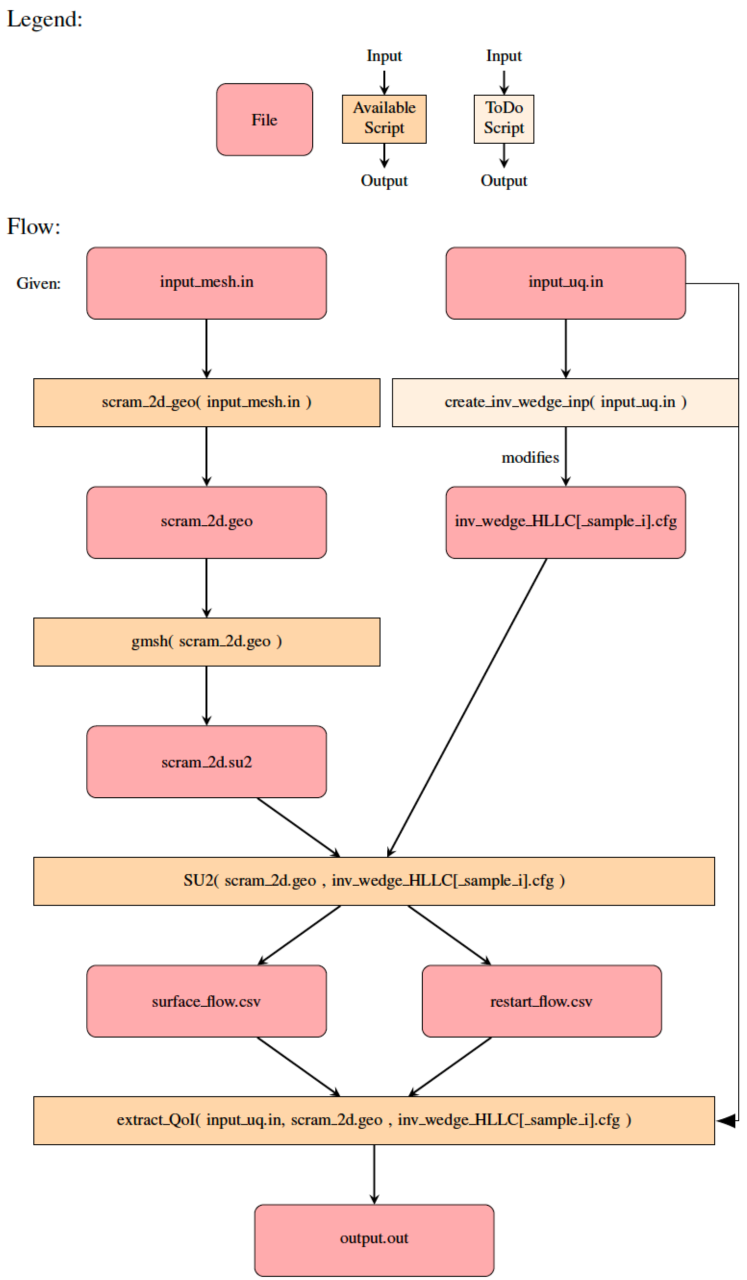
dakota_su2_mlmc.out

```
##########################
# begin UQ specification #
##########################
method,
        id_method = 'UQ'
        model_pointer = 'HIERARCH'
      multilevel_sampling
          pilot_samples = 25 5
          final_moments central
          max_iterations = 0
          seed = 12347
          #sample_type random # use MC error estimates
#         fixed_seed
          output silent
#       final_moments central

model,
        id_model = 'HIERARCH'
        variables_pointer = 'UQ_V'
        responses_pointer = 'UQ_R'
        surrogate hierarchical
          ordered_model_fidelities = '2D'

model,
        id_model = '2D'
        variables_pointer = 'UQ_V'
        interface_pointer = 'UQ_I'
        responses_pointer = 'UQ_R'
        simulation
          solution_level_control = 'mesh_density'
          solution_level_cost = 0.1 1.0 # relative cost of 2DCoarse, 2DFine

variables,
        id_variables = 'UQ_V'
        continuous_design = 5
        normal_uncertain = 3
          means            =  1.48E+6  1550E+0 2.51
          std_deviations   =  0.0074E+6 7.75E+0 0.01255 # 0.5% std
          descriptors      =   'P'     'T'     'Ma'
          discrete_state_set string = 1
          initial_state = 'COARSE'
          set_values = 'COARSE' 'MEDIUM'
          descriptors = 'mesh_density'

interface,
        id_interface = 'UQ_I'
        fork asynchronous evaluation_concurrency = 4
          analysis_driver = 'run_DAK2SU2_interface.sh'
          parameters_file = 'params.in'
          results_file = 'results.out'
          file_save file_tag
          #file_tag file_save

responses,
        id_responses = 'UQ_R'
        response_functions = 2
        no_gradients
        no_hessians
---------------------
End DAKOTA input file
---------------------
-:**-  dakota_su2_mlmc.out    3% L100   SVN:2974  (Fundamental)
```

ries



- Black box driver based on fork + file I/O
- Asynchronous local concurrency with work directories
- Multiple levels of parallelism: optimizer, UQ, SU2



