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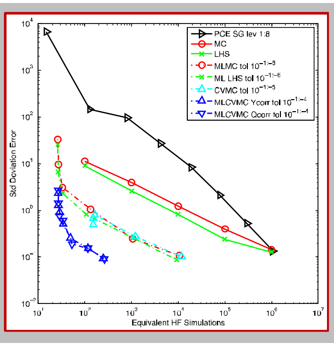
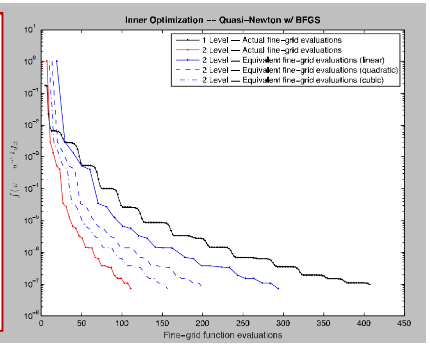
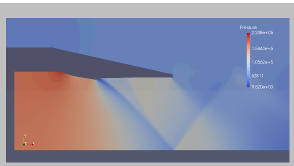
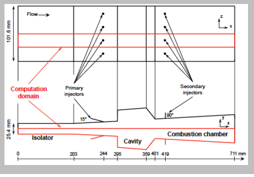


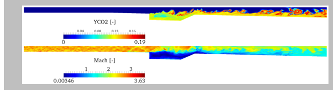


DAKOTA

Explore and predict with confidence







Multilevel-Multifidelity Expansions with Application to Forward UQ, OUU, and Emulator-Based Bayesian Inference

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Sandia National Laboratories, Albuquerque, NM

14th U.S. National Congress on Computational Mechanics, Montreal, CA, July 19, 2017

U.S. DEPARTMENT OF ENERGY

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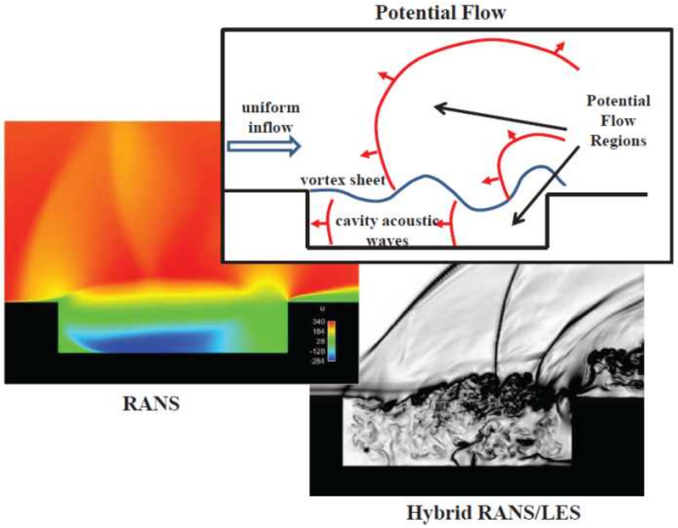
Multiple Model Forms in UQ & Opt

Discrete model choices for simulation of same physics

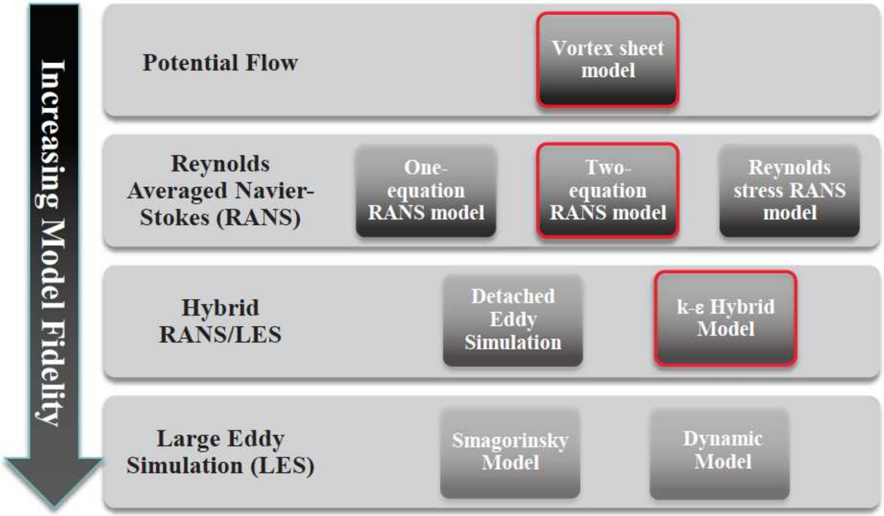
A clear hierarchy of fidelity (from low to high)

- 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 characterizatior
  - 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 and Multifidelity Sampling Methods

Monte Carlo estimator: $\hat{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i$ → analytic variance $Var[\hat{Q}] = \frac{\sigma_Q^2}{N}$

Geometrical MLMC – targeting discretization levels

Multilevel Monte Carlo estimator

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

$$\left.\begin{aligned} \mathcal{C}(\hat{Q}_M^{ML}) &= \sum_{\ell=0}^{L} N_\ell \mathcal{C}_\ell \\ \sum_{\ell=0}^{L} N_\ell^{-1} \mathbb{V}ar\left(Y_\ell\right) &= \varepsilon^2/2 \end{aligned}\right\} \xrightarrow{\textit{Lagrange multipliers}} N_\ell = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L} \left(\mathbb{V}ar\left(Y_k\right)\mathcal{C}_k\right)^{1/2}\right] \sqrt{\frac{\mathbb{V}ar\left(Y_\ell\right)}{\mathcal{C}_\ell}}$$

[Giles, 2008]

Control variate MC – targeting hierarchical model forms

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

[Pasupathy et al., 2012,
Ng & Willcox, 2014:
estimated control means]

$$\underset{\beta, r_l}{\operatorname{argmin}}\, Var\left[\hat{Q}_N^{MCCV}\right] \Rightarrow \beta^* = \rho_{HL}\frac{\sigma_{HF}}{\sigma_{LF}} \quad r_l^* = \frac{N_l^{LF}}{N_l^{HF}} = \sqrt{\frac{w_l\, \rho_{HL}^2}{1-\rho_{HL}^2}}$$

where $w_\ell = \mathcal{C}_\ell^{\mathrm{HF}} / \mathcal{C}_\ell^{\mathrm{LF}}$

Multilevel-Multifidelity UQ: Multilevel-control variate MC

MLCV MC – both model forms & discretization levels

- Apply control variate to discrepancy at each level:

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

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

- Optimal CV parameter and LF sampling increment remain the same as before
- Multilevel sampling allocation becomes

MLCV Y-correlation:

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

$$\Lambda_k = 1 - \rho_k^2 \frac{1-r_k}{r_k}$$

G. Geraci, E., G. Iaccarino, “A multifidelity control variate approach for the multilevel Monte Carlo technique,” Center for Turbulence Research, Ann Res Briefs 2015, pp. 169—181.

Multilevel Control Variate MC: 1D transient diffusion

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MLCV Y-correlation:

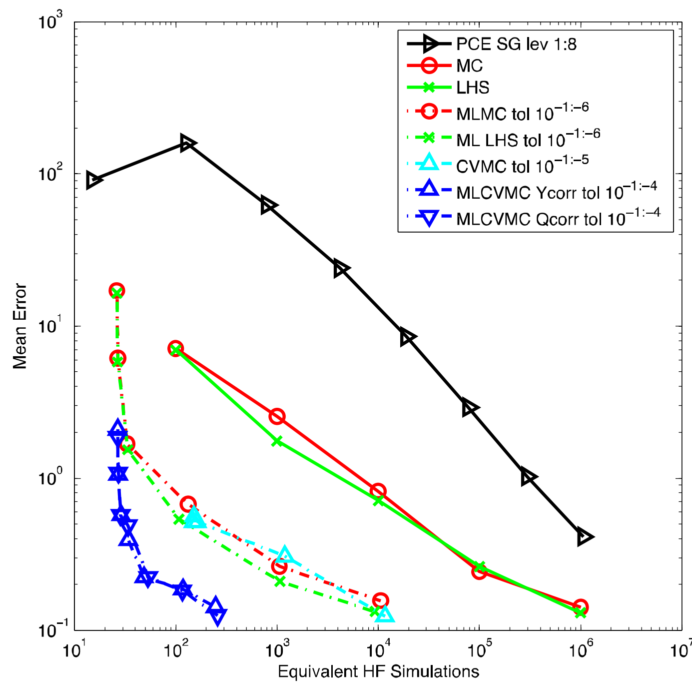
$$N_\ell^{\mathrm{HF}} = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L_{\mathrm{HF}}} \left(\frac{\mathbb{V}ar\left(Y_k^{\mathrm{HF}}\right)\mathcal{C}_k^{\mathrm{HF}}}{1-\rho_\ell^2}\right)^{1/2} \Lambda_k(r_k)\right]\sqrt{\left(1-\rho_\ell^2\right)\frac{\mathbb{V}ar\left(Y_\ell^{\mathrm{HF}}\right)}{\mathcal{C}_\ell^{\mathrm{HF}}}}$$

