Exceptional service in the national interest

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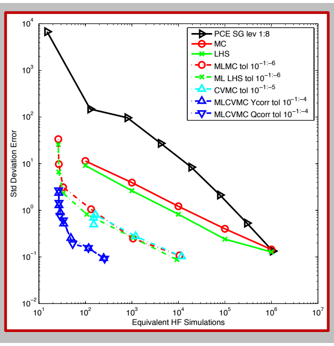
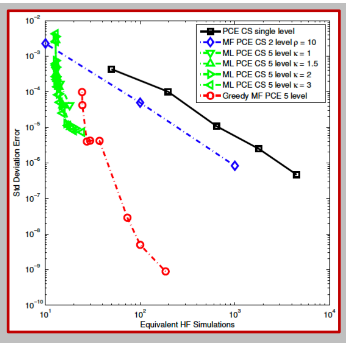
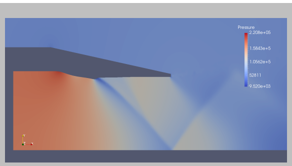
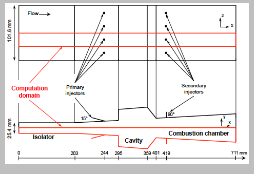


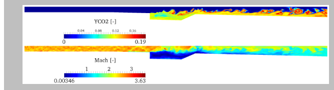


DAKOTA

Explore and predict with confidence







Multilevel-Multifidelity Sampling and Emulation for Forward UQ

Michael S. Eldred, Gianluca Geraci, Alex A. Gorodetsky, John D. Jakeman
Sandia National Laboratories, Albuquerque NM / University of Michigan, Ann Arbor MI

IPAM Workshop: HPC and Data Science for Scientific Discovery, UCLA, October 15-19, 2018

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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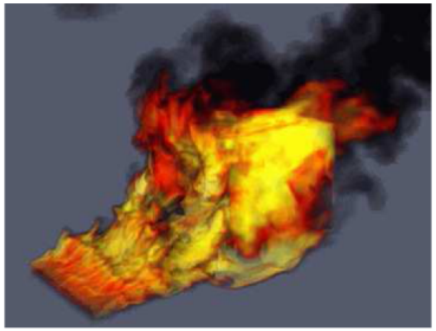
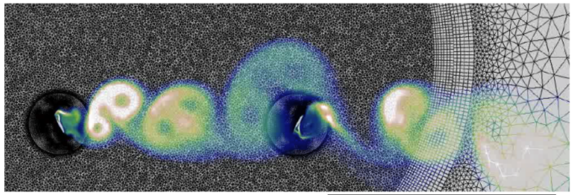
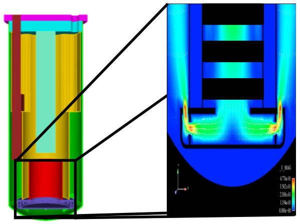
UQ & Optimization: DOE/DOD Mission Deployment

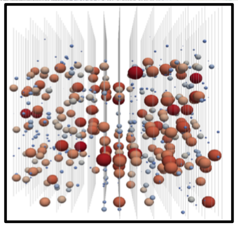
Stewardship (NNSA ASC)
Safety in abnormal environments



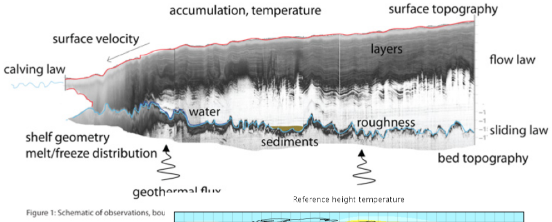
Energy (ASCR, EERE, NE)
Wind turbines, nuclear reactors

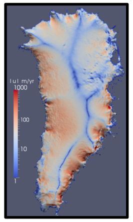


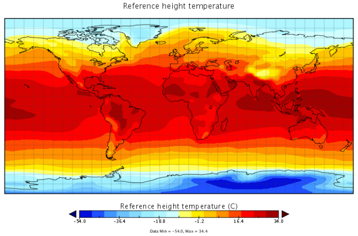




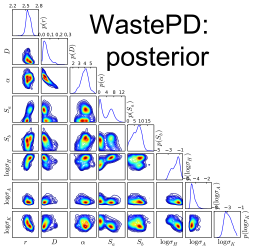
Climate (SciDAC, CSSEF, ACME)
Ice sheets, CISM, CESM, ISSM, CSDMS

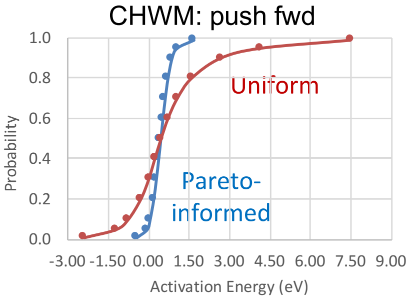


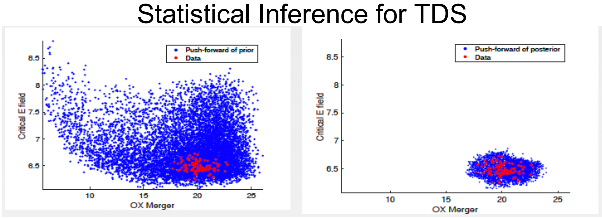




Addtnl. Office of Science:
(SciDAC, EFRC)
Comp. Matls: waste forms / hazardous matls (WastePD, CHWM)
MHD: Tokamak disruption (TDS)







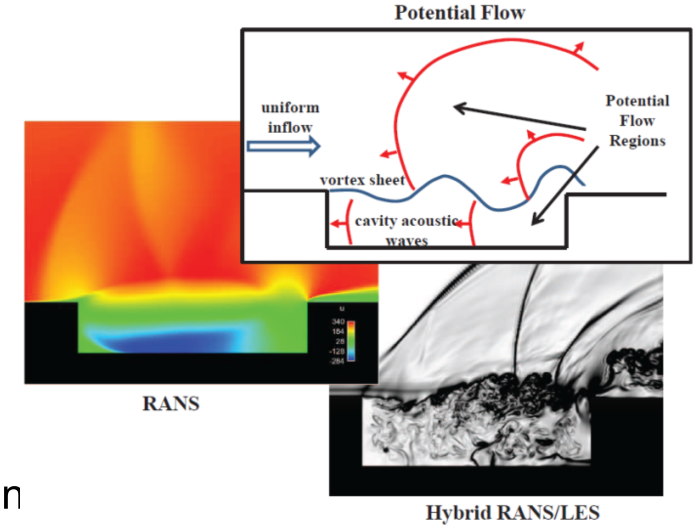
Common theme across these applications:

- High-fidelity simulation models: 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, multiscale)

Focus on scalable algorithms in combination with approaches that can exploit a modeling hierarchy.

Multiple Model Forms in UQ & Opt

Discrete model choices for simulation of same physics



A clear hierarchy of fidelity (from low to high)

- Exploit less expensive models to render HF practical
  - *Multifidelity Opt, UQ, inference*
- Support general case of discrete model forms
  - Discrepancy does not go to 0 under refinement

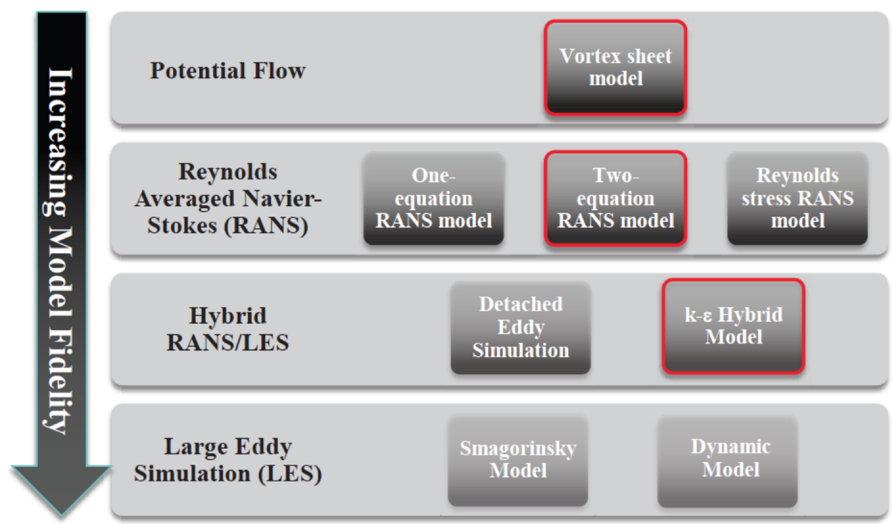
An ensemble of peer models lacking clear preference structure / cost separation: e.g., SGS models

- *With data:* model selection, inadequacy characterization
  - Criteria: predictivity, discrepancy complexity
- *Without (adequate) data:* epistemic model form uncertainty propagation
  - Intrusive, nonintrusive
- *Within MF context:* CV correlation

Discretization levels / resolution controls

- Exploit special structure: discrepancy → 0 at order of spatial/temporal convergence

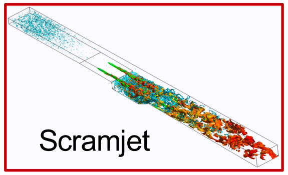
Combinations for multiphysics, multiscale

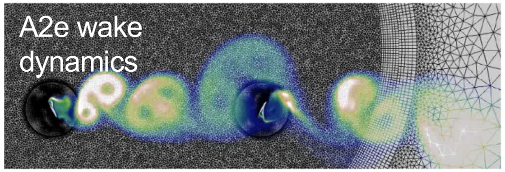


Multilevel-Multifidelity Concepts Have Broad Relevance

Recurring R&D theme: couple scalable algorithms with exploiting a (multi-dimensional) model hierarchy

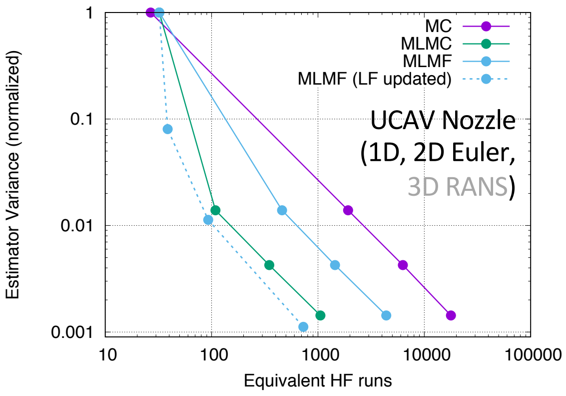
- address scale and expense for high fidelity M&S applications in defense, energy, and climate
- render UQ / optimization / OUU tractable for cases where only a handful of HF runs are possible





Monte Carlo Methods (UQ)

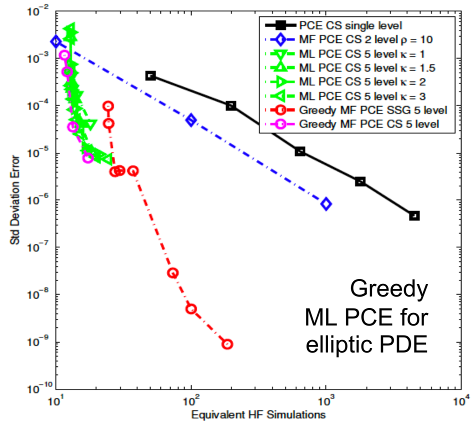
Optimal resource allocation: multilevel (ML), multifidelity (MF), and combined (MLMF)



- More than order of magnitude speedup vs. MC
- Render HF UQ possible (e.g., only 9 LES in 24D)
- Integrate w/ active subspaces (enhance ρ, link ξ)
- Unification of ML, MF, MI approaches

Polynomial Chaos Methods (UQ)

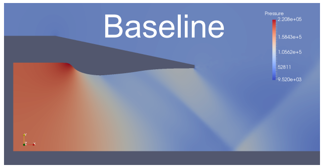
- ML rate estimation, greedy ML adaptation
- Sparse grids, compressed sensing, fn train

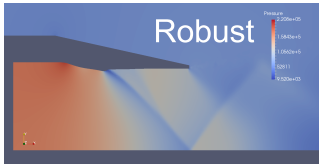


- Exploit problem structure: sparsity, low rank
- Additional orders of magn. when regular
- Sparse grids in model space

Recursive Trust Region Methods (OUU)

- Extend trust-region model mgmt. to deep hierarchies
- Manage both simulation and stochastic fidelity





UCAV Nozzle OUU (Aero, Structural, Thermal)

- Order of magnitude fewer HF runs
- More aggressive profile shaping than MG/Opt

Monte Carlo Methods

Monte Carlo Sampling Methods

MSE for mean estimator

Problem statement: We are interested in the expected value of $Q_M = \mathcal{G}(\mathbf{X}_M)$ where

- M is (related to) the number of spatial degrees of freedom
- $\mathbb{E}[Q_M] \xrightarrow{M\to\infty} \mathbb{E}[Q]$ for some RV $Q : \Omega \to \mathbb{R}$

Monte Carlo:

$$\hat{Q}^{MC}_{M,N} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{i=1}^{N} Q_M^{(i)},$$

two sources of error:

- Sampling error: replacing the expected value by a (finite) sample average
- Spatial discretization: finite resolution implies $Q_M \approx Q$

Looking at the Mean Square Error:

$$\mathbb{E}\left[(\hat{Q}^{MC}_{M,N} - \mathbb{E}[Q])^2 \right] = N^{-1} \mathbb{V}ar(Q_M) + (\mathbb{E}[Q_M - Q])^2$$

Accurate estimation $\Rightarrow$ **Large number** of samples at high (spatial) resolution

Multilevel and Multifidelity Sampling Methods
Multilevel MC: decomposition of variance

Multilevel MC: Sampling from several approximations Q_M of Q (Multigrid...)