Deterministic

```
Using Dakota input file 'dakota_su2_nowpac.in'
Writing new restart file dakota.rst

>>>>> Executing environment.

>>>>> Running nowpac iterator.

------------------------------
Begin     UQ_I Evaluation    1
------------------------------
Parameters for evaluation 1:
                      2.0000000000e+00 hb
                      1.1000000000e+01 lt
                      3.0000000000e+00 ltp
                      1.8000000000e+01 lb
                      8.5000000000e+01 xb
                                MEDIUM mesh_density

blocking fork: run_DAK2SU2_interface.sh params.in.1 results.out.1

Active response data for UQ_I evaluation 1:
Active set vector = { 1 1 }
                      5.1986449332e-01 obj_fn
                      5.9890487703e+02 nln_ineq_con_1



------------------------------
Begin     UQ_I Evaluation    2
------------------------------
Parameters for evaluation 2:
                      2.3000000000e+00 hb
                      1.1000000000e+01 lt
                      3.0000000000e+00 ltp
                      1.8000000000e+01 lb
                      8.5000000000e+01 xb
                                MEDIUM mesh_density

blocking fork: run_DAK2SU2_interface.sh params.in.2 results.out.2

Active response data for UQ_I evaluation 2:
Active set vector = { 1 1 }
                      5.2606601776e-01 obj_fn
                      6.1195189499e+02 nln_ineq_con_1



------------------------------
Begin     UQ_I Evaluation    3
------------------------------
Parameters for evaluation 3:
                      2.0000000000e+00 hb
                      1.0400000000e+01 lt
                      3.0000000000e+00 ltp
                      1.8000000000e+01 lb
                      8.5000000000e+01 xb
                                MEDIUM mesh_density

blocking fork: run_DAK2SU2_interface.sh params.in.3 results.out.3

Active response data for UQ_I evaluation 3:
Active set vector = { 1 1 }
-:---  dakota_su2_nowpac_medium.out    5% L77    SVN-2974  (Fundamental)
```

MC

```
dakota_su2_snowpac_medium.out

Using Dakota input file 'dakota_su2_snowpac.in'
Writing new restart file dakota.rst

>>>>> Executing environment.

>>>>> Running snowpac iterator.

-------------------------------------------------
NestedModel Evaluation    1: running sub_iterator
-------------------------------------------------

NonD random Samples = 20 Seed (user-specified) = 12347

Blocking synchronize of 20 asynchronous UQ_I evaluations
First pass: initiating 4 local asynchronous jobs
Second pass: scheduling 16 remaining local asynchronous jobs

Active response data from sub_iterator:
Active set vector = { 1 0 1 0 }
                      5.2004116715e-01 mean_r1
                      6.0016183017e+02 mean_r2



---------------------------
NestedModel Evaluation    1 results:
---------------------------

Active response data from nested mapping:
Active set vector = { 1 1 }
                      5.2004116715e-01 obj_fn
                      6.0016183017e+02 nln_ineq_con_1



-------------------------------------------------
NestedModel Evaluation    2: running sub_iterator
-------------------------------------------------

NonD random Samples = 20 Seed not reset from previous LHS execution

Blocking synchronize of 20 asynchronous UQ_I evaluations
First pass: initiating 4 local asynchronous jobs
Second pass: scheduling 16 remaining local asynchronous jobs

Active response data from sub_iterator:
Active set vector = { 1 0 1 0 }
                      5.2419844639e-01 mean_r1
                      6.1227624902e+02 mean_r2



---------------------------
NestedModel Evaluation    2 results:
---------------------------

Active response data from nested mapping:
Active set vector = { 1 1 }
                      5.2419844639e-01 obj_fn
                      6.1227624902e+02 nln_ineq_con_1
-:---  dakota_su2_snowpac_medium.out    6% L129   SVN-2974  (Fundamental)
```

MLMC

```
>>>>> Executing environment.

>>>>> Running snowpac iterator.

---------------------------------------------------
NestedModel Evaluation    1: running sub_iterator
---------------------------------------------------

MLMC pilot sample:
                                    25
                                     5


NonD random Samples = 25 Seed (user-specified) = 12347

Blocking synchronize of 25 asynchronous UQ_I evaluations
First pass: initiating 4 local asynchronous jobs
Second pass: scheduling 21 remaining local asynchronous jobs

NonD random Samples = 5 Seed not reset from previous LHS execution

Blocking synchronize of 10 asynchronous UQ_I evaluations
First pass: initiating 4 local asynchronous jobs
Second pass: scheduling 6 remaining local asynchronous jobs

Blocking synchronize of 0 asynchronous UQ_I evaluations

MLMC iteration 1 sample increments:
                                 98683
                                 12172


Active response data from sub_iterator:
Active set vector = { 1 0 1 0 }
                      5.2149926761e-01 mean_r1
                      5.9745882158e+02 mean_r2



----------------------------
NestedModel Evaluation    1 results:
----------------------------

Active response data from nested mapping:
Active set vector = { 1 1 }
                      5.2149926761e-01 obj_fn
                      5.9745882158e+02 nln_ineq_con_1



---------------------------------------------------
NestedModel Evaluation    2: running sub_iterator
---------------------------------------------------

MLMC pilot sample:
                                    25
                                     5


NonD random Samples = 25 Seed not reset from previous LHS execution

Blocking synchronize of 25 asynchronous UQ_I evaluations
-:---  dakota_su2_mlmc.out    5% L167  SVN-2974  (Fundamental)
```