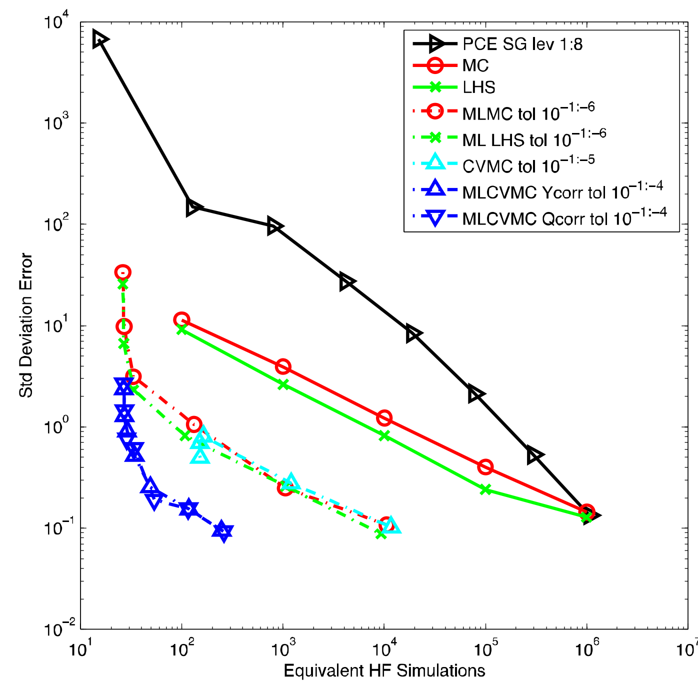
MLCV Q-correlation:

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

G. Geraci, E., G. Iaccarino, "A multifidelity multilevel Monte Carlo method for uncertainty propagation in aerospace applications," 19th AIAA Non-Deterministic Approaches Conf., Jan 9 – 13, 2017, Grapevine, TX.

MLCV MC (blue) is effective; LF/HF correlation at level 0 dominates





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

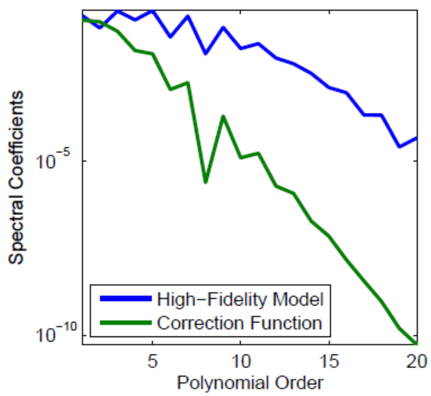
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity "design" codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

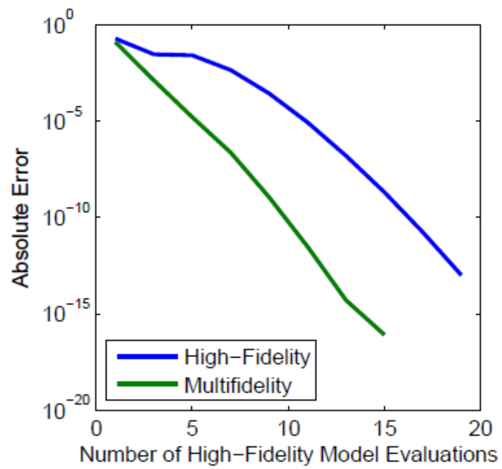
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

$$N_{lo} >> N_{hi}$$

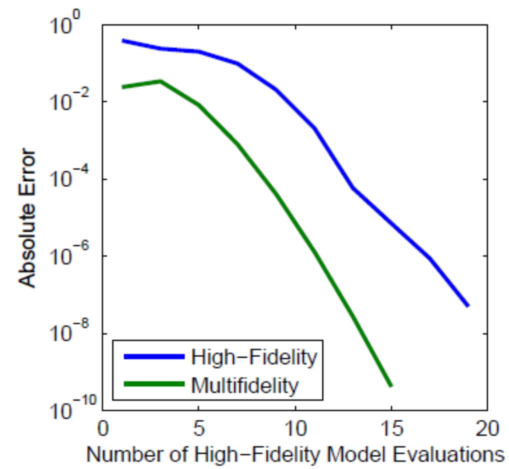
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi \underbrace{- 0.5 e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

$$R_{\text{low}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi,$$





(a) Error in mean



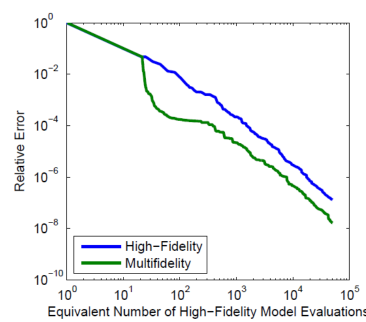
(b) Error in standard deviation

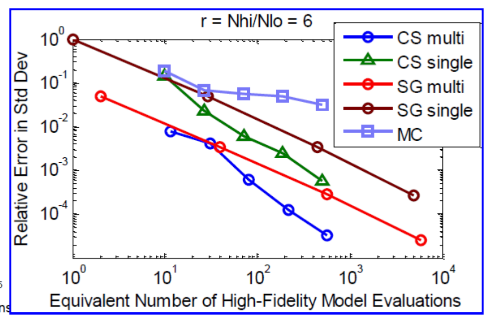
Adaptive sparse grid multifidelity algorithm:

- Gen. sparse grids for LF & discrepancy levels
- Greedy selection from grids: max ΔQoI/ΔCost
- Refine discrepancy where LF is less predictive

Compressed sensing multifidelity algorithm:

- Target sparsity within the model discrepancy





Elliptic PDE with FEM

$$-\frac{d}{dx}\left[\kappa(x,\omega)\frac{du(x,\omega)}{dx}\right] = 1, \qquad x \in (0,1), \qquad u(0,\omega) = u(1,\omega) = 0$$

$$\kappa(x,\omega) = 0.1 + 0.03\sum_{k=1}^{10}\sqrt{\lambda_k}\phi_k(x)Y_k(\omega), \qquad Y_k \sim \text{Uniform}[-1,1]$$

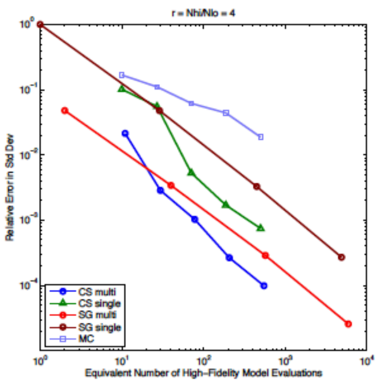
$$C_{\kappa\kappa}(x,x') = \exp\left[-\left(\frac{x-x'}{0.2}\right)^2\right]$$

QoI is u(0.5, ω).

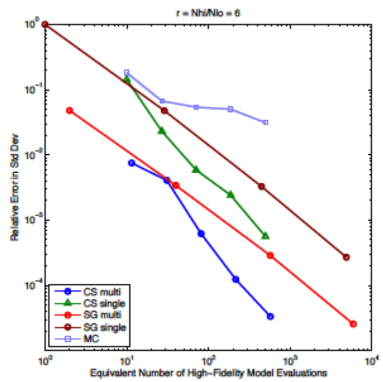
LF = coarse spatial grid with 50 states.

HF = fine spatial grid with 500 states.

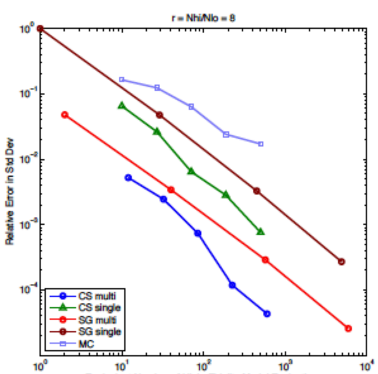
r_{work} = 40.



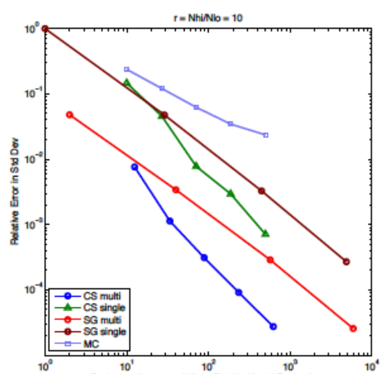
(a) $\rho_{\text{points}} = 4$



(b) $\rho_{\text{points}} = 6$



(c) $\rho_{\text{points}} = 8$



(d) $\rho_{\text{points}} = 10$

This particular case is multilevel, rather than general multifidelity. LF model is accurate predictor of HF results.

Good LF models result in discrepancy with one or more of the following properties:

- lower complexity than HF model (sparse grid)
  → faster conv rate (affects exponent)
- lower variance than HF model
  → reduction in initial error (affects leading const)
- more sparse than HF model (CS)
  → fewer samples to recover coefficients

Existing multifidelity machinery provides a foundation for multilevel PCE approaches
→ augment with optimal sample allocation.

Improve ML estimator: replace MC avg w/ sparse PCE recovery → Multilevel sampling with parameterized estimator variance

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Assume parameterized form for estimator variance $V[\hat{Q}]$ and derive optimal N_l

$$V[\hat{Q}] = \frac{\sigma_Q^2}{\gamma N^\kappa}$$

$$N_l = \sqrt[\kappa]{\frac{2}{\varepsilon^2 \gamma} \sum_{k=0}^{L} \sqrt[\kappa+1]{Var[Y_k]\, C_k^\kappa}} \sqrt[\kappa+1]{\frac{Var[Y_l]}{C_l}}$$

for positive κ and γ.