Ingredients:

- $\{M_\ell : \ell = 0, \ldots, L\}$ with $M_0 < M_1 < \cdots < M_L \stackrel{\text{def}}{=} M$
- Estimation of $\mathbb{E}[Q_M]$ by means of correction w.r.t. the next lower level

$$Y_\ell \stackrel{\text{def}}{=} Q_{M_\ell} - Q_{M_{\ell-1}} \xrightarrow{linearity} \mathbb{E}[Q_M] = \mathbb{E}[Q_{M_0}] + \sum_{\ell=1}^{L} \mathbb{E}\left[Q_{M_\ell} - Q_{M_{\ell-1}}\right] = \sum_{\ell=0}^{L} \mathbb{E}[Y_\ell]$$

- Multilevel Monte Carlo estimator

$$\hat{Q}_M^{\text{ML}} \stackrel{\text{def}}{=} \sum_{\ell=0}^{L} \hat{Y}_{\ell,N_\ell}^{\text{MC}} = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left(Q_{M_\ell}^{(i)} - Q_{M_{\ell-1}}^{(i)} \right)$$

- The Mean Square Error is

$$\mathbb{E}\left[(\hat{Q}_M^{ML} - \mathbb{E}[Q])^2\right] = \sum_{\ell=0}^{L} N_\ell^{-1} \mathbb{V}ar(Y_\ell) + (\mathbb{E}[Q_M - Q])^2$$

Note If $Q_M \to Q$ (in a mean square sense), then $\mathbb{V}ar(Y_\ell) \xrightarrow{\ell \to \infty} 0$

Multilevel and Multifidelity Sampling Methods

Multilevel MC: optimal resource allocation

Let us consider the numerical cost of the estimator

$$\mathcal{C}(\hat{Q}_M^{ML}) = \sum_{\ell=0}^{L} N_\ell \mathcal{C}_\ell$$

Determining the ideal number of samples per level (i.e. minimum cost at fixed variance)

$$\underbrace{\left.\begin{aligned} \mathcal{C}(\hat{Q}_M^{ML}) &= \sum_{\ell=0}^{L} N_\ell \mathcal{C}_\ell \\ \sum_{\ell=0}^{L} N_\ell^{-1} \mathbb{V}ar\left(Y_\ell\right) &= \varepsilon^2/2 \end{aligned}\right\}}_{\text{Balance ML estimator variance (stochastic error) and residual bias (deterministic error)} \rightarrow \text{don't over-resolve one at the expense of the other}} \xrightarrow{Lagrange\ multiplier} \underbrace{\boxed{N_\ell = \underbrace{\frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L} \left(\mathbb{V}ar\left(Y_k\right)\mathcal{C}_k\right)^{1/2}\right]}_{\text{Level independent}} \underbrace{\sqrt{\frac{\mathbb{V}ar\left(Y_\ell\right)}{\mathcal{C}_\ell}}}_{\text{Level dependent}}}}_{\text{Optimal sample profile}}$$

M. Giles, "Multilevel Monte Carlo path simulation," 2008.

Multilevel and Multifidelity Sampling Methods

Classical Control Variate → Multifidelity MC

A Control Variate MC estimator (function G with $\mathbb{E}[G]$ known)

$$\hat{Q}_N^{MCCV} = \hat{Q}_N^{MC} - \beta\left(\hat{G}_N^{MC} - \mathbb{E}[G]\right)$$

$$\underset{\beta}{\operatorname{argmin}}\, \mathbb{V}ar\left(\hat{Q}_N^{MCCV}\right) \rightarrow \beta = -\rho \frac{\mathbb{V}ar^{1/2}(Q)}{\mathbb{V}ar^{1/2}(G)} \qquad \mathbb{V}ar\left(\hat{Q}_N^{MCCV}\right) = \mathbb{V}ar\left(\hat{Q}_N^{MC}\right)\left(1-\rho^2\right)$$

In our context, *G* is a low fidelity approximation of *Q* and its expectation is not known *a priori*

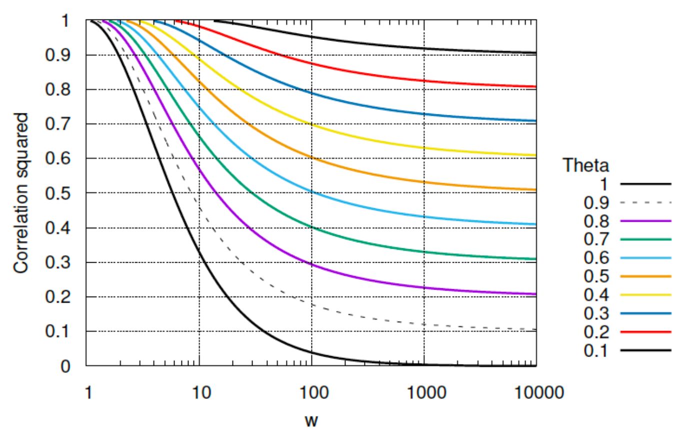
Let's modify the high-fidelity QoI, Q_M^{HF}, to decrease its variance

$$\hat{Q}_{M,N}^{\mathrm{HF},CV} = \hat{Q}_{M,N}^{\mathrm{HF}} + \alpha\left(\hat{Q}_{M,N}^{\mathrm{LF}} - \mathbb{E}\left[Q_M^{\mathrm{LF}}\right]\right).$$

additional and independent set $\Delta^{\mathrm{LF}} = rN^{\mathrm{HF}}$

$$\mathbb{V}ar\left(\hat{Q}_{M,N}^{\mathrm{HF},CV}\right) = \mathbb{V}ar\left(\hat{Q}_M^{\mathrm{HF}}\right)\left(1 - \frac{r}{1+r}\rho_{HL}^2\right)$$

MFMC cost relative to MC



Minimize CV estimator variance → control param. as before:

$$\frac{\mathrm{d}\,\mathbb{V}ar\left(\hat{Q}_M^{\mathrm{HF,MF}}\right)}{\mathrm{d}\,\alpha} = 0 \quad \rightarrow \quad \alpha = -\rho\frac{\mathbb{V}ar^{1/2}(Q_M^{\mathrm{HF}})}{\mathbb{V}ar^{1/2}(Q_M^{\mathrm{LF}})}$$

Minimize total cost → optimal sample ratio: $r^\star = -1 + \sqrt{\dfrac{w\rho^2}{1-\rho^2}}$

Multilevel – Multifidelity Sampling Methods
Combining ML and CV for multidimensional model hierarchies

- OUTER SHELL – Multi-level

$$\mathbb{E}\left[Q_M^{\mathrm{HF}}\right] = \sum_{l=0}^{L_{\mathrm{HF}}} \mathbb{E}\left[Y_\ell^{\mathrm{HF}}\right] = \sum_{l=0}^{L_{\mathrm{HF}}} \hat{Y}_\ell^{\mathrm{HF}}$$

- INNER BLOCK – Multi-fidelity (*i.e.* control variate on each level)

$$Y_\ell^{\mathrm{HF},\star} = \hat{Y}_\ell^{\mathrm{HF}} + \alpha_\ell \left(\hat{Y}_\ell^{\mathrm{LF}} - \mathbb{E}\left[Y_\ell^{\mathrm{LF}}\right] \right)$$

- Cost per level is now $\mathcal{C}_\ell^{\mathrm{eq}} = \mathcal{C}_\ell^{\mathrm{HF}} + \mathcal{C}_\ell^{\mathrm{LF}} \left(1 + r_\ell\right)$
- the (constrained) optimization problem is

$$\underset{N_\ell^{\mathrm{HF}}, r_\ell, \lambda}{\mathrm{argmin}} \ (\mathcal{L}), \quad \text{where} \quad \mathcal{L} = \sum_{\ell=0}^{L_{\mathrm{HF}}} N_\ell^{\mathrm{HF}} \mathcal{C}_\ell^{\mathrm{eq}} + \lambda \left(\sum_{\ell=0}^{L_{\mathrm{HF}}} \frac{1}{N_\ell^{\mathrm{HF}}} \mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right) \Lambda_\ell(r_\ell) - \varepsilon^2/2 \right)$$

- $\Lambda_\ell(r_\ell) = 1 - \rho_\ell^2 \dfrac{r_\ell}{1 + r_\ell}$

Optimal sample allocation across discretizations and model forms

$$\begin{cases} r_\ell^\star = -1 + \sqrt{\dfrac{\rho_\ell^2}{1-\rho_\ell^2} w_\ell}, \quad \text{where} \quad w_\ell = \mathcal{C}_\ell^{\mathrm{HF}} / \mathcal{C}_\ell^{\mathrm{LF}} \\ N_\ell^{\mathrm{HF},\star} = \dfrac{2}{\varepsilon^2} \left[\sum_{k=0}^{L_{\mathrm{HF}}} \left(\dfrac{\mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right) \mathcal{C}_\ell^{\mathrm{HF}}}{1-\rho_\ell^2} \right)^{1/2} \Lambda_\ell \right] \sqrt{\left(1-\rho_\ell^2\right) \dfrac{\mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right)}{\mathcal{C}_\ell^{\mathrm{HF}}}} \end{cases}$$

Multilevel – Multifidelity Sampling Methods
Combining ML and CV for multidimensional model hierarchy

- Algorithmic-contained correlation improvement
  - Optimality of the LF discrepancy

$$\mathring{Y}_\ell^{\mathrm{LF}} = \gamma_\ell Q_\ell^{\mathrm{LF}} - Q_{\ell-1}^{\mathrm{LF}},$$

where γ is chosen in order to maximize the correlation between Y_ℓ^{HF} and $\mathring{Y}_\ell^{\mathrm{LF}}$

Cost min s.t. error balance

$$N_\ell^{\mathrm{HF},\star} = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L_{\mathrm{HF}}} \left(\frac{\mathbb{V}ar\left(Y_k^{\mathrm{HF}}\right) \mathcal{C}_k^{\mathrm{HF}}}{1-\rho_\ell^2 \frac{\theta_\ell^2}{\tau_\ell}}\right)^{1/2} \Lambda_k(r_k^\star)\right] \sqrt{\left(1-\rho_\ell^2 \frac{\theta_\ell^2}{\tau_\ell}\right) \frac{\mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right)}{\mathcal{C}_\ell^{\mathrm{HF}}}}$$

where

$$\theta_\ell = \frac{\mathrm{Cov}\left(Y_\ell^{\mathrm{LF}}, \mathring{Y}_\ell^{\mathrm{LF}}\right)}{\mathrm{Cov}\left(Y_\ell^{\mathrm{LF}}, Y_\ell^{\mathrm{LF}}\right)} \qquad \tau_\ell = \frac{\mathbb{V}ar\left(\mathring{Y}_\ell^{\mathrm{LF}}\right)}{\mathbb{V}ar\left(Y_\ell^{\mathrm{LF}}\right)} \qquad \Lambda_\ell = 1-\rho_\ell^2 \frac{\theta_\ell^2}{\tau_\ell} \frac{r_\ell^\star}{1+r_\ell^\star} \qquad r_\ell^\star = -1 + \sqrt{\frac{\rho_l^2 \frac{\theta_\ell^2}{\tau_\ell}}{1-\rho_\ell^2 \frac{\theta_\ell^2}{\tau_\ell}} w_\ell}$$

Can be rewritten as

$$\boxed{N_\ell^{\mathrm{HF}} = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L_{\mathrm{HF}}} \left(\frac{\mathbb{V}ar\left(Y_k^{\mathrm{HF}}\right) \mathcal{C}_k^{\mathrm{HF}}}{1-\mathring{\rho}_{HL}^2}\right)^{1/2} \Lambda_k(r_k)\right] \sqrt{\left(1-\mathring{\rho}_{HL}^2\right) \frac{\mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right)}{\mathcal{C}_\ell^{\mathrm{HF}}}}}$$

Compared to previous

$$\boxed{N_\ell^{\mathrm{HF}} = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L_{\mathrm{HF}}} \left(\frac{\mathbb{V}ar\left(Y_k^{\mathrm{HF}}\right) \mathcal{C}_k^{\mathrm{HF}}}{1-\rho_\ell^2}\right)^{1/2} \Lambda_k(r_k)\right] \sqrt{\left(1-\rho_\ell^2\right) \frac{\mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right)}{\mathcal{C}_\ell^{\mathrm{HF}}}}}$$

Multilevel – Multifidelity Sampling Methods

Results on model problem: wave propagation in composites

Sandia National Laboratories

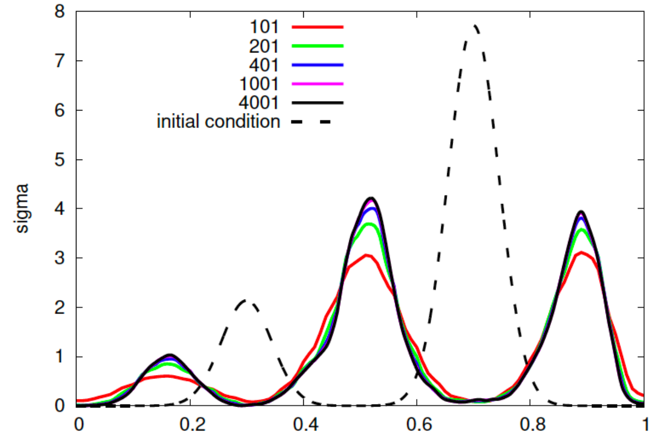
- Rod constituted by 50 layers, two alternated materials (A and B) with constitutive laws

$$\begin{cases} \sigma_A = K_1^A \epsilon + K_2^A \epsilon^2, \quad K_1^A = 1 \quad \text{and} \quad K_2^A = \xi_j \quad \xi_j \sim \mathcal{U}(0.01, 0.02) \\ \sigma_B = K_1^B \epsilon + K_2^B \epsilon^2, \quad K_1^A = 1.5 \quad \text{and} \quad K_2^A = 0.8 \end{cases}$$

- Uncertain initial static $(u(x, t=0) = 0)$ pre-tension state:

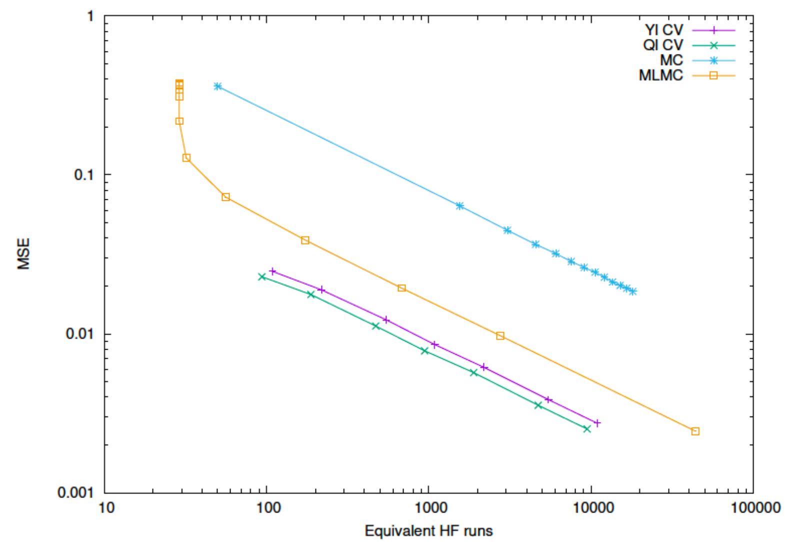
$$\sigma(x) = \begin{cases} \xi_3 \exp\left(-\dfrac{(x-0.35)(x-0.25)}{2 \times 0.002}\right) & \text{if} \quad 0 < x < 1/2 \quad \xi_3 \sim \mathcal{U}(0.5, 2) \\ \xi_2 \exp\left(-\dfrac{(x-0.65)(x-0.75)}{2 \times 0.002}\right) & \text{if} \quad 1/2 < x < 1 \quad \xi_2 \sim \mathcal{U}(0.5, 6.5) \end{cases}$$

- Spatially varying uncertain density: $\rho(x) = \xi_1 + 0.5 \sin(2\pi x)$, $\xi_1 \sim \mathcal{U}(1.5, 2)$
- Clamped rod as B.C.



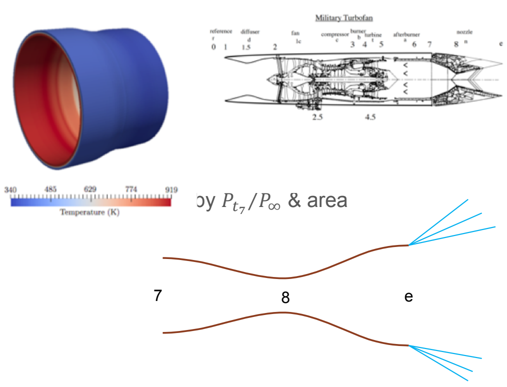
28 random variables
Two fidelities, each with 4 discretizations

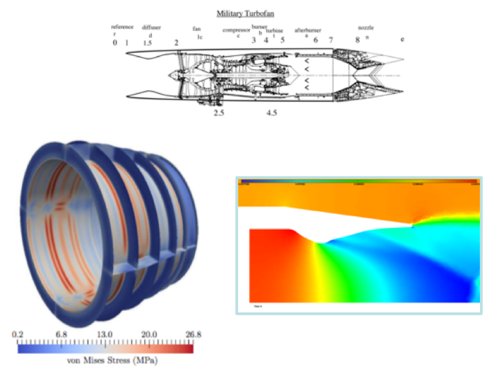
	N_x	N_t	Δ_t
Low-fidelity (GODUNOV)	21	50	3.6×10^{-3}
	41	100	1.8×10^{-3}
	81	150	1.2×10^{-3}
	151	288	6.25×10^{-4}
High-fidelity (MUSCL)	101	200	9×10^{-4}
	201	400	4.5×10^{-4}
	401	900	2×10^{-4}
	1001	2000	9×10^{-5}

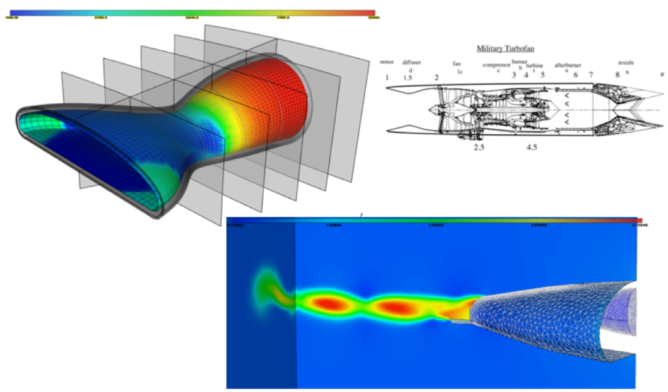


Level	MLMC	MLMF-YI				MLMF-QI			
	N_ℓ	N_ℓ^{HF}	N_ℓ^{LF}	r_ℓ	ρ_ℓ^2	N_ℓ^{HF}	N_ℓ^{LF}	r_ℓ	$\mathring{\rho}_\ell^2$
0	80029	5960	243178	40	0.97	4682	192090	40	0.97
1	6282	2434	12487	4	0.49	1049	13781	12	0.83
2	1271	262	3877	14	0.82	151	3657	23	0.92
3	212	47	966	19	0.84	34	754	21	0.86

DARPA SEQUOIA: Hierarchy of Fidelity Levels







Low fidelity model

- Quasi 1D ideal/non ideal nozzle aero
- 1D heat transfer
- Coarse axisymmetric FEM model
- 30 seconds on one core

Medium fidelity model

- 2D Euler/RANS axisymmetric CFD
- 1D heat transfer
- Coarse axisymmetric FEM model
- 5 minutes on one core (2D Euler)

High fidelity model

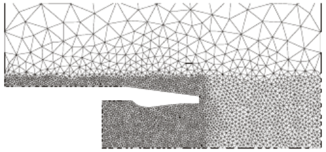
- 3D non-axisymmetric Euler/RANS CFD
- 1D heat transfer
- Full 3D FEM model
- 2 hours on 20 cores (3D RANS, coarse mesh)

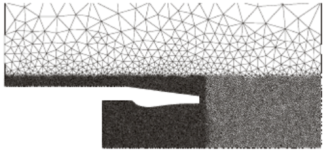
Multiple mesh refinements available for Medium & High (ragged ML-MF)

Initial Deployment of MLCV MC to UCAV Nozzle UQ

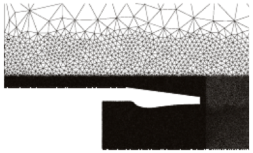
Context: Analysis of performance of UCAV nozzles subject to environmental, material, and manufacturing uncertainties.

Goal: Explore utility of low fidelity model (potential flow, hoop stress) alongside discretizations for medium fidelity (Euler, FEM)





(a) Coarse



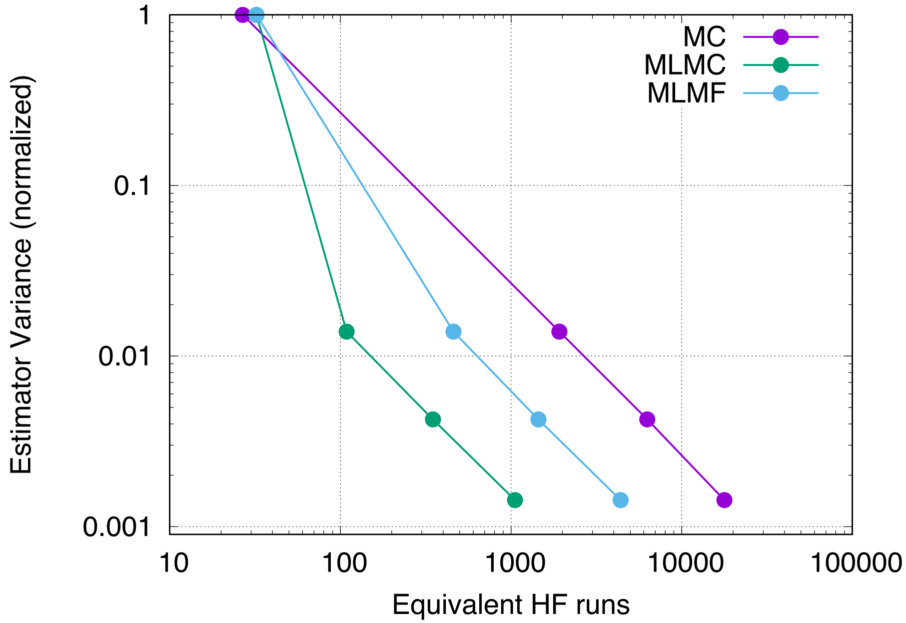
(c) Fine

	Triangles
Coarse	6,119
Medium	29,025
Fine	142,124

TABLE: Number of triangles.

	LF	MF
Coarse	0.016	0.053
Medium	N/A	0.253
Fine	N/A	1.0

TABLE: Computational cost.

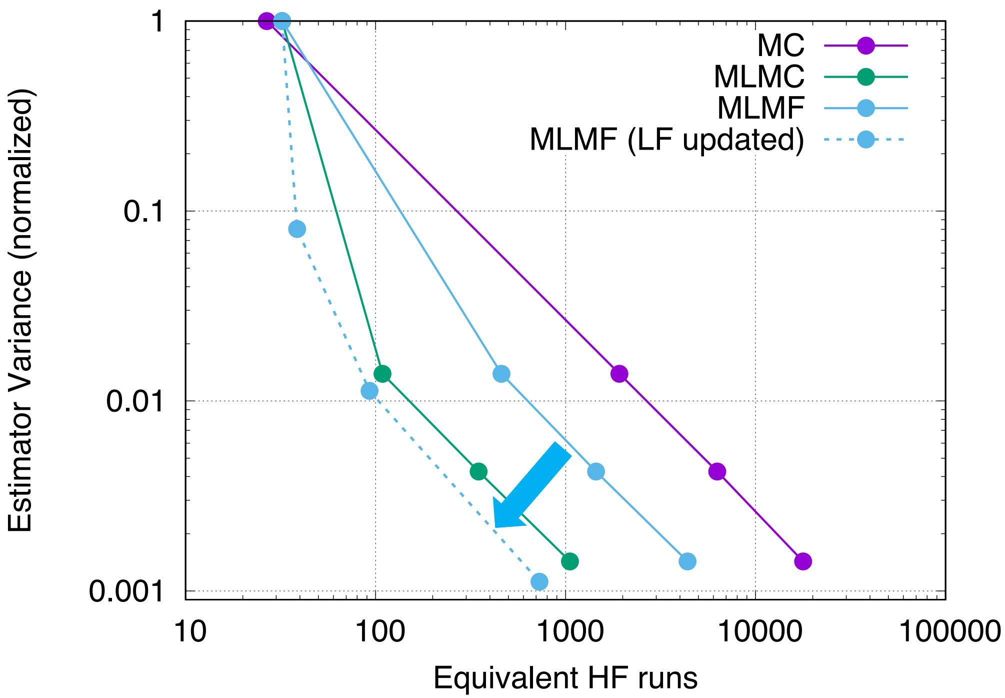


Optimal sample allocations based on relative cost, observed correlation between models, and observed variance distribution across levels

Target accuracy	LF	MF		
	Coarse	Coarse	Medium	Fine
0.01	21143	1757	20	20
0.003	69580	5775	36	20
0.001	212828	17715	109	34

Updated Deployment of MLCV MC to UCAV Nozzle UQ

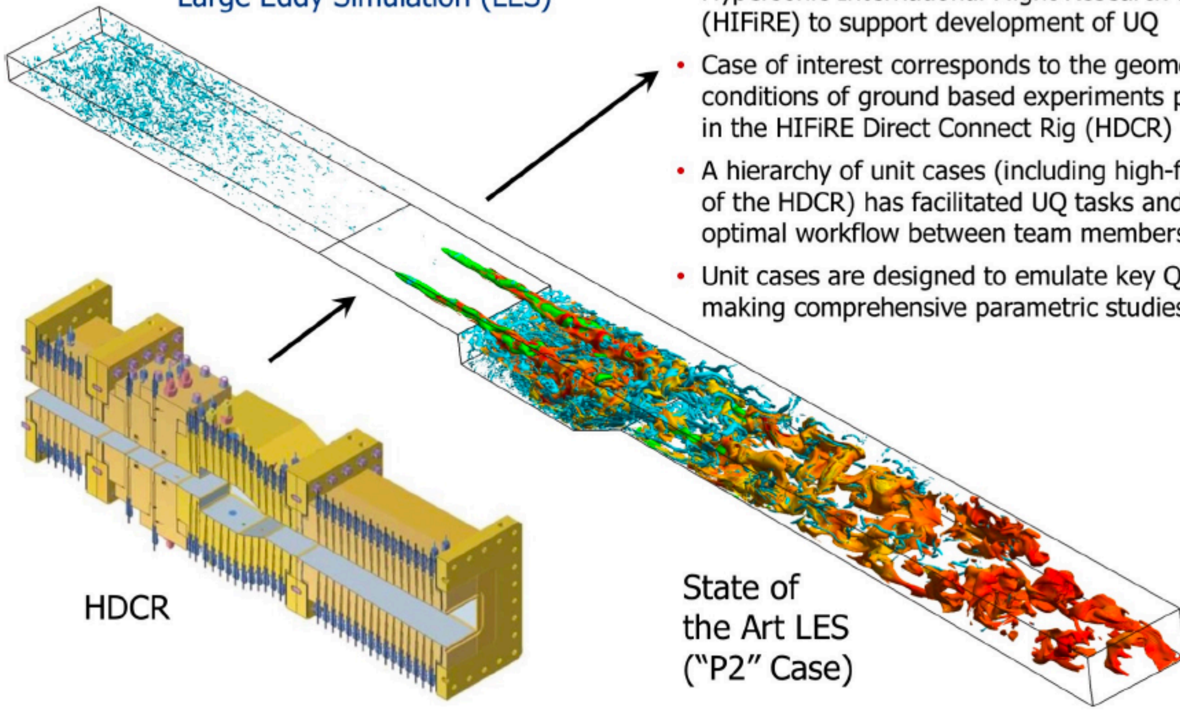
	LF		LF (updated)	
	correlation	Variance reduction [%]	correlation	Variance reduction [%]
Thrust	0.997	91.42	0.996	94.2
Mechanical Stress	2.31e-5	2.12e-3	0.944	89.2
Thermal Stress	0.391	12.81	0.987	93.4