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

Note: γ does not affect *relative* sample allocation

- Given ε target and omitting $\gamma > 1$, N_l may overshoot (MSE < target level)

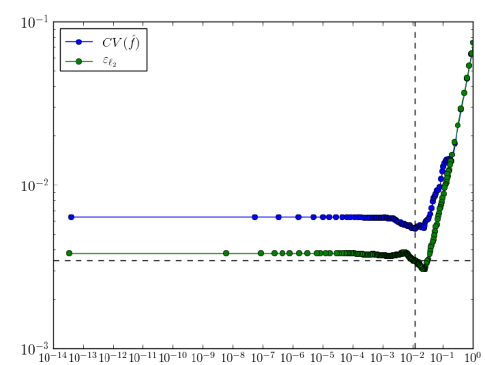
Estimation/update of κ (and γ if ε is important)

- Initial approximation (for CS) from Gauss-Markov theorem (OLS is BLUE)

$$Var[\hat{\alpha}] = \sigma_Q^2 (\Psi^T \Psi)^{-1}$$

- Optionally update with cross validation results: estimate $Var[\hat{Q}]$ from k-fold results
  - σ_Q^2 known from recovered PCE
  - Fit κ, γ across level profile for each ML iteration

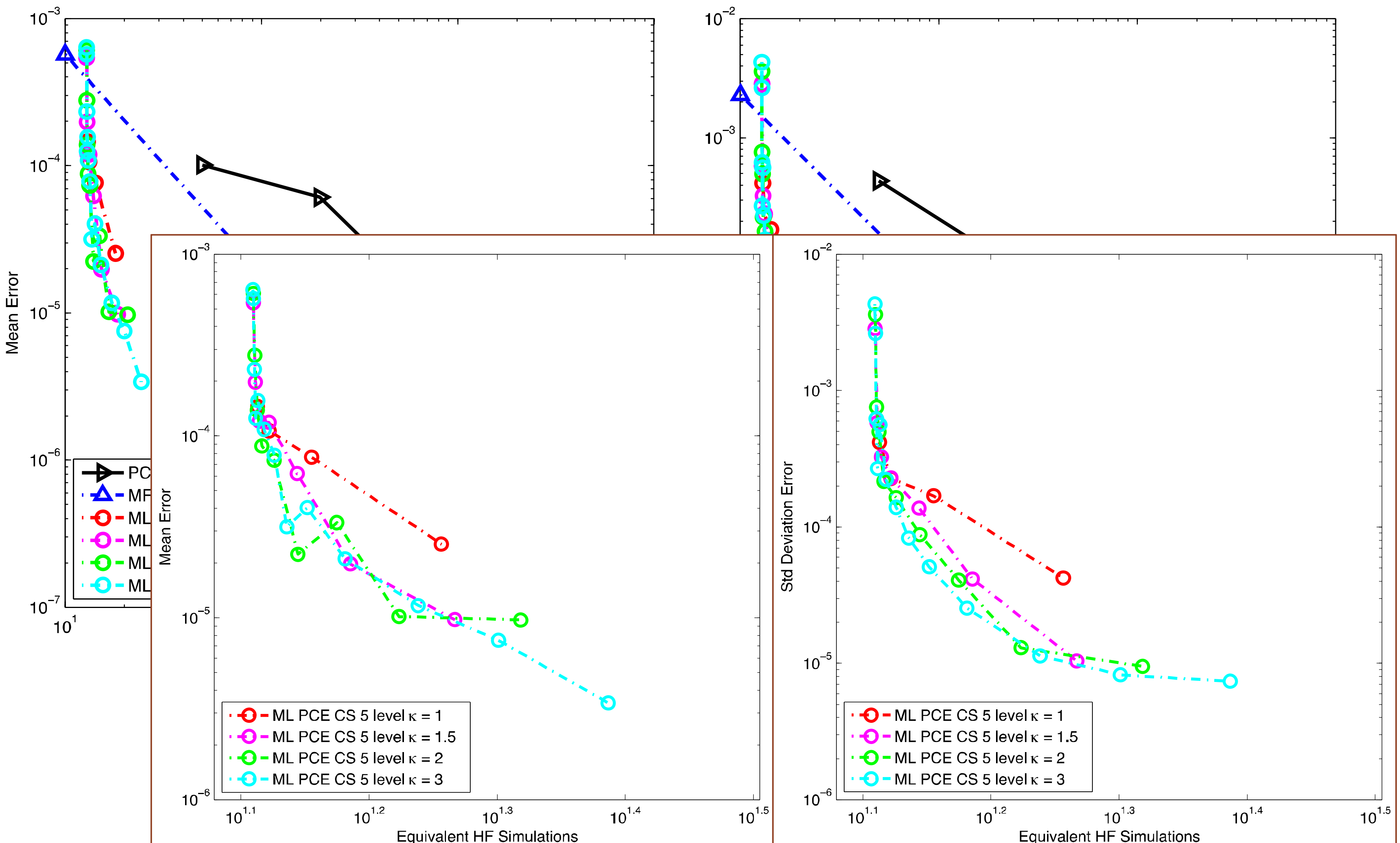
$$\kappa = \log \frac{\sigma_Q^2}{\gamma V[\hat{Q}]} / \log N$$



Identical process as for MF PCE with CS, but now with optimal N_l

Multilevel PCE Regression: SS diffusion

Single and multi-fidelity CS compared to multilevel CS (assumed κ values)



Current focus: improve recovery for large systems at coarse level using low rank

MLMF Deployment for DOE/DOD

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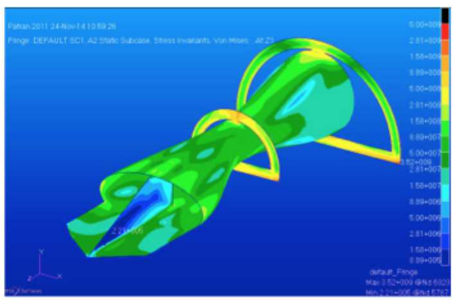
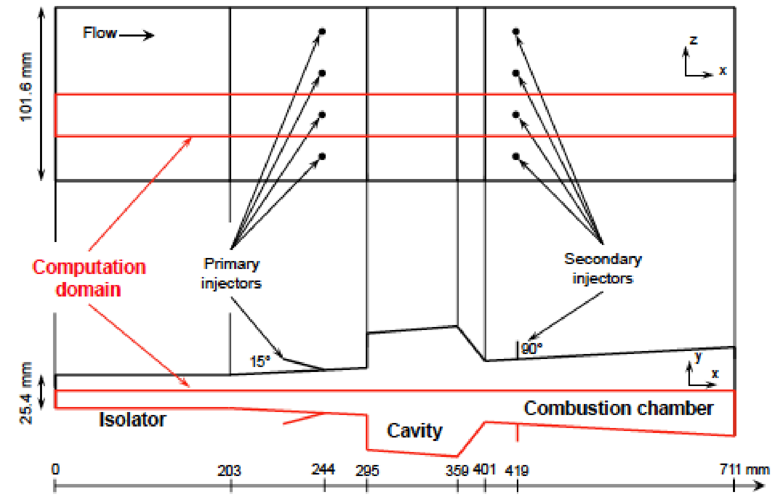
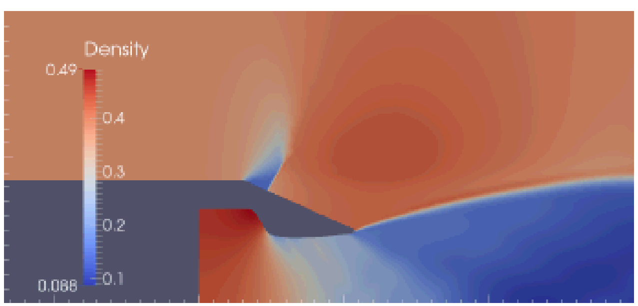
DARPA (EQUiPS)

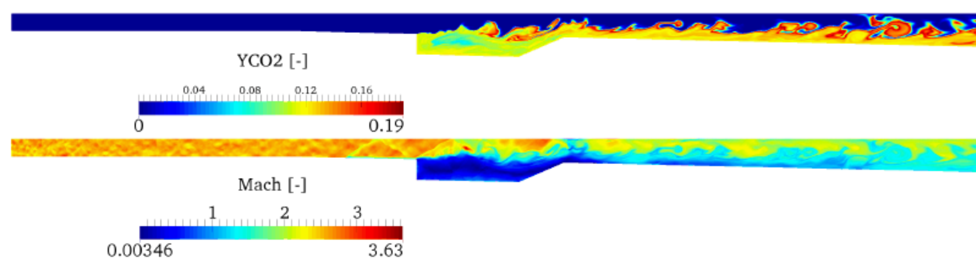
SEQUOIA
High perf UCAV nozzle



ScramjetUQ
HiFIRE hypersonic test facility







A2e HFM Wind (EERE)

EFRC WastePD (SciDAC QUEST)