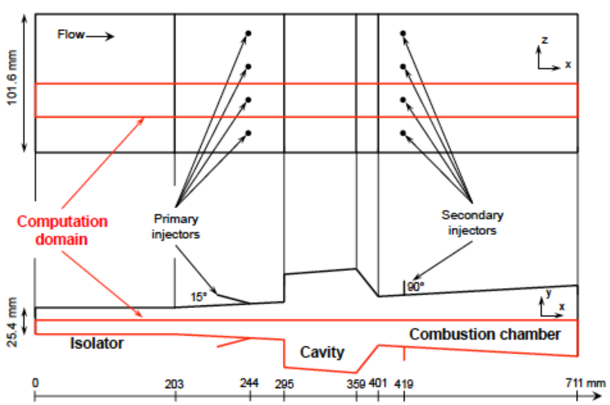
Accuracy ($\varepsilon^2/\varepsilon_0^2$)	LF	Medium Fidelity			LF (updated)	Medium Fidelity		
	Coarse	Coarse	Medium	Fine	Coarse	Coarse	Medium	Fine
0.1	N/A	N/A	N/A	N/A	404	20	20	20
0.01	21,143	1,757	20	20	3,091	177	31	20
0.003	69,580	5,775	36	20	N/A	N/A	N/A	N/A
0.001	212,828	17,715	109	34	32,433	1,773	314	20

DARPA EQUiPS (Scramjet UQ):
LES Models for Turbulent Reacting Flow in HIFiRE

Multiscale-multiphysics application of Large Eddy Simulation (LES)

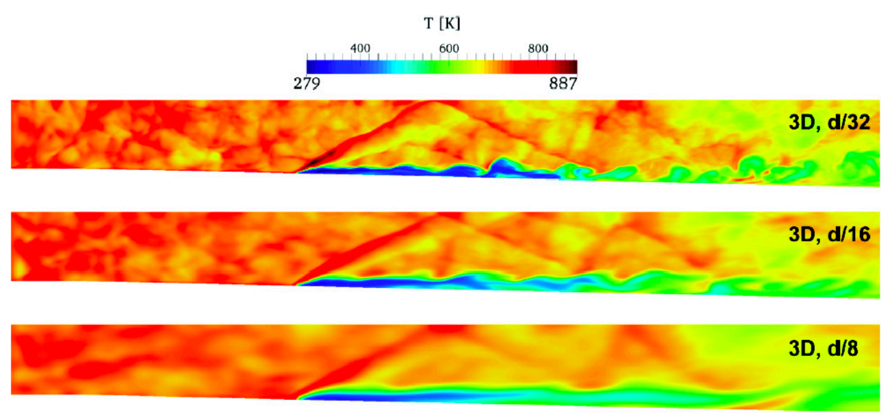


- Provided benchmark LES calculations of the Hypersonic International Flight Research Experiment (HIFiRE) to support development of UQ
- Case of interest corresponds to the geometry and conditions of ground based experiments performed in the HIFiRE Direct Connect Rig (HDCR)
- A hierarchy of unit cases (including high-fidelity LES of the HDCR) has facilitated UQ tasks and provided optimal workflow between team members
- Unit cases are designed to emulate key QoIs while making comprehensive parametric studies possible



Model forms:
- 2D, 3D

Discretizations:
- d/{8,16,32,64}

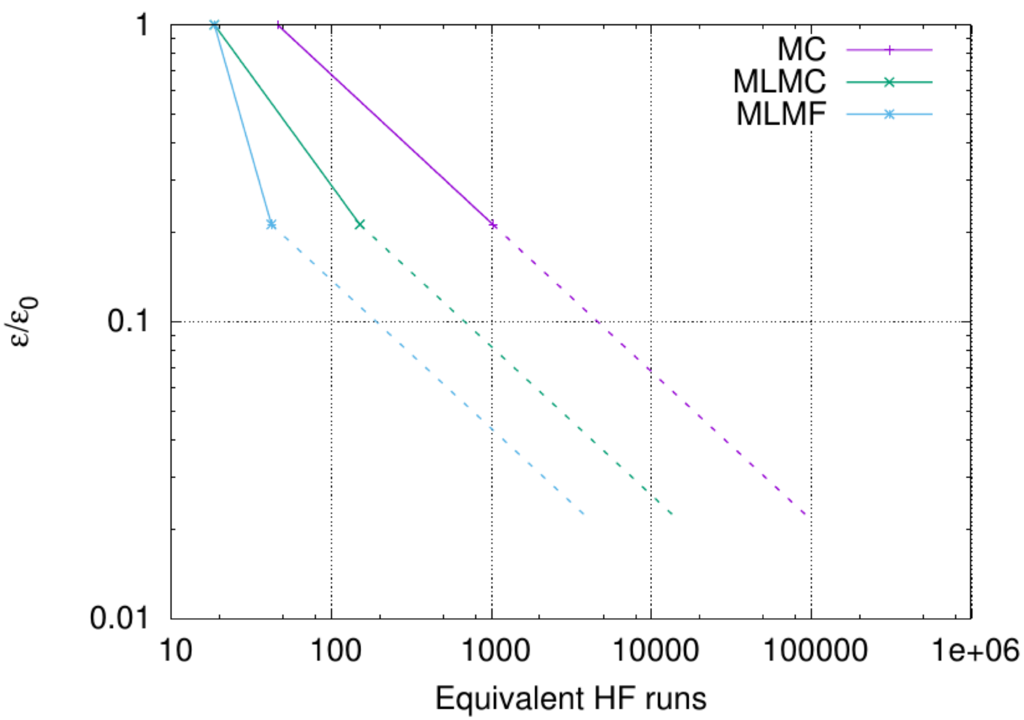


Initial Deployment of MLCV MC for Scramjet UQ

Context: 3D LES simulation of scramjets is extremely expensive and a significant challenge for UQ; even more so for OUU.

Goal: Demonstrate UQ in moderately high D using only a "handful" of HF simulations, by leveraging lower fidelity 2D models and coarsened 2D/3D discretizations

UQ Approach: MLCV algorithm described previously.



	2D	3D
$d/8$	5E-4	0.11
$d/16$	0.014	1

TABLE: Computational cost.

	2D	3D
$d/8$	4,191	263
$d/16$	68	9

Optimal sample allocations based on relative cost, observed correlation between models, observed variance distribution across levels, and MSE target (.045 of pilot MSE)

Optimized allocation: achieve MSE target for 3D LES in 24D using only 9 HF sims. (50 equiv HF)

Updated Deployment of MLCV MC for Scramjet UQ

P1 updated: re-formulate inputs in order to obtain an higher level of turbulence and, in turn, a more non-linear response of the system

	$P_{0,mean}$	$P_{0,rms,mean}$	M_{mean}	TKE_{mean}	χ_{mean}
	P1				
$d/8$	4.02554e-03	1.90524e-06	1.99236e-02	3.34905e-07	4.24520e-03
$d/16$	4.03350e-07	7.77838e-08	6.68974e-05	1.74847e-08	4.40048e-05
	P1 updated				
$d/8$	4.05795e-03	1.90612e-06	1.60029e-02	7.53353e-07	9.41403e-04
$d/16$	2.85017e-04	7.36978e-07	2.07638e-03	2.99744e-07	2.57399e-02

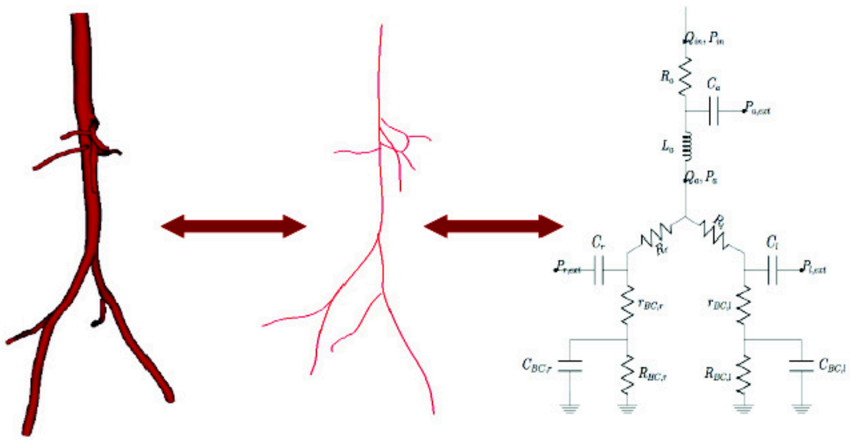
Table 2: Variance for the five QoIs of the P1 unit problem.

Observations from pilot sample: decay in variance across discretizations (LF d/8 and discrepancy d/16 – d/8) no longer observed for all QoI

Implications: requires more focused analysis of deterministic convergence properties → Need to engage additional refinement levels (i.e., d/32, d/64) in order to converge QoI statistics that are closely tied to resolution of turbulence.

Multilevel – Multifidelity Sampling Methods

Cardiovascular flow

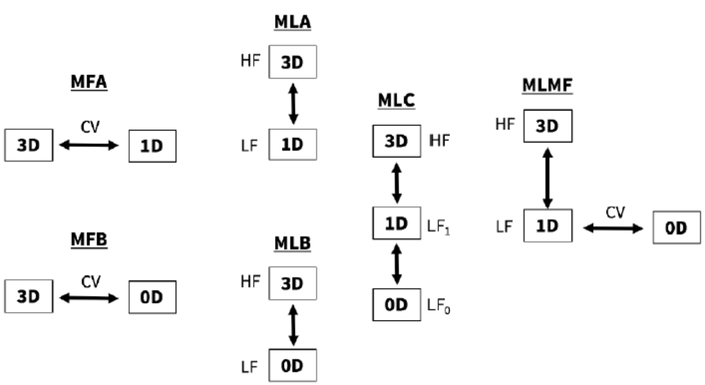


3D Model 1D Model 0D Model

Solver	Cost (1 simulation)	Effective Cost (No. 3D Simulations)
3D	96 hr	1
1D	11.67 min	2E-3
0D	5 sec	1.45E-5

Courtesy of C. Fleeter (Stanford), Prof. D. Schiavazzi (Notre Dame), Prof. A. Marden (Stanford)

Model relationships / graph topologies



(a) Multifidelity (CV) (b) Multilevel (c) Multilevel-Multifidelity

Costs to achieve prescribed error tolerance

Method	Effective Cost (3D Simulations)	No. 3D Simulations	No. 1D Simulations	No. 0D Simulations
MC	9 885	9 885	–	–
MFA	56	21	15 681	–
MFB	39	36	–	154 880
MLA	305	212	41 990	–
MLB	156	150	–	342 060
MLC	165	156	1 324	351 940
MLMF	165	156	1 249	362 590

Implies need for not presuming a fixed topology…

Multilevel – Multifidelity Sampling Methods

Research Direction: Leveraging active directions (ECCOMAS, WCCM)

- Active subspaces, ridge approximation, adapted basis, …

  - Let's introduce the $m \times m$ matrix $\mathbf{C}$

$$\mathbf{C} = \int \left(\vec{\nabla} f\right)\left(\vec{\nabla} f\right)^{\mathrm{T}} \rho(\mathbf{x})\mathrm{d}\,\mathbf{x}$$

  - Since $\mathbf{C}$ is I) Positive semidefinite and II) Symmetric, it exists a real eigenvalue decomposition

$$\mathbf{C} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^{\mathrm{T}}, \text{ where}$$

  - $\mathbf{W}$ is the $m \times m$ orthogonal matrix whose columns are the normalized eigenvectors
  - $\mathbf{\Lambda} = \mathrm{diag}\{\lambda_1, \ldots, \lambda_m\}$ and $\lambda_1 \geq \cdots \geq \lambda_m \geq 0$

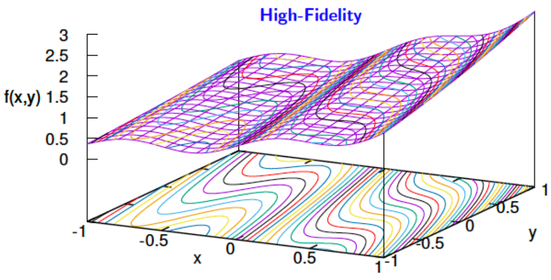
  Let's define two sets of variables

$$\begin{cases} \mathbf{y} = \mathbf{W}_A^{\mathrm{T}}\mathbf{x} \in \mathbb{R}^n & \text{(Active)} \\ \mathbf{z} = \mathbf{W}_I^{\mathrm{T}}\mathbf{x} \in \mathbb{R}^{(m-n)} & \text{(Inactive)} \end{cases} \implies \mathbf{x} = \mathbf{W}_A\mathbf{y} + \mathbf{W}_I\mathbf{z} \approx \mathbf{W}_A\mathbf{y}$$

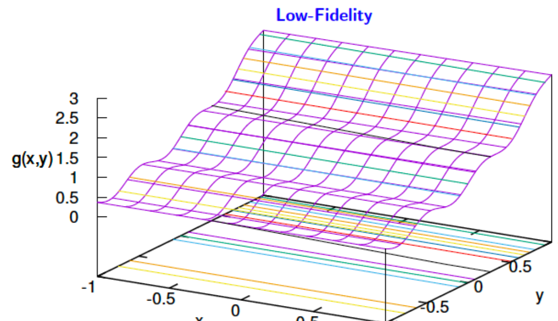
- Main ideas:
  - For each model independently one can compute active directions
  - Sample along these shared active directions and map back to original model coords.
  - Principal directions for a shared QoI can bridge dissimilar parameterizations and demonstrate underlying shared processes