Initial Deployment of MLCV MC for Scramjet UQ

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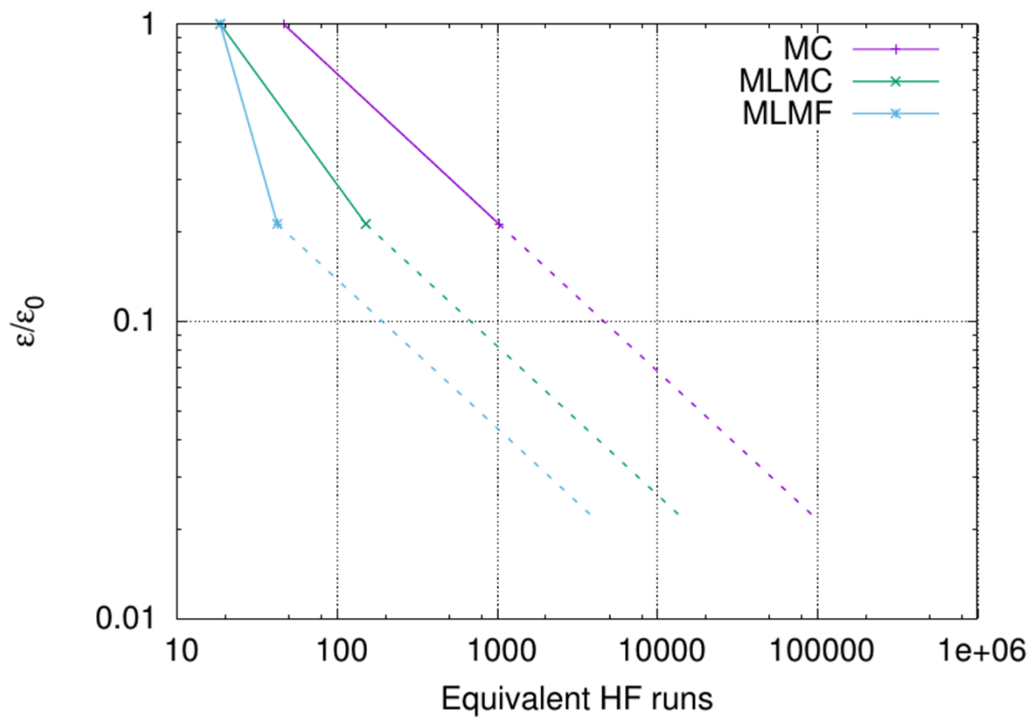
Context: 3D LES simulation of scramjets is extremely expensive and a significant challenge for UQ; even more so for OUU.

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

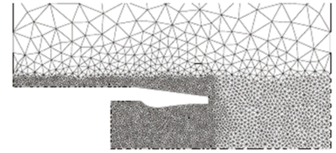
Implications: pursuing a more focused analysis of deterministic convergence properties. Anticipated outcome is the need to engage additional refinement levels (i.e., d/32, d/64) in order to converge QoI statistics that are closely tied to resolution of turbulence.

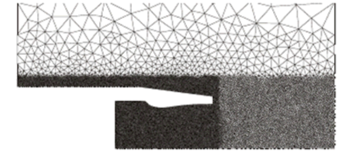
Initial Deployment of MLCV MC to UCAV Nozzle UQ

Sandia National Laboratories

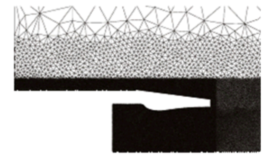
Context: Analysis of performance of UCAV nozzles subject to environmental, material, and manufacturing uncertainties.

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





(a) Coarse



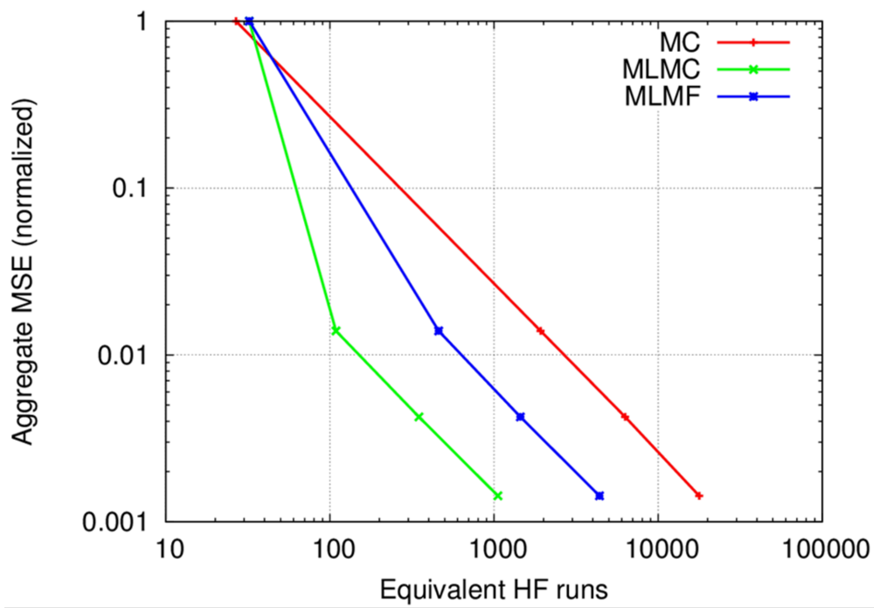
(c) Fine

	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

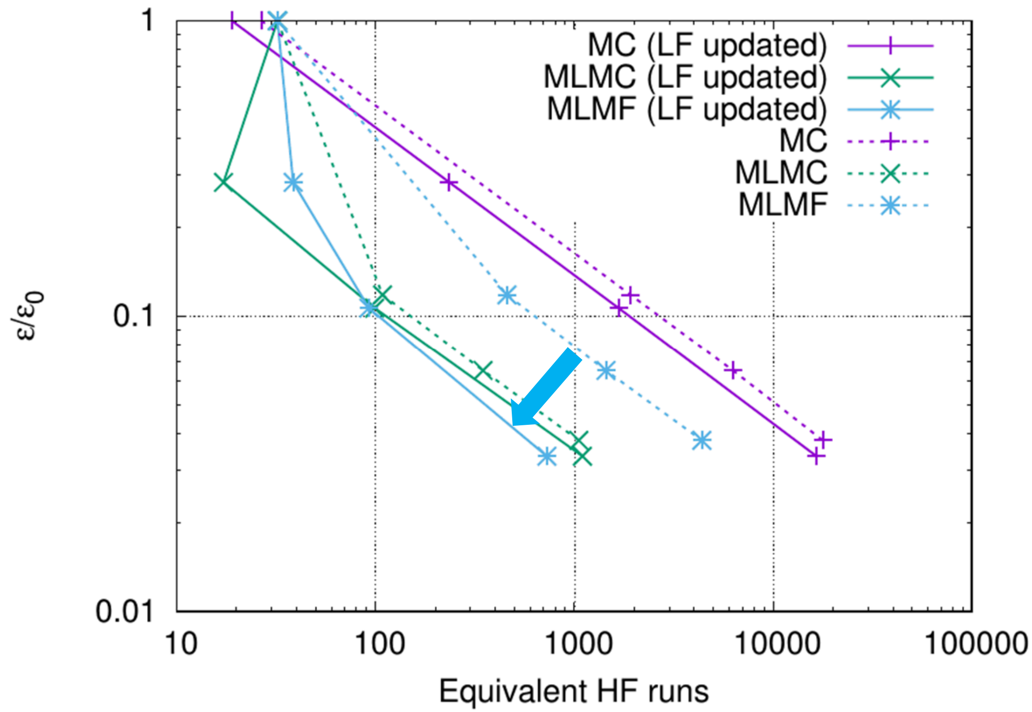
Target accuracy	LF	MF		
	Coarse	Coarse	Medium	Fine
0.01	21143	1757	20	20
0.003	69580	5775	36	20
0.001	212828	17715	109	34

MLMC is effective across MF discretizations, CV is hampered by LF corr

Results leading to improvements in LF structural models + algorithm refinements to adaptively manage (discard) models with low correlation

Updated Deployment of MLCV MC to UCAV Nozzle UQ

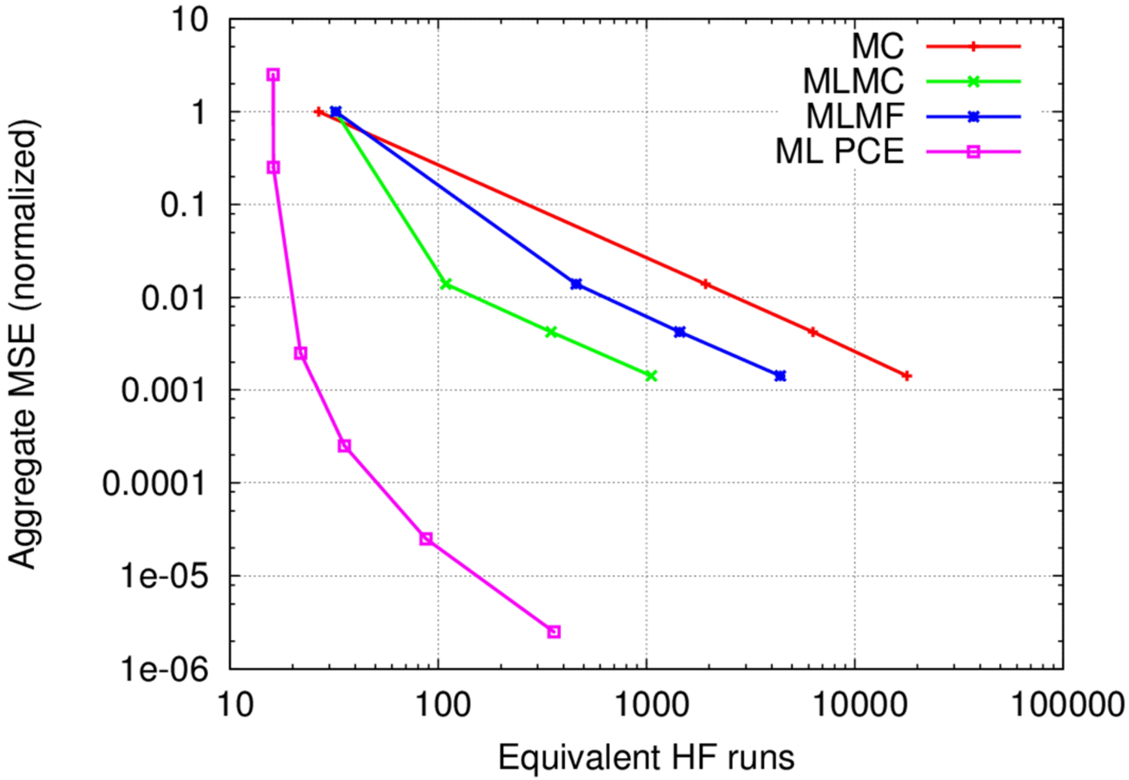
	LF		LF (updated)	
	correlation	Variance reduction [%]	correlation	Variance reduction [%]
Thrust	0.997	91.42	0.996	94.2
Mechanical Stress	2.31e-5	2.12e-3	0.944	89.2
Thermal Stress	0.391	12.81	0.987	93.4



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

Current Focus: Deployment of ML PCE to UCAV Nozzle UQ

Sandia National Laboratories



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

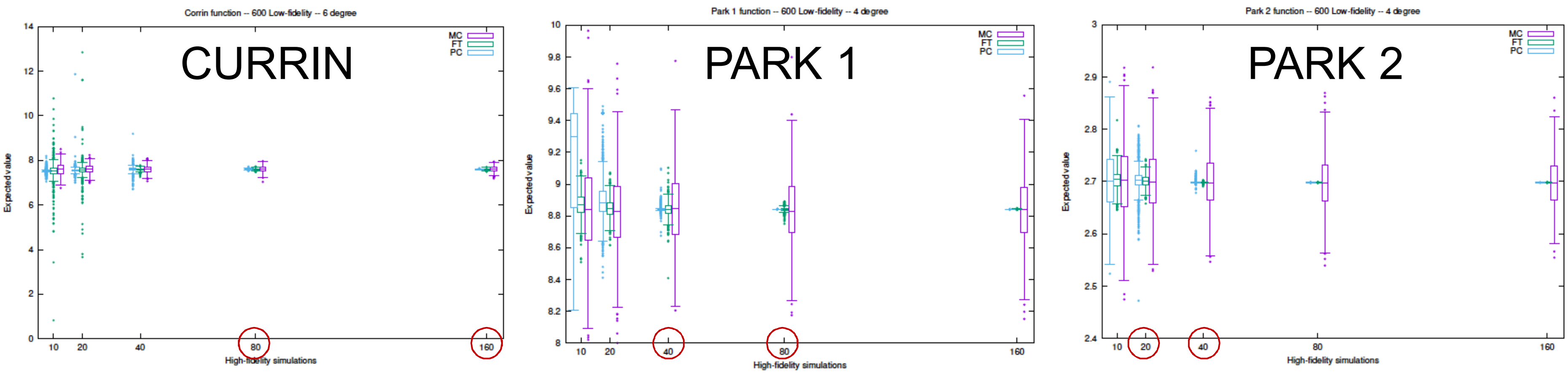
Target accuracy	MF		
1E-1	11	10	10
1E-3	118	10	10
1E-4	374	10	10
1E-5	1182	35	11
1E-6	4048	132	70

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

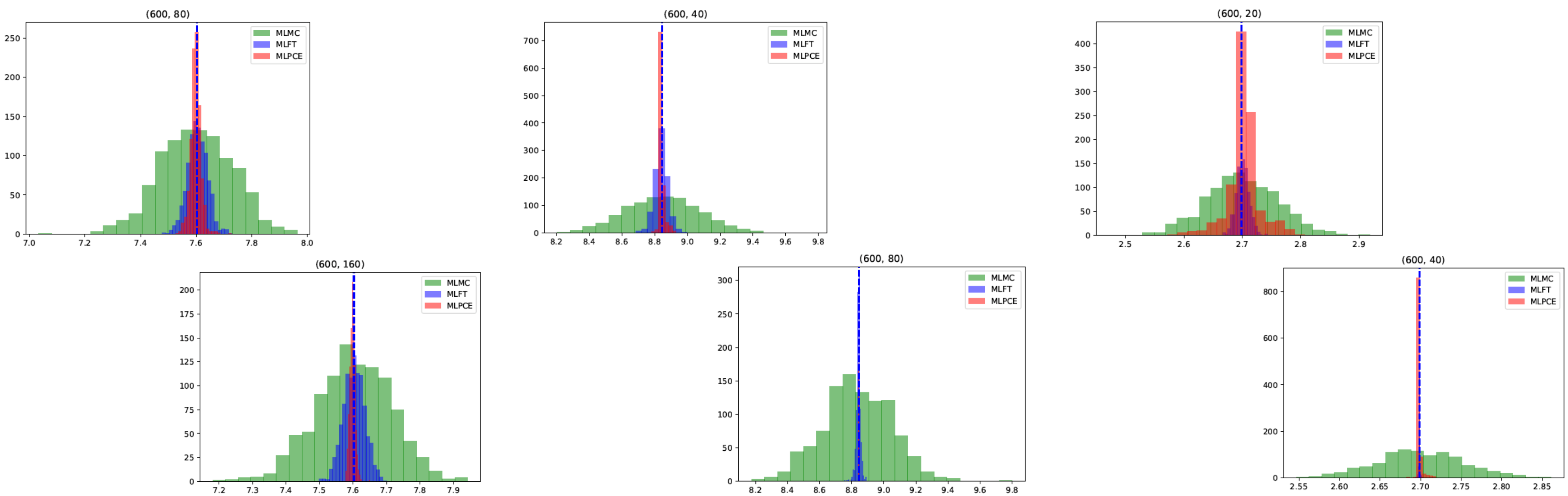
- Exploits smoothness in moderate dimension
- MC approaches expected to be competitive at higher dimension

Next steps: κ estimation, alternate PCE recovery methods, MLMF PCE

Latest ML PCE and ML FT



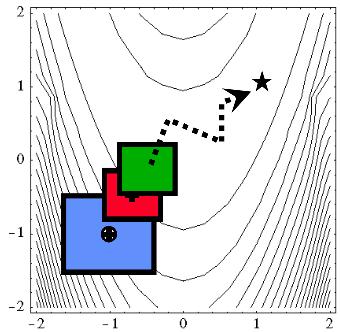
$N_{low} = 600$, **degree=6** $N_{low} = 600$, **degree=4** $N_{low} = 600$, **degree=4**



Multilevel-Multifidelity OUU: MG/Opt + recursive TRMM

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)

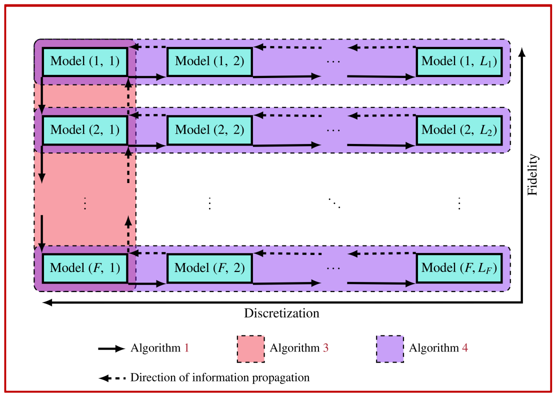
- targets *hierarchy of discretization levels*
- multigrid V cycle to hierarchy of *optimization solves*
- coarse optim. generates search direction for fine optim.
  - corrections + line search globalization → provable convergence

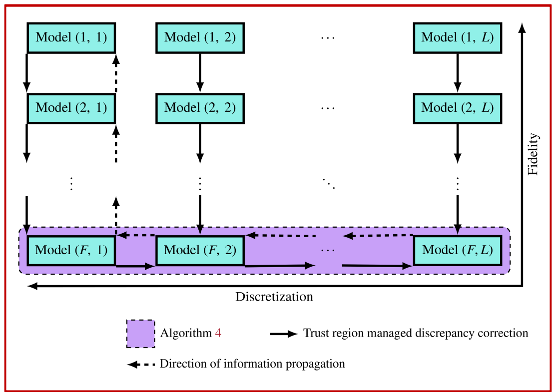
Algorithm 1 Multigrid Optimization

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

MLMF combining MG/Opt and TRMM

- both *model forms* and *discretization levels*
- Flexible hybridization of MG/Opt + recursive TRMM
- Prototype code now implemented in Dakota





Emulator-Based Bayesian Inference

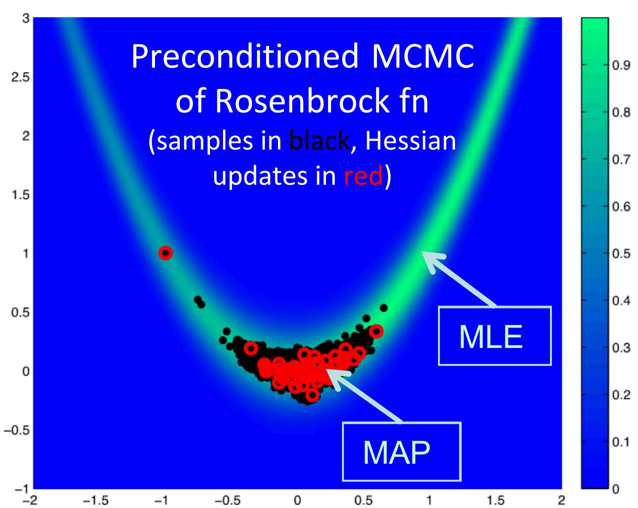
Objectives

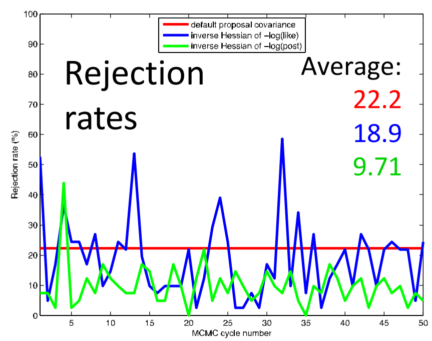
- Avoid direct interfacing of Markov Chain Monte Carlo (MCMC) with expensive high fidelity models
- Exploit analytic gradients/Hessians from emulators
  - DRAM: Pre-solve for posterior mode and form accurate proposal density for efficient MCMC
  - MALA/HMC: efficient SDE solves from emulator grads
- Parallel MCMC to identify multimodal posteriors