Multilevel – Multifidelity Sampling Methods

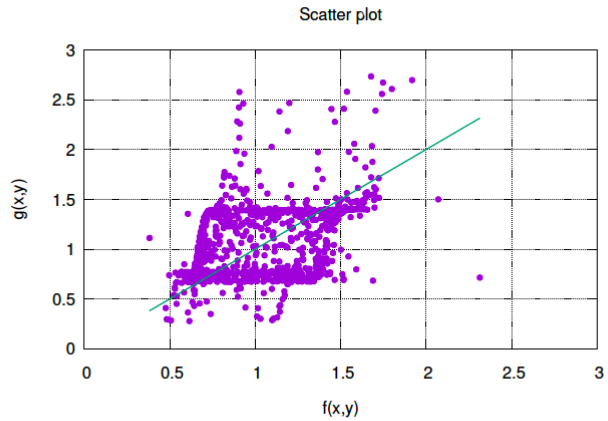
Research Direction: leveraging active directions (example 1)



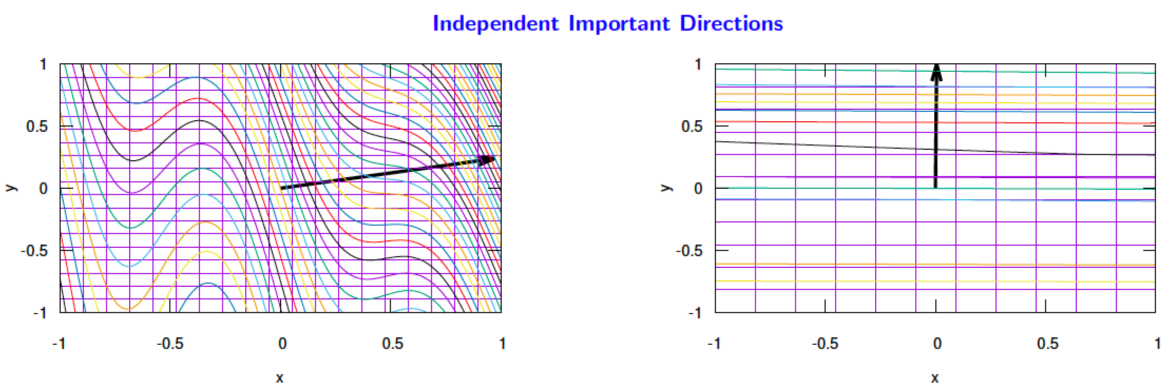
$$f(x, y) = \exp(0.7x + 0.3y) + 0.15\,(2\pi x)$$

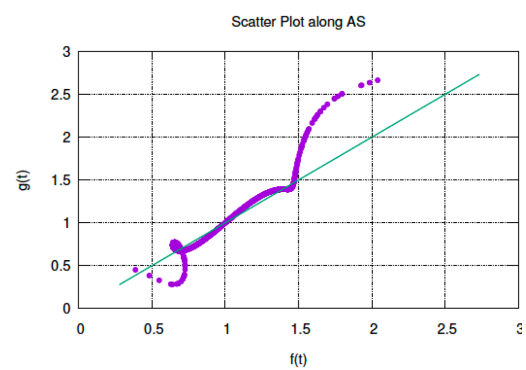


$$g(x, y) = \exp(0.01x + 0.99y) + 0.15\,(3\pi y)$$



$\rho^2 = 0.05$



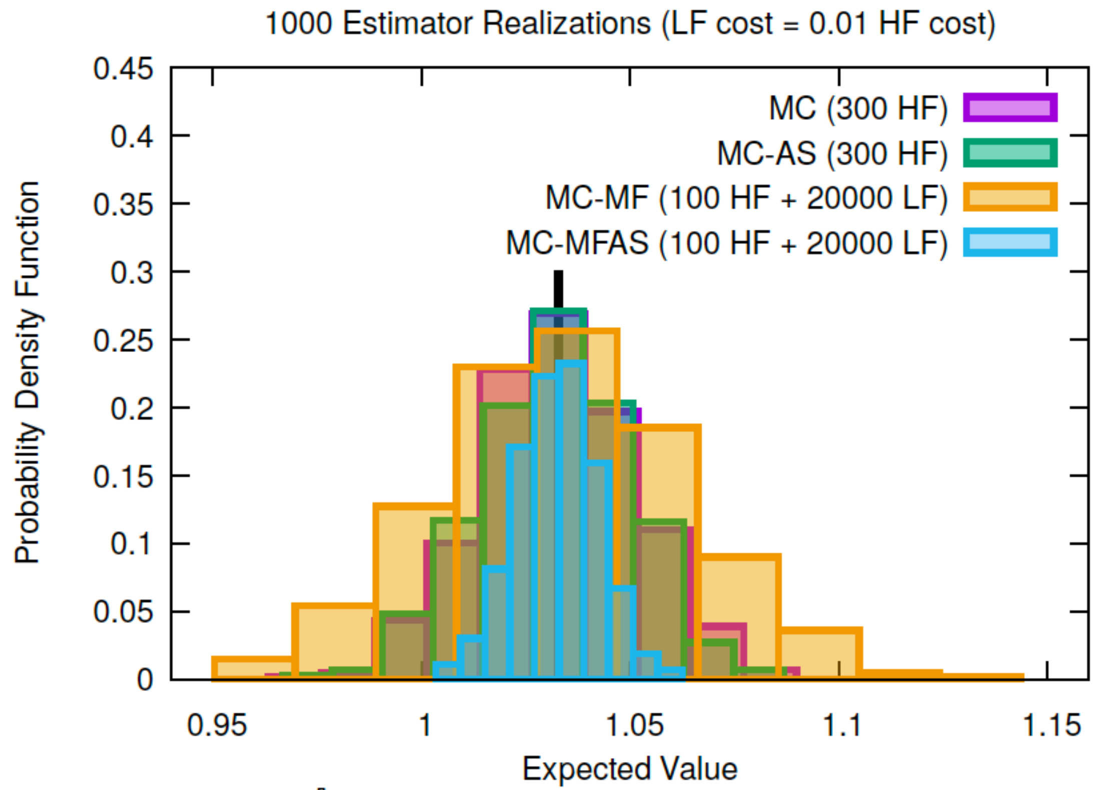


$\rho^2 = 0.9$

G. Geraci, E., "Leveraging Intrinsic Principal Directions for Multifidelity Uncertainty Quantification," SAND2018-10817, Sept. 2018

Multilevel – Multifidelity Sampling Methods

Research Direction: leveraging active directions (example 1)

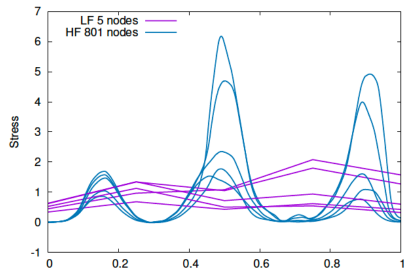


- Fixed computational budget of equivalent of 300 HF runs (LF cost ratio = 100)
- 1000 realizations for each estimator → pdf of estimated Expected Value
- Active subspace discovery for each realization during the pilot sample phase

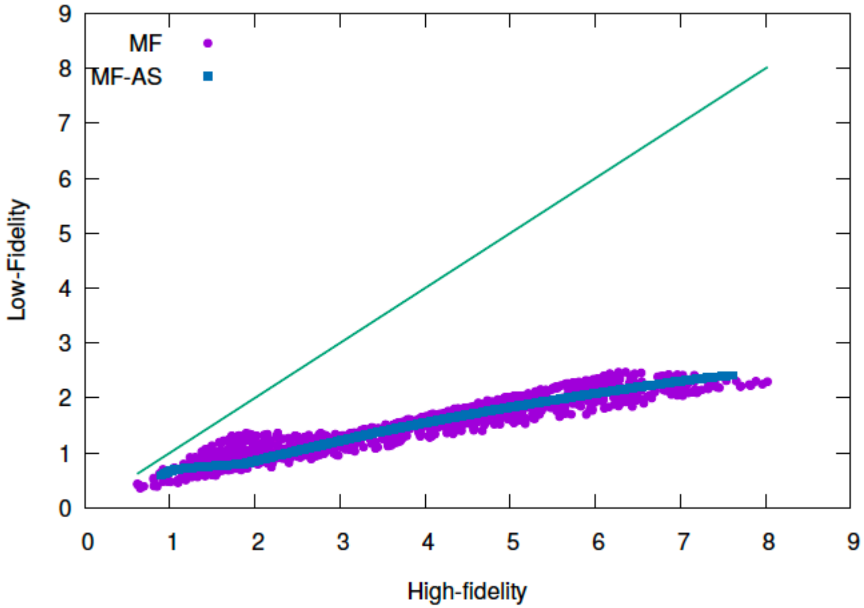
Multilevel – Multifidelity Sampling Methods

Research Direction: leveraging active directions (example 2)

Wave propagation test problem

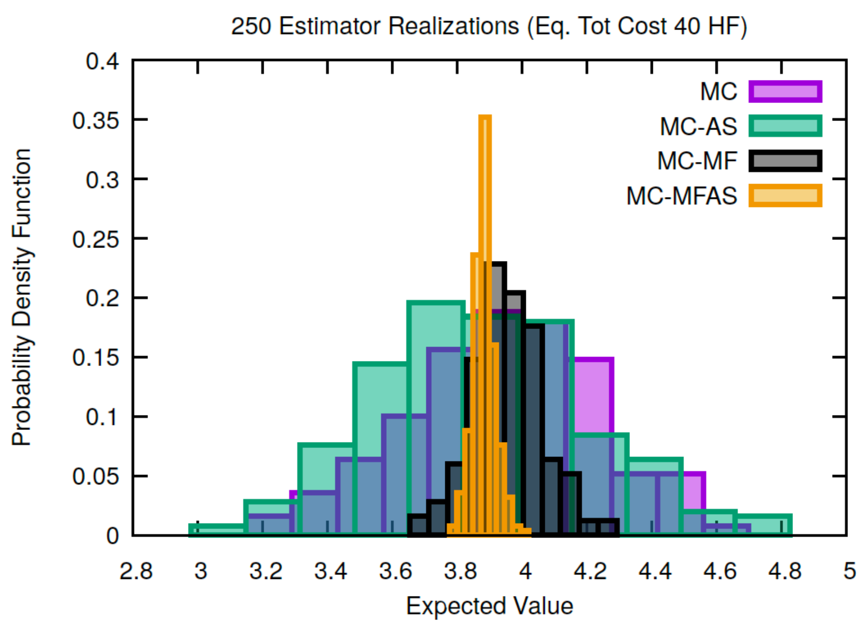


	N_x	N_t	Δ_t
Low-fidelity	5	50	36×10^{-4}
High-fidelity	801	600	30×10^{-5}



Active Direction Agnostic sampling: $\rho^2 = 0.89$

Active Direction Aware sampling:
$\rho^2 = 0.99$



Method	HF runs	LF runs
MC	40	-
MC-MF	38	5946
MC-MFAS	32	21185

Enhances correlation (even if initially high) and links (dissimilar) model parameterizations

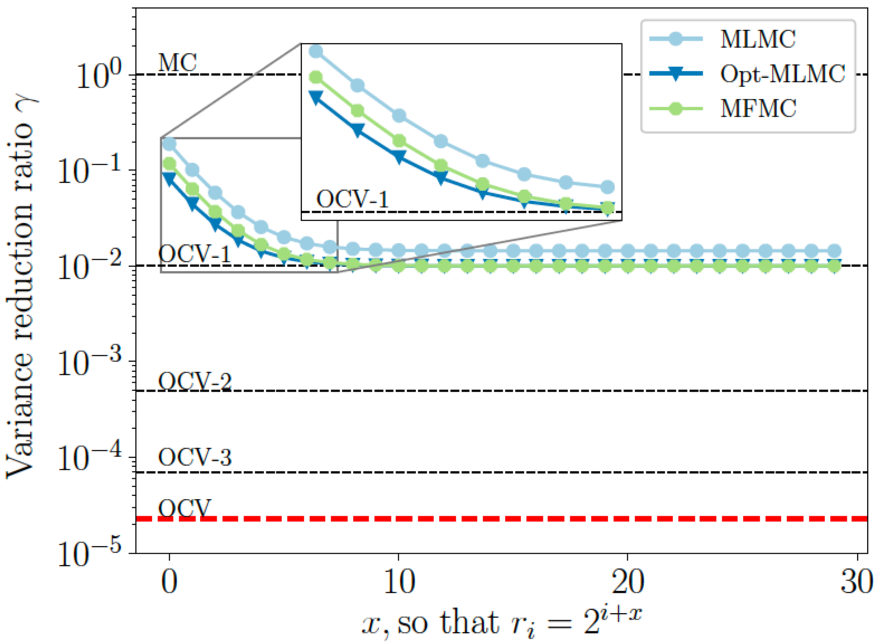
Multilevel – Multifidelity Sampling Methods

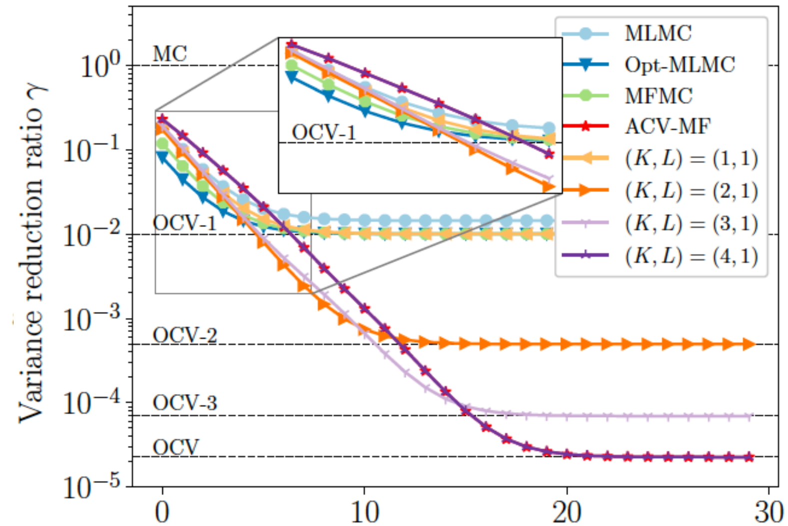
Research Direction: Generalized control variates (in internal Sandia review)