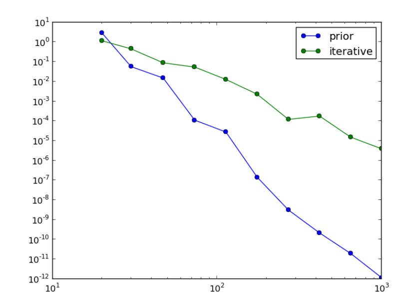
Impact

- Provides a scalable approach for inference
  - Interface of MCMC with scalable emulators for UQ
  - Laplace approximation of posterior distribution provides accurate proposal, eliminating high rejection rates for high-dimensional MCMC
- Integration of latest inference algorithms into production tools for broad SAP deployment
  - PISCEES, multi-scale climate, EFRC (CHWM)

Accomplishments







- Pre-solve for maximum a posteriori probability (MAP) = mode of posterior
  - Full Newton minimization of –log(posterior) using analytic Hessians of priors & emulators
- Accurate MCMC proposal distribution reduces sample rejection in high dimensions
  - 10D: 98% rejection reduced to 30%
- Posterior Hessian-based proposal (green) balances likelihood (blue) and prior (red)
- Emulator refinement: pivoted LU on chain

Summary Remarks

The case for multilevel – multifidelity methods

- Push towards higher simulation fidelity can make opt, UQ, OUU untenable
- Multiple model fidelities and discretizations are often available that trade accuracy for reduced computational cost

Towards multilevel-multifidelity UQ tailored for smoothness and dimensionality

- Multilevel sampling fmwk for cost-optimized variance reduction is quite general
  - ML-MF MC accounts for LF control variate at each HF discretization level within multilevel MC
  - ML PCE with CS: Adds optimal sample allocation to previous MF PCE approach. Initial prototype appears promising, but multiple refinements (estimator var, ML FT, MLMF) in progress.

Directions

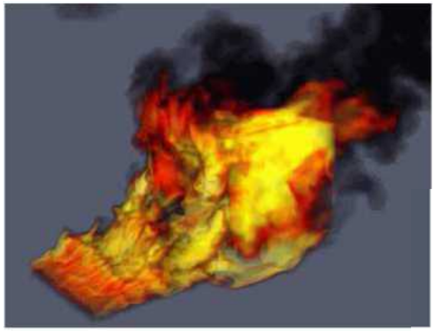
- OUU: move beyond common bi-fidelity approaches; push evals down hierarchy
- Inference: Exploit efficient ML-MF forward emulators for inference

Extra Slides

UQ & Optimization: DOE Mission Deployment

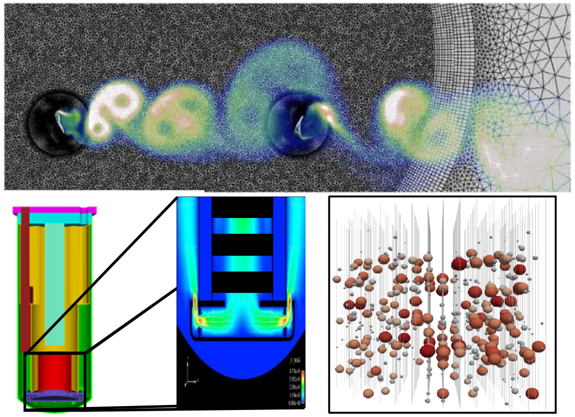
Stewardship (NNSA ASC)

Safety in abnormal environments



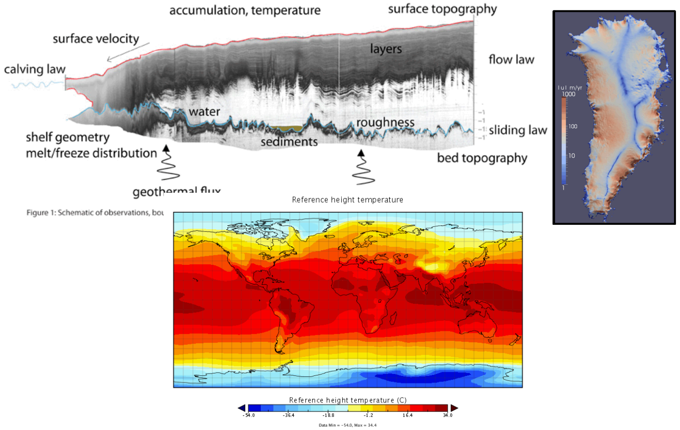
Energy (ASCR, EERE, NE)

Wind turbines, nuclear reactors



Climate (SciDAC, CSSEF, ACME)

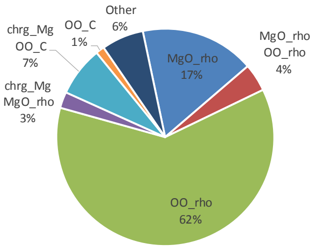
Ice sheets, CISM, CESM, ISSM, CSDMS

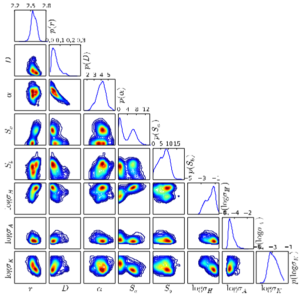


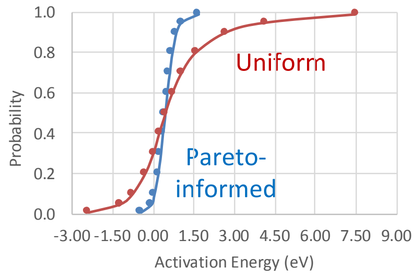
Computational Materials

(SciDAC+EFRC: CHWM, WastePD)

GSA, inference, forward UQ for waste forms / hazardous matls



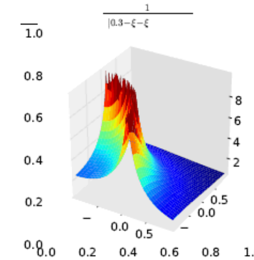




Common theme across these applications:

- 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)

Emphasis on Scalable Methods for High-fidelity UQ on HPC

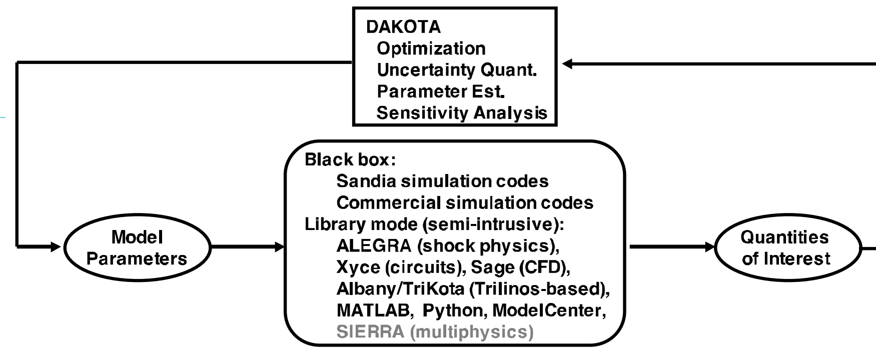


Compounding effects:

- Mixed aleatory-epistemic uncertainties (segregation → nested iteration)
- Requirement to evaluate probability of rare events (resolve PDF tails for QoI)
- Nonsmooth QoI (exp conv in spectral methods exploits smoothness)

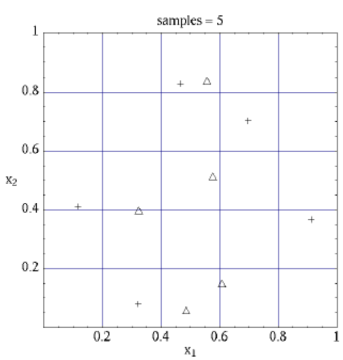
Steward Scalable Algorithms within DAKOTA

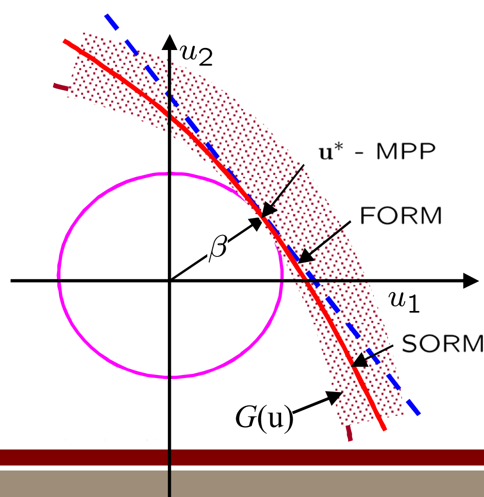
Explore and predict with confidence

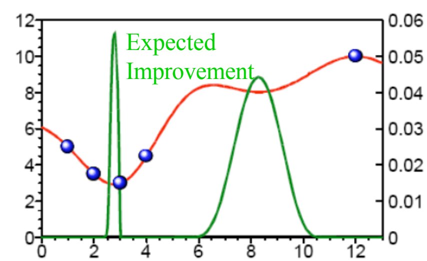


Core (Forward) UQ Capabilities:

- 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

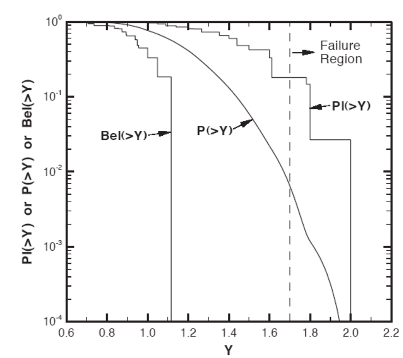






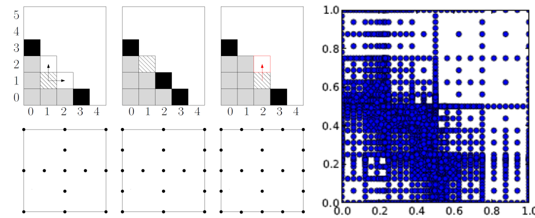
$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

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

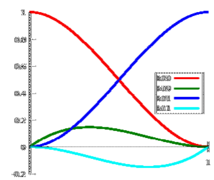


Research Thrusts for UQ

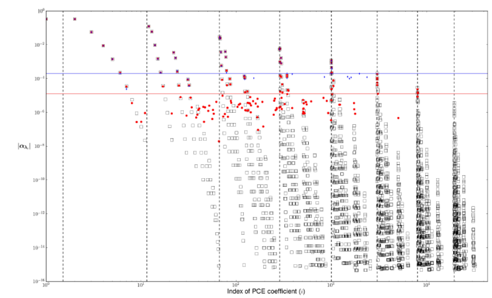
- *Focus:* Compute dominant uncertainty effects despite key challenges



- Emphasize scalability and exploitation of structure
  - *Adaptivity:* p- and h- refinement of stochastic expansions
  - *Adjoints:* gradient enhancement for PCE / SC / GP
  - *Sparsity:* compressed sensing
  - *Low Rank:* tensor / function train
  - *Dimension reduction:* active subspaces, adapted basis PCE

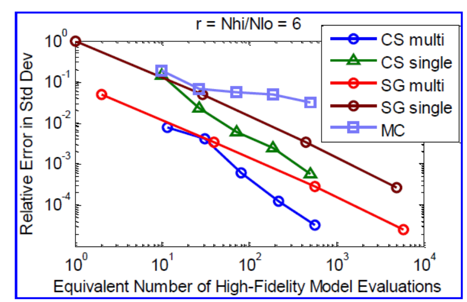


$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i)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



- Compound efficiencies
  - Multilevel-Multifidelity, Active subspaces + optimal quadrature

- Address complexity w/ component-based approach
  - Bayesian inference, Mixed aleatory-epistemic, OUU



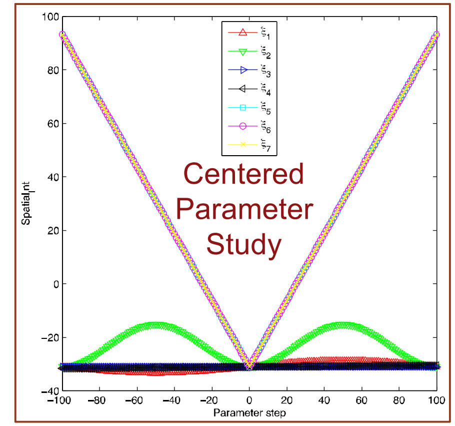
- Position UQ for next generation architectures
  - *Current (imperative):* multilevel parallelism
  - *Future (declarative):* exploit DAG + AMT for ensemble workflows

1D transient diffusion (parabolic PDE)

$$\frac{\partial\, u(x,\xi,t)}{\partial\, t} - \alpha(\xi)\frac{\partial^2\, u(x,\xi,t)}{\partial\, x^2} = 0, \quad \alpha > 0,\ x \in [0,L] = \Omega \subset \mathbb{R}$$

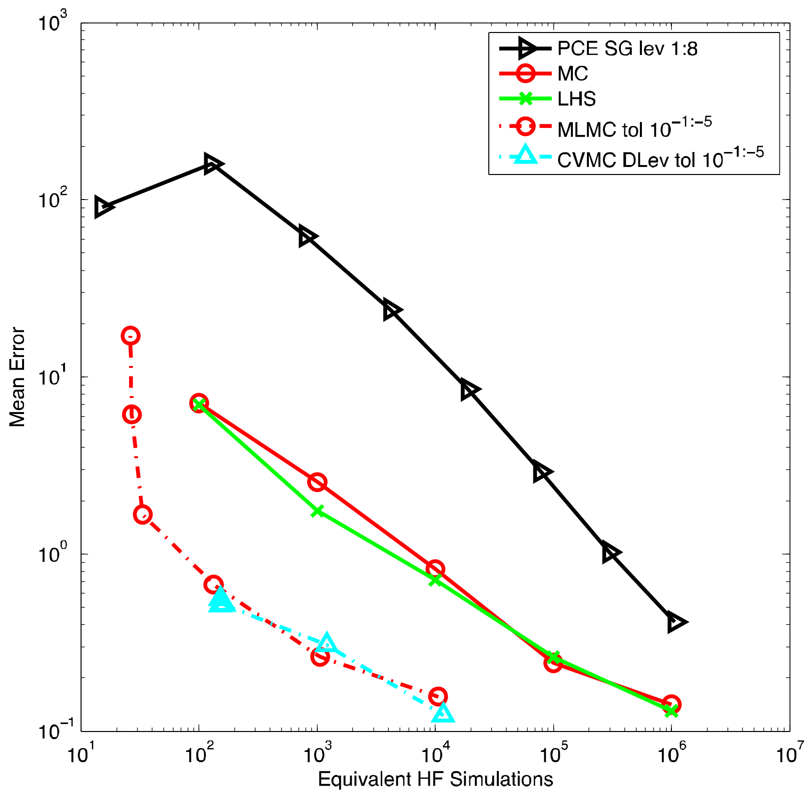
$$u(x,\xi,0) = u_0(x,\xi), \quad t \in [0,t_F] \quad \text{and} \quad \xi \in \Xi \subset \mathbb{R}^d$$

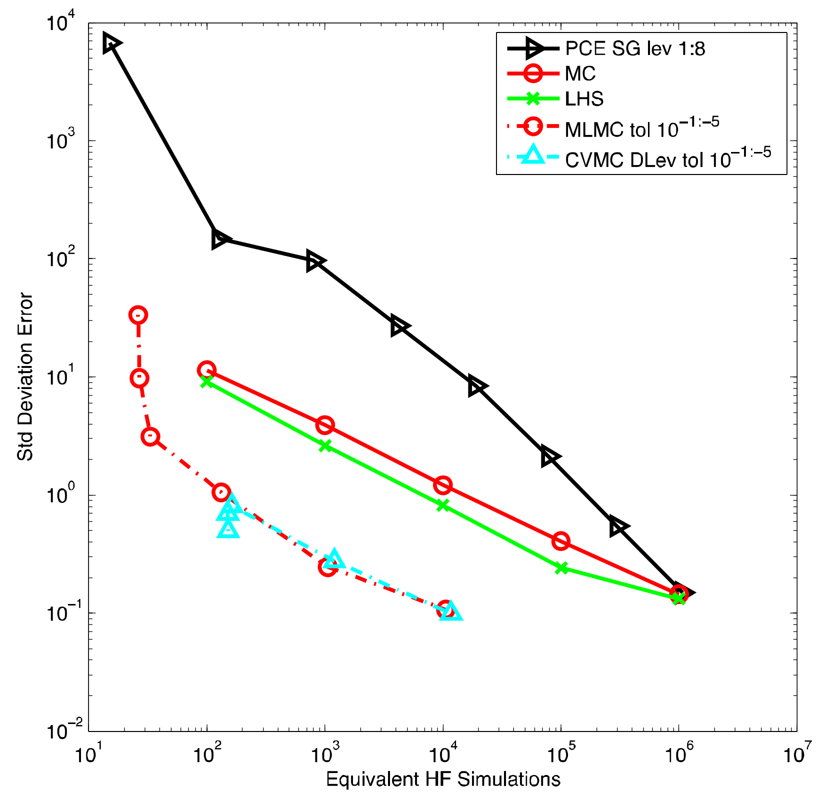
$$u(x,\xi,t)|_{\partial\Omega} = 0.$$



$$\mathcal{G}(\xi_5,\xi_6,\xi_7) = 50\frac{|4\xi_5-2|+a_i}{1+a_i}\,\frac{|4\xi_6-2|+a_i}{1+a_i}\,\frac{|4\xi_7-2|+a_i}{1+a_i}$$

Model forms: 2 (N_m = 3, 21)
Discretization levels: 4 per form (N_x)
Dimensionality: 7 *QoI:* 1
Cost model: linear in N_m, cubic in N_x