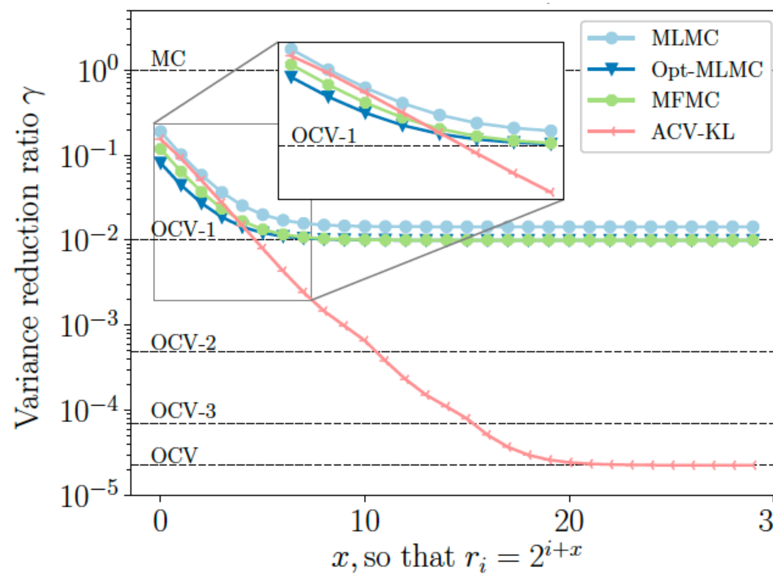
- Unification of ML and CV approaches
- Look beyond (recursive) model pairings

$$\hat{Q}^{\mathrm{CV}} = \hat{Q} + \sum_{i=1}^{M} \alpha_i \left(\hat{Q}_i - \mu_i \right)$$

$$\underset{\underline{\alpha}}{\arg\min}\, \mathbb{V}\mathrm{ar}\left[\hat{Q}^{\mathrm{CV}}(\underline{\alpha}) \right] \Rightarrow \begin{cases} \boldsymbol{C} \in \mathbb{R}^{M \times M} & \text{covariance matrix among } Q_i \\ \boldsymbol{c} \in \mathbb{R}^{M} & \text{vector of covariances between } Q \\ \underline{\alpha}^* = \boldsymbol{C}^{-1}\boldsymbol{c} & \end{cases}$$







A. Gorodetsky, G. Geraci, E., J. Jakeman "Approximate Control Variates," (in internal SNL R&A; expected on arxiv next week).

Multilevel – Multifidelity Sampling Methods

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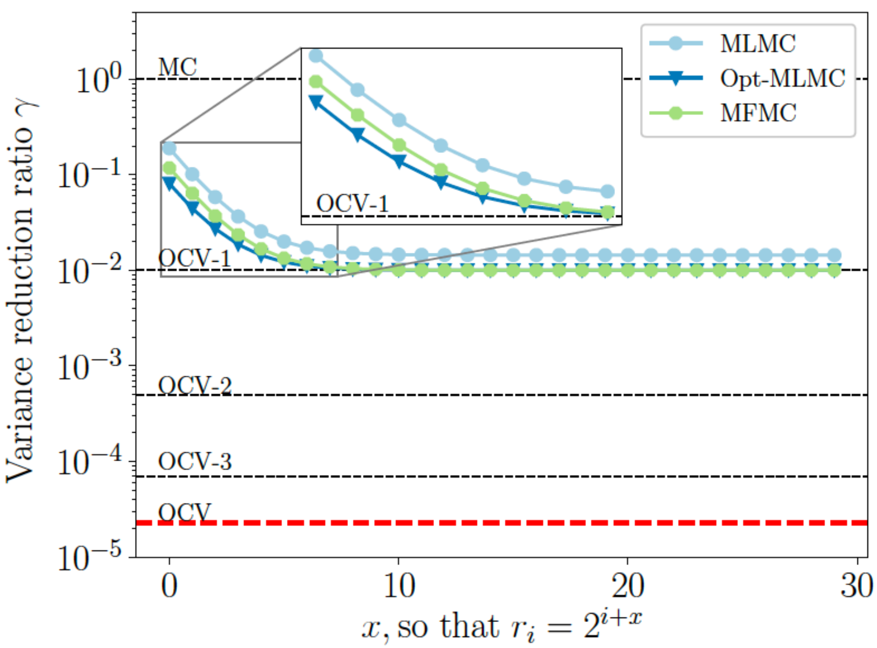

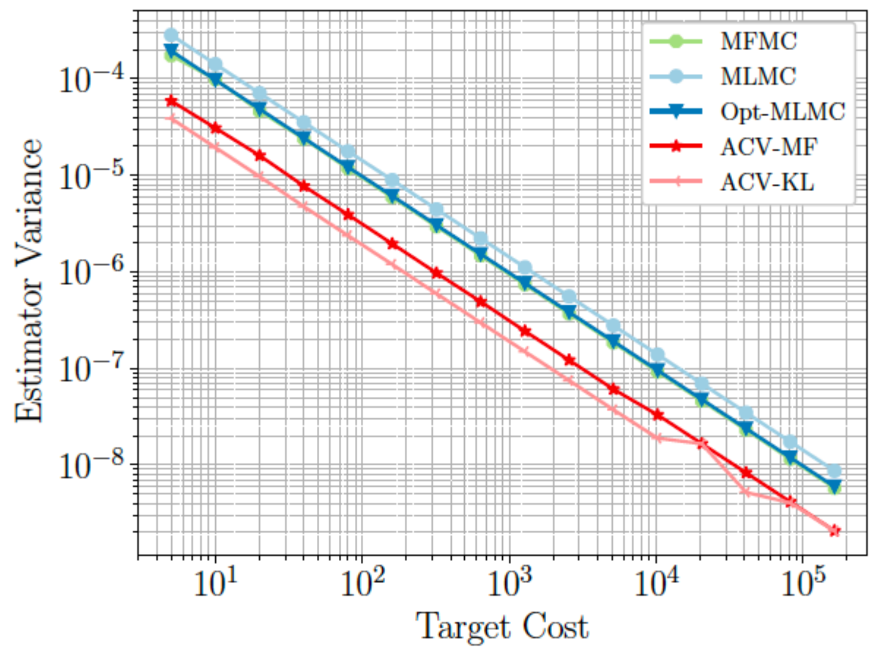

A. Gorodetsky, G. Geraci, E., J. Jakeman “Approximate Control Variates,” (in internal SNL R&A; expected on arxiv next week).

Summary: Monte Carlo Methods

The case for multilevel and multifidelity methods

- Push towards higher simulation fidelity can make propagation / inference / OUU untenable
- Multiple model fidelities / discretizations are often available that trade accuracy for cost
- Realistic deployments (nozzle, scramjet, cardio) → rich model ensemble, challenging QoI

Towards multilevel-multifidelity UQ tailored for smoothness and dimensionality

- Multilevel-multifidelity MC framework for cost-optimized variance reduction
  - ML MC targets *variance decay* within a discretization hierarchy
  - MF MC (control variates) targets *correlation* between HF and 1 or more LF models
  - ML-MF MC employs LF control variate at each HF discretization level
    → tailors approach to hierarchy type; leverages multiple variance reduction opportunities
  - Well suited for high dimensionality and/or low regularity

Research Directions

- Leverage active directions to enhance correlation and bridge dissimilar parameterizations
- Relax assumed model relationships / graph topologies to expose additional performance

Stochastic Polynomial Expansion Methods

- Projection, Regression, Interpolation
- Multilevel | Multifidelity expansions (heuristic)

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

$$L_j = \prod_{\substack{k=1 \\ k \neq j}}^{m} \frac{\xi - \xi_k}{\xi_j - \xi_k} \Rightarrow R(\boldsymbol{\xi}) \cong \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n}\right)$$

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

MF UQ with Spectral Stochastic Discrepancy Models

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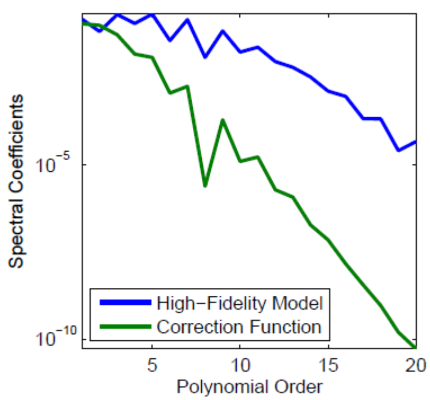
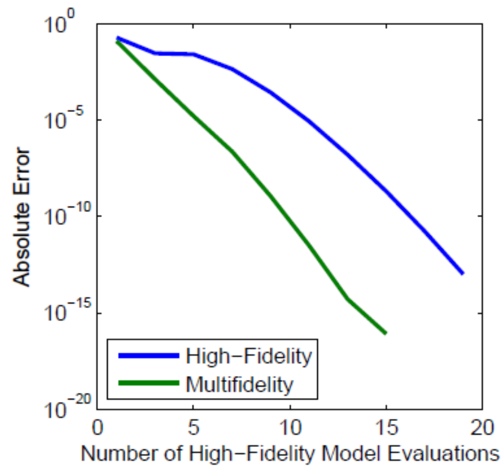
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity "design" codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

$$\boxed{\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)}$$

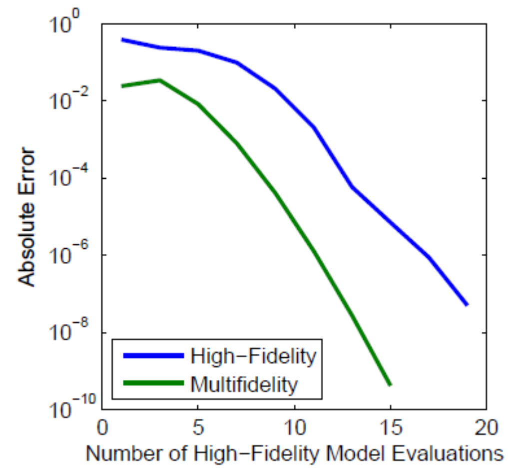
$$\boxed{N_{lo} >> N_{hi}}$$

$$\boxed{\begin{aligned} R_{\text{high}}(\xi) &= e^{-0.05\xi^2}\cos 0.5\xi \underbrace{- 0.5e^{-0.02(\xi-5)^2}}_{\text{discrepancy}} \\ R_{\text{low}}(\xi) &= e^{-0.05\xi^2}\cos 0.5\xi, \end{aligned}}$$





(a) Error in mean

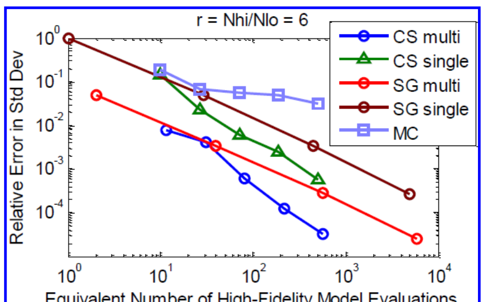


(b) Error in standard deviation

Sparse grid bi-fidelity: target reduced complexity in model discrepancy

Compressed sensing bi-fidelity: target sparsity

(Functional) tensor train bi-fidelity: target low rank



E., Ng, Barone, Domino, "Multifidelity Uncertainty Quantification Using Spectral Stochastic Discrepancy Models," Handbook of UQ, 2015.

Stochastic Polynomial Expansion Methods

- Projection, Regression, Interpolation
- Multilevel | Multifidelity expansions (heuristic)
- Multilevel | Multifidelity expansions (optimized)

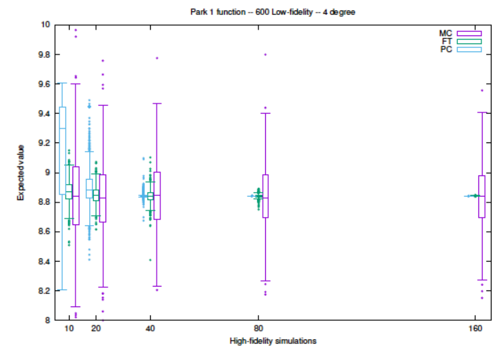
Formulations for Multilevel PCE / SC

1. Optimal resource allocation: parameterize estimator variance → optimal N_l

Global κ and $\gamma > 0$

$$\boxed{Var[\hat{Y}_l] = \frac{Var[Y_l]}{\gamma N^{\kappa}} \quad \rightarrow \quad N_l = \sqrt[\kappa]{\frac{2}{\epsilon^2 \gamma} \sum_{q=0}^{L} \sqrt[\kappa+1]{Var[Y_q] C_q^{\kappa}}} \sqrt[\kappa+1]{\frac{Var[Y_l]}{C_l}}}$$

E., G. Geraci, J.D. Jakeman, "Multilevel Monte Carlo Hybrids Exploiting Multidelity Modeling and Sparse Polynomial Chaos Estimation," SIAM UQ 2016, Lausanne.



Main challenge: abrupt transitions in sparse / low rank recovery

$N_{low} = 600$, **degree=4**

2. Restricted Isometry Property (RIP) for sparse recovery

$$\boxed{N_l \geq s_l \; log^3(s_l) \; L_l \; log(C_l)}$$

Jakeman, Narayan, and Zhou, 2016

Main challenge: compressible fns

→ increasing *s*

→ feedback not well controlled

3. Greedy Multilevel refinement

ML competition with multiple level candidate generators

Main challenges: scalable refinement schemes, loss of precision

ML PCE with rate estimation: Model Problem & UCAV Nozzle

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$$-\frac{d}{dx}\left[a(x,\xi)\frac{du}{dx}(x,\xi)\right] = 10, \quad (x,\xi) \in (0,1) \times I_{\xi}, \tag{22}$$

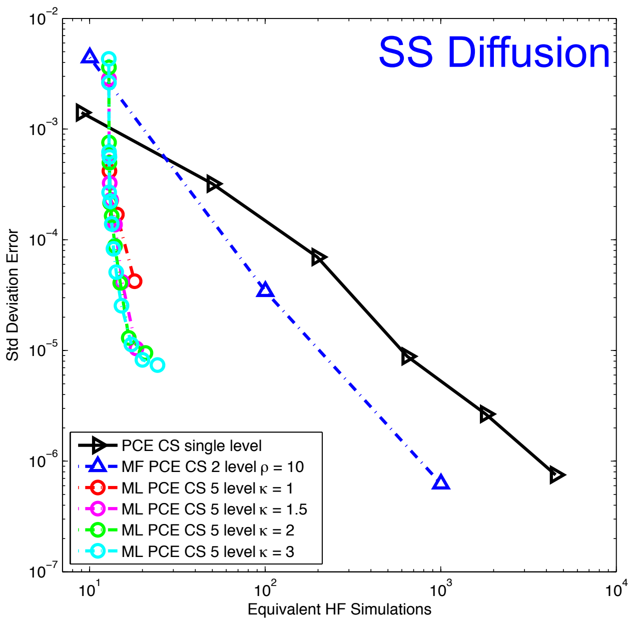
where x is the spatial coordinate, ξ a vector of independent random input parameters and $a(x,\xi)$ denotes the (random) diffusivity field. The following Dirichlet boundary conditions are also assumed

$$u(0,\xi) = 0, \quad u(1,\xi) = 0. \tag{23}$$

We are interested in quantifying the uncertainty in the solution u at specified spatial locations: $\bar{x} = 0.05, 0.5, 0.95$.

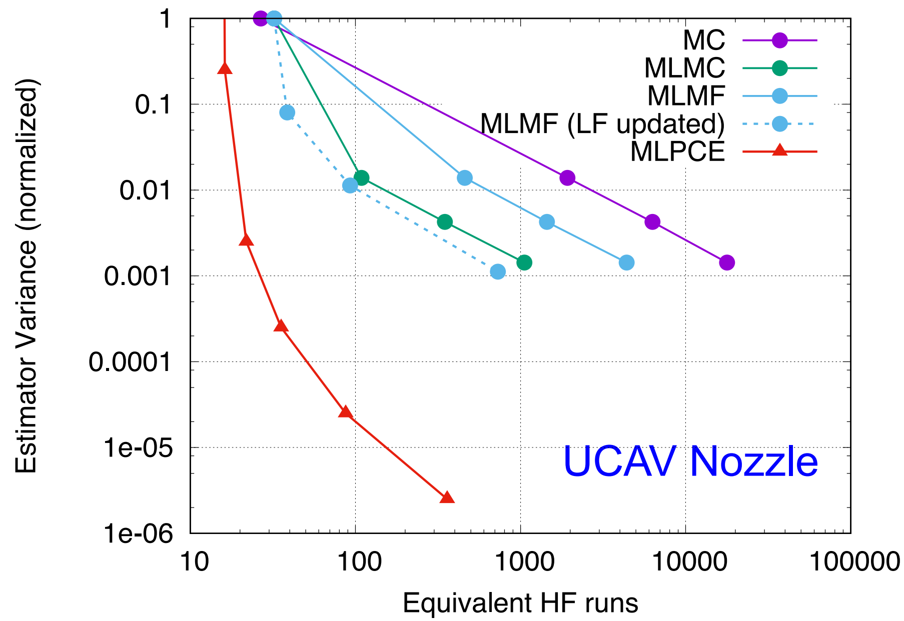
We represent the random diffusivity field a using the following expansion

$$a(x,\xi) = 1 + \sigma \sum_{k=1}^{d} \frac{1}{k^2\pi^2}\cos(2\pi k x)\xi_k \tag{24}$$



Optimized resource allocation outperforms previous heuristics: $\kappa > 1$ is effective

Optimal sample allocations based on relative cost, variance distribution across levels and $\kappa = 2$



ML PCE shows **more rapid convergence** using coarse/medium/fine discretizations:

- Exploits smoothness in moderate dim.

Initial results were promising, but rate estimation impeded by abrupt transition in recovery

Formulations for Multilevel PCE / SC

1. Optimal resource allocation: parameterize estimator variance → optimal N_l

   Global κ and $\gamma > 0$

$$\boxed{Var[\hat{Y}_l] = \frac{Var[Y_l]}{\gamma N^\kappa} \quad \to \quad N_l = \sqrt[\kappa]{\frac{2}{\epsilon^2 \gamma} \sum_{q=0}^{L} \sqrt[\kappa+1]{Var[Y_q] C_q^\kappa}} \; \sqrt[\kappa+1]{\frac{Var[Y_l]}{C_l}}}$$

   E., G. Geraci, J.D. Jakeman, "Multilevel Monte Carlo Hybrids Exploiting Multidelity Modeling and Sparse Polynomial Chaos Estimation," SIAM UQ 2016, Lausanne.

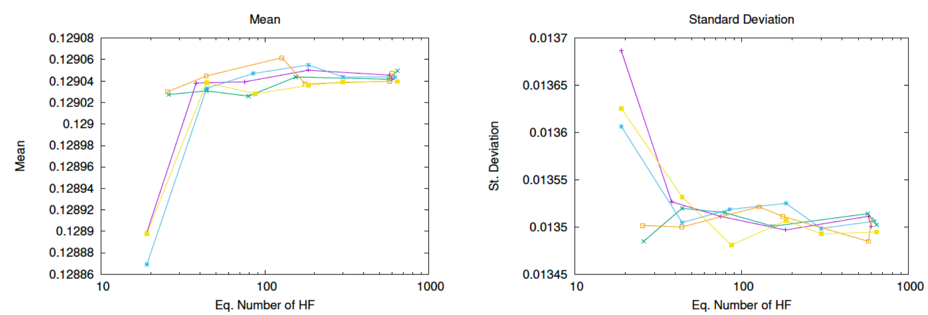
   Main challenge: abrupt transitions in sparse / low rank recovery

2. Restricted Isometry Property (RIP) for sparse recovery

$$\boxed{N_l \geq s_l \, log^3(s_l) \; L_l \, log(C_l)}$$

   Jakeman, Narayan, and Zhou, 2016

   Main challenge: compressible fns
   → increasing *s*
   → feedback not well controlled



3. Greedy Multilevel refinement

   ML competition with multiple level candidate generators

   Main challenges: scalable refinement schemes, loss of precision

Multilevel-Multifidelity expansions – Greedy refinement

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Compete level refinement candidates to maximize induced change per unit cost:

- 1 or more refinement candidates per level
- Measure impact on final QoI statistics (roll up multilevel estimates),
  - norm of change in response covariance (default)
  - norm of change in level mappings (goal-oriented: $z/p/\beta/\beta^*$)

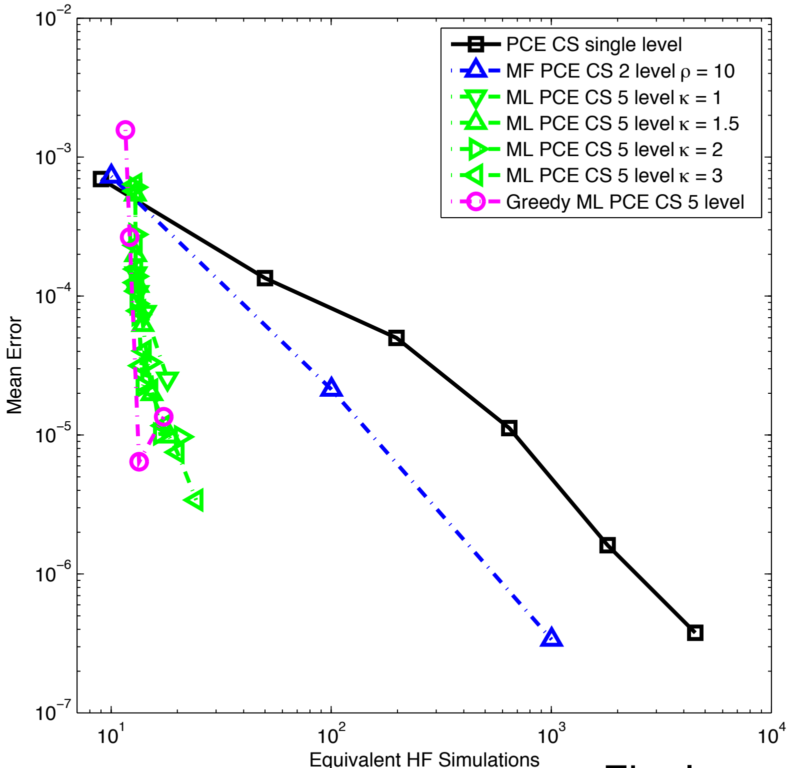
  normalized by relative cost of level increment (# new points * cost / point)
- Greedy selection of best candidate, which generates new candidate(s) for selected level

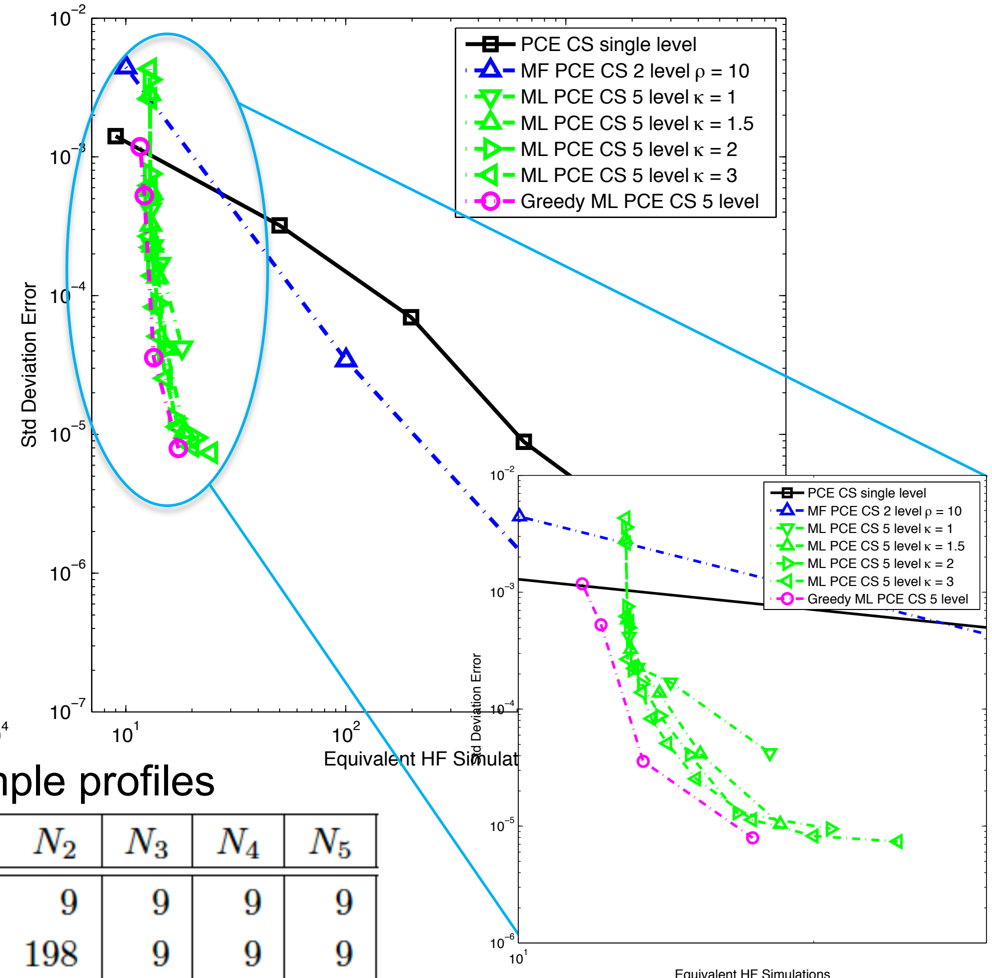
Level candidate generators:

- Uniform refinement of orders / levels (coarse-grained, 1 candidate per level)
  - Tensor / sparse grids: PCE and nodal/hierarchical SC
  - Regression PCE: least sq. / compressed sensing using fixed sample ratio
- Anisotropic refinement of orders / levels (coarse-grained, 1 candidate per level)
  - Tensor / sparse grids
- Index-set-based refinement (fine-grained, many candidates per level: exp growth w/ dim)
  - Generalized sparse grids: PCE and nodal/hierarchical SC
  - Regression PCE
- Adapted basis (coarse-grained, a few exp order frontier advancements per level)
  - Regression PCE

Jakeman, E., Sargsyan, “Enhancing ℓ1-minimization estimates of polynomial chaos expansions using basis selection,” *J. Comp. Phys.,* Vol. 289, May 2015.)

Multilevel-multifidelity expansion methods: Greedy ML PCE: CS + uniform basis refinement

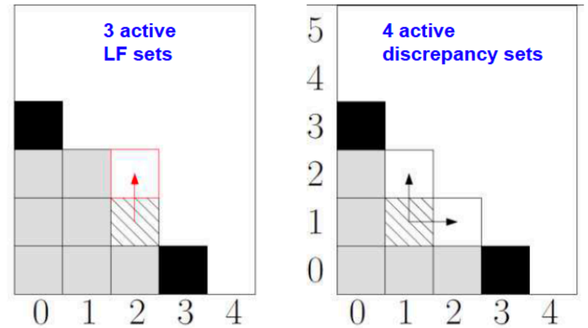




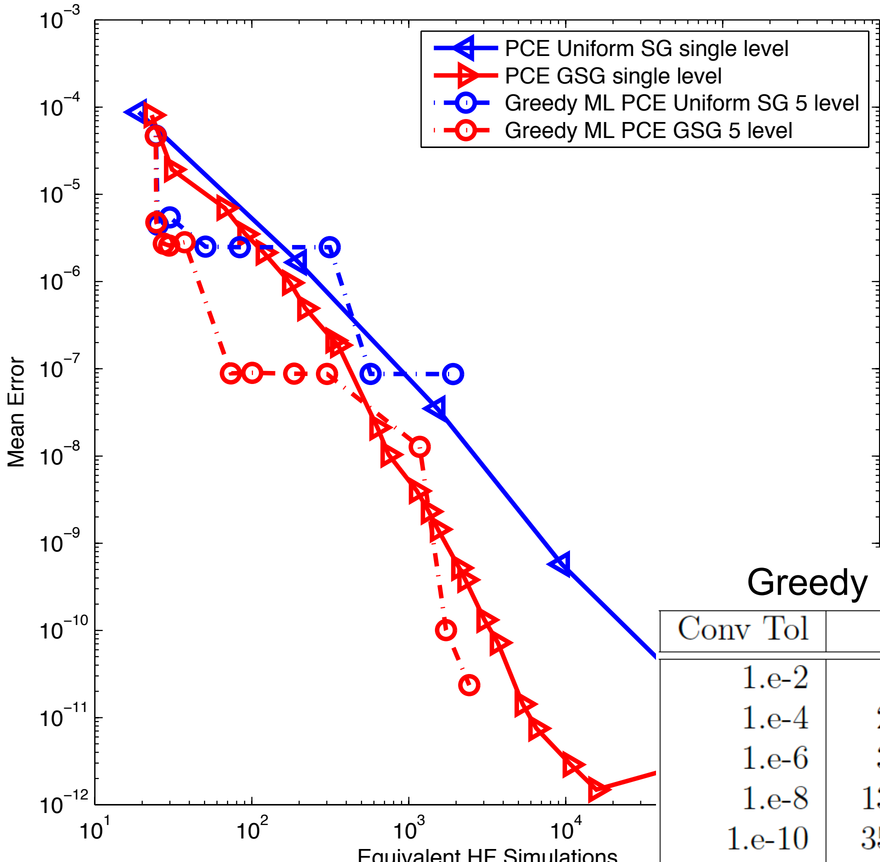
Final sample profiles

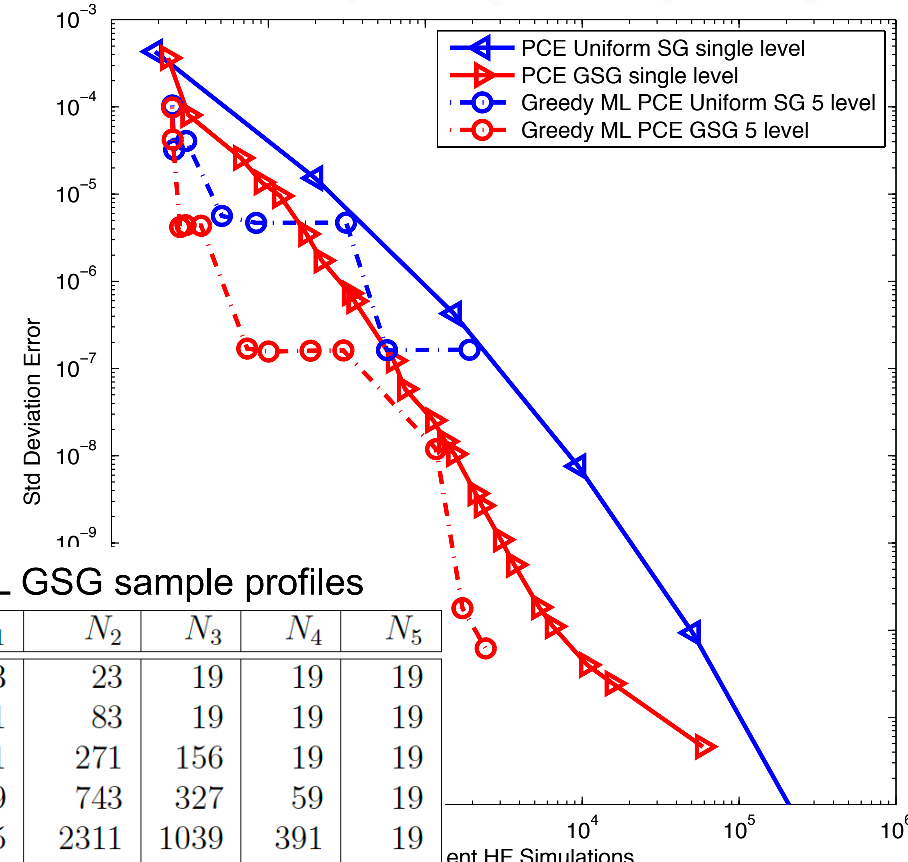
Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-1	198	9	9	9	9
1.e-2	644	198	9	9	9
1.e-3	1802	644	9	9	9
1.e-4	4505	1802	50	9	9

Multilevel-multifidelity expansion methods
Greedy ML PCE: uniform/generalized sparse grids



Generalized sparse grid @ each level:
- Combinatorial growth in refinement candidates

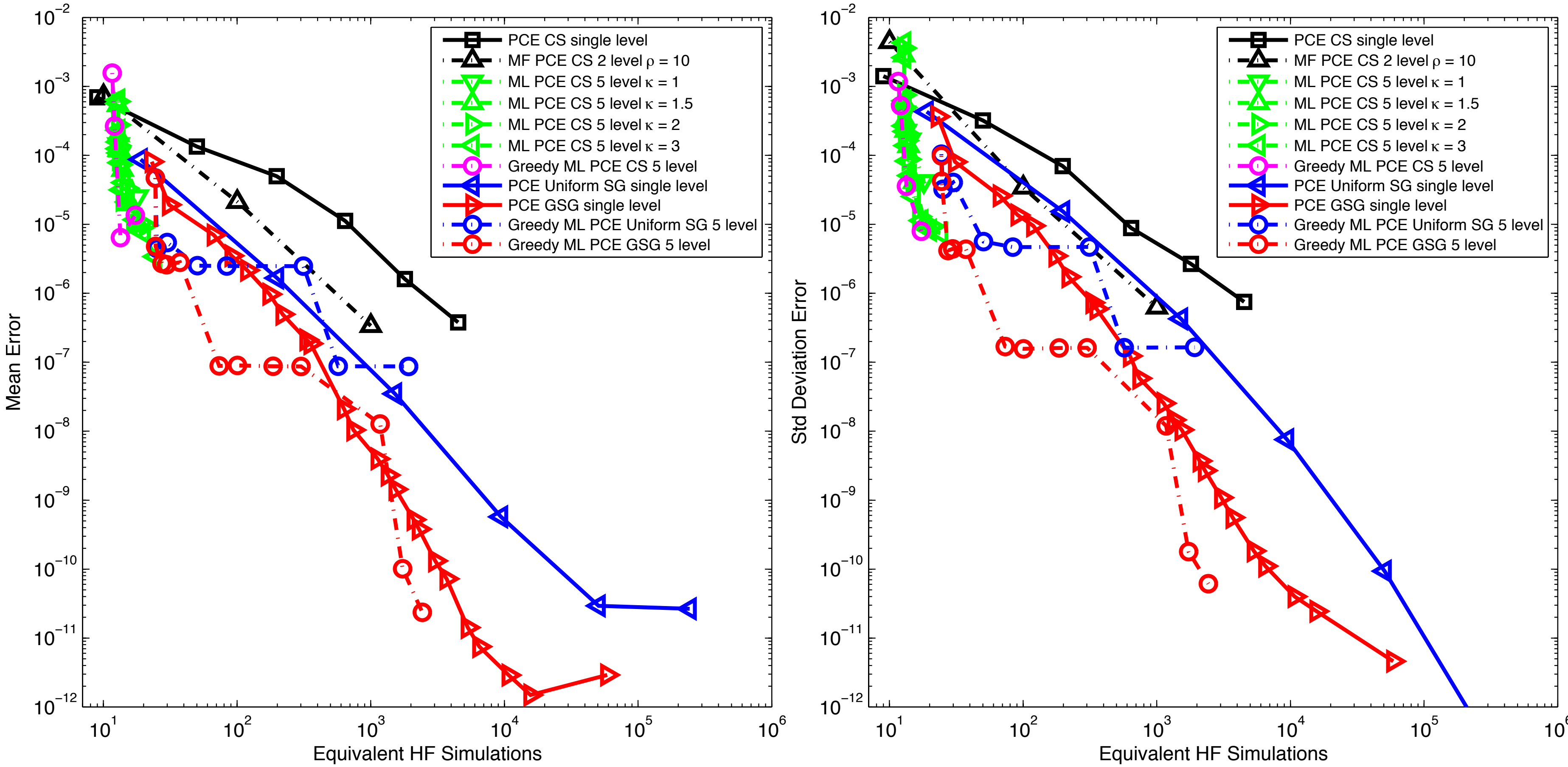




Greedy ML GSG sample profiles

Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-2	43	23	19	19	19
1.e-4	211	83	19	19	19
1.e-6	391	271	156	19	19
1.e-8	1359	743	327	59	19
1.e-10	3535	2311	1039	391	19
1.e-12	10319	5783	2783	1343	43
1.e-14	26655	14991	8063	3703	1535

Multilevel-multifidelity expansion methods
Greedy ML PCE: overlay all cases & references



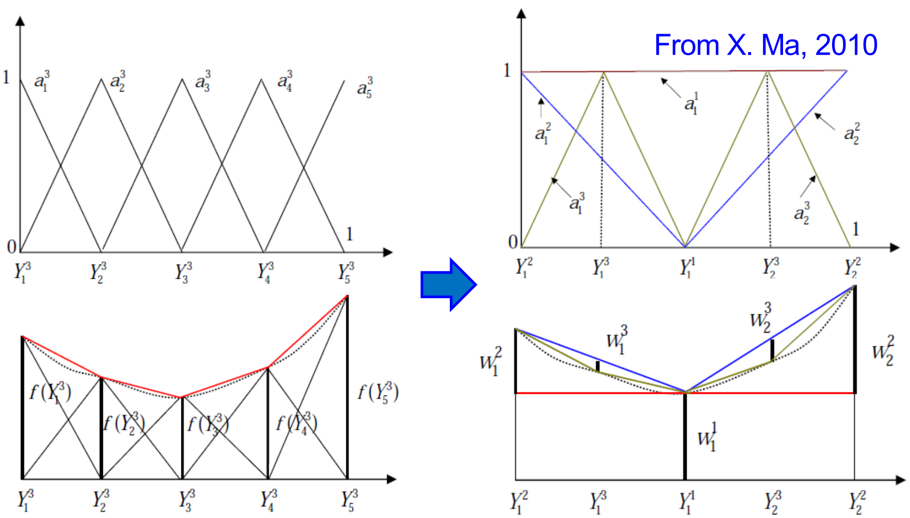
CS approaches have greater flexibility at low sample levels (lower initialization cost), but accuracy currently limited by numerical issues for large systems allocated at coarse levels

ML PCE / SC: Directions

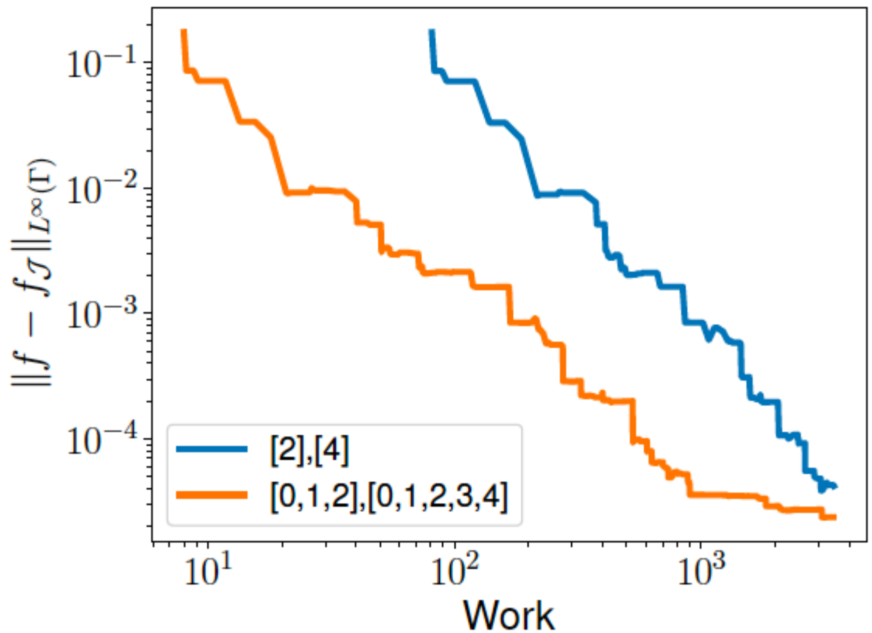
Current developmental areas:

- Hierarchical interpolation (Δ precision for small grid increments)
- Functional tensor train (large systems: scalability of level solver, especially @ LF)
- Limiting number of level candidates (expanding front: MLMF scalability)
- Multidimensional model hierarchies → greedy sparse grids in model space

Interpolation via hierarchical surplus



UCAV Nozzle for structural/thermal fidelity



J.D Jakeman, E., G. Geraci, A. Gorodetsky, "Adaptive Multi-index Collocation and Sensitivity Analysis" (in internal review)

Summary Remarks (ML PCE)

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The case for multilevel and multifidelity methods

- Push towards higher simulation fidelity can make propagation / inference / OUU untenable
- Multiple model fidelities / discretizations are often available that trade accuracy for cost
- Deployments for CFD (nozzle, scramjet, wind) → rich model ensemble, challenging QoI

Towards multilevel-multifidelity UQ tailored for smoothness and dimensionality

- Multilevel-multifidelity MC framework for cost-optimized variance reduction
  - ML-MF MC employs LF control variate at each HF discretization level; tailor to hierarchy type
  - Well suited for high dimensionality and/or low regularity
- Multilevel PCE/SC: extend ML MC machinery with higher performance estimators
  extend heuristic multifidelity PCE/SC with optimal allocations
  - PCE CS / FT: exploit sparsity / low rank in δ; SC hierarchical interp: direct Δ calculation
  - *Rate estimation of estimator variance:* complicated by abrupt transitions in CS/FT recovery
  - *RIP sampling:* shape sample profile based on observed sparsity; issues w/ feedback
  - *Greedy refinement:* competition among multiple candidates per level, normalized by cost
    - ML compressed sensing with expansion order candidates
    - ML (generalized) sparse grids with level and index set candidates
  - Achieve more rapid convergence (sufficient regularity, moderate dimensionality)

Related Efforts:

- Multilevel Bayesian inference → exploit ML PCE/FT within emulator-based inference
- Multilevel Opt/OUU → move beyond common bi-fidelity to exploit deep / multi-D hierarchy