Latest ML PCE and ML FT

- All the results obtained in this numerical investigation suggest that we should use γ_ℓ and κ_ℓ

$$\mathbb{V}ar\left(\hat{Y}_\ell\right) = \frac{\mathbb{V}ar\left(Y_\ell\right)}{\gamma_\ell {N_\ell}^{\kappa_\ell}}$$

- The optimal samples allocation in this case is

$$N_\ell = \sqrt[\kappa_\ell+1]{\frac{\sum_{q=0}^{L} \frac{\kappa_\ell}{\kappa_q} N_q C_q}{\gamma_\ell \varepsilon^2/2}} \sqrt[\kappa_\ell+1]{\mathbb{V}ar\left(Y_\ell\right) C_\ell}$$

- The optimization problem is now more complex and requires non-linear iterations

Optimization Foundational Components for ML and MF:

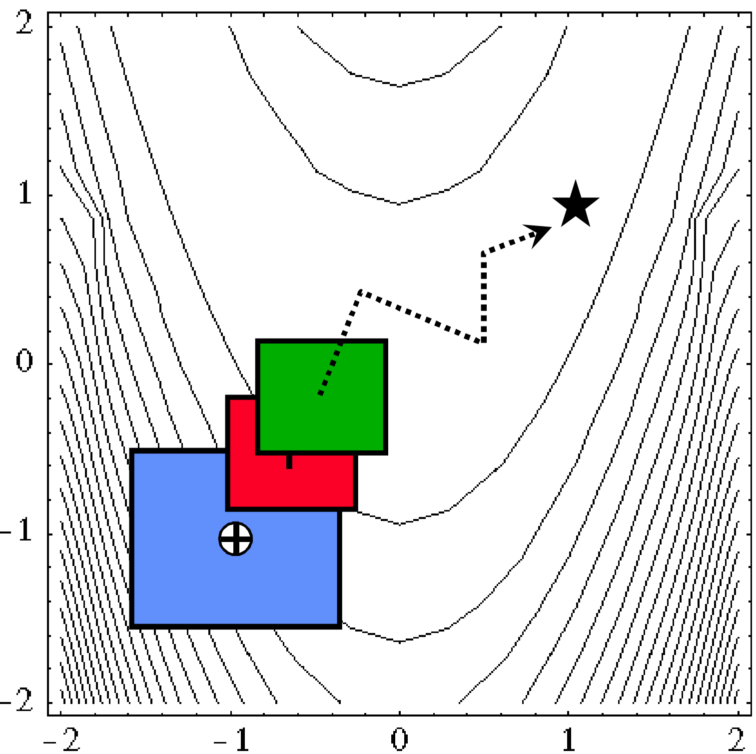
- Trust Region Model Management (TRMM)
- Multigrid Optimization (MG/Opt)

Trust-Region Model Management – Multifidelity Case

TRMM solves a series of approximate subproblems:

- Data fit (global, local, multipoint)
- Multifidelity
- ROM

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**
    $A_0 = f_{hi}(x_c) - f_{lo}(Rx_c)$, $B_0 = \frac{f_{hi}(x_c)}{f_{lo}(Rx_c)}$
  end if
  if (correction order ≥ 1) **then**
    $A_1 = R\left[\nabla f_{hi}(x_c)\right] - \nabla f_{lo}(Rx_c)$, $B_1 = \frac{1}{f_{lo}(Rx_c)} R\left[\nabla f_{hi}(x_c)\right] - \frac{f_{hi}(x_c)}{f_{lo}^2(Rx_c)} \nabla f_{lo}(Rx_c)$
  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

Note: bi-fidelity approaches dominate

Multigrid optimization (MG/Opt)

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MODEL PROBLEMS FOR THE MULTIGRID OPTIMIZATION OF SYSTEMS GOVERNED BY DIFFERENTIAL EQUATIONS*

ROBERT MICHAEL LEWIS† AND STEPHEN G. NASH‡

SIAM REVIEW
Vol. 51, No. 2, pp. 361–395

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Multigrid Methods for PDE Optimization*

Alfio Borzì†
Volker Schulz‡

As in multilevel Monte Carlo, exploit discretization hierarchy within optimization/OUU:

- Apply multigrid V cycle to hierarchy of *optimal* solns
  - Distinct from applying multigrid to KKT system
  - Distinct from successive refinement of optimal solns (employs bi-directional prolongation / restriction)

Recursively uses coarse resolution problems to generate search directions for finer-resolution solves

- Line search used to compute fine-resolution iterate from coarse-resolution search direction
- Globalization enables provable convergence

Special case of / component within generalized model management framework

- Requires effective subproblem solver to generate a new iterate at a particular level
- Leverages 1st and (quasi, finite diff.) 2nd-order additive & combined corrections

Algorithm 1 Multigrid Optimization

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

Dive

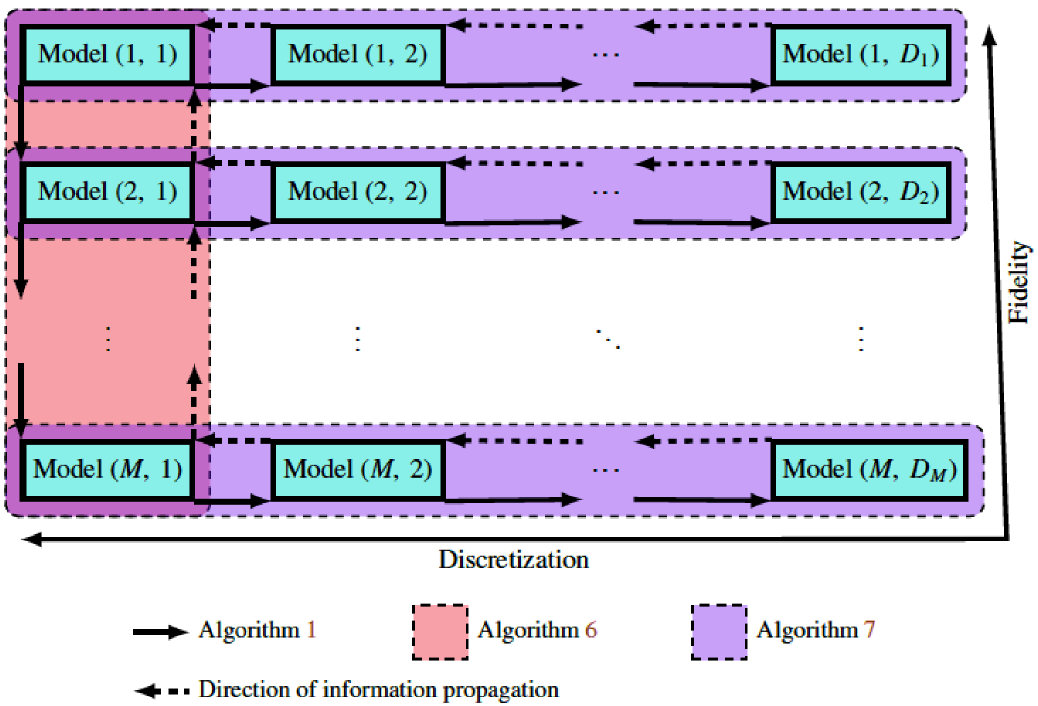
Return

TRMM + MG/Opt for Multilevel-Multifidelity Hierarchies

- Nested Multigrid
- Trust Region-Managed Multigrid
- Nested TRMM

MLMF 1: Nested Multigrid

- **Outer iteration until convergence**
- **MFOPT: V cycle over model forms**
- **MLOPT: V cycle over discretizations for each form**



- **Partial optimization applied to every discretization for every model form**

Algorithm 5 Nested Multigrid

procedure MLMFOPT1
  Initialize optimization at a lower fidelity and/or level:
  Partially solve: $x_n^{(M,D)} = \arg\min_x f^{(M,D)}(x)$
  $x_{n+1} = \prod_{m=M-1}^{1} P_{m,1} \prod_{d=D-1}^{1} P_{M,d}\, x_n^{(M,D)}$
  repeat
    $x_n = x_{n+1}$
    $x_{n+1} = \text{MFOPT}(1,\ x_n,\ f^{(1,1)}(x))$
  until convergence
  return x_{n+1}
end procedure

Algorithm 6 Recursive Multifidelity Optimization

procedure MFOPT(m, $x_0^{(m,1)}$, $f_{\text{CORR}}^{(m,1)}(x)$)
  if $m = M$ **then**
    $x_1^{(m,1)} = \text{MLOPT}(k,\ 1,\ x_0^{(m,1)},\ f_{\text{corr}}^{(m,1)}(x))$
    return $x_1^{(m,1)}$
  else
    Partially solve: $x_1^{(m,1)} = \text{MLOPT}(m,\ 1,\ x_0^{(m,1)},\ f_{\text{corr}}^{(m,1)}(x))$
    $x_1^{(m+1,1)} = R_{m,1}\left[x_1^{(m,1)}\right]$
    $f_{\text{corr}}^{(m+1,1)}(x) = \text{CORRECTION}(x_1^{(m,1)},\ R_{m,1},\ f_{\text{corr}}^{(m,1)}(x),\ f^{(m+1,1)}(x))$
    $x_2^{(m+1,1)} = \text{MFOPT}(f+1,\ x_1^{(m+1,1)},\ f_{\text{corr}}^{(m+1,1)}(x))$
    $e = P_{m,1}\left[x_2^{(m+1,1)} - x_1^{(m+1,1)}\right]$
    return result of linesearch along direction e
  end if
end procedure

Algorithm 7 Recursive Multilevel Optimization

procedure MLOPT(m, l, $x_0^{(m,d)}$, $f_{\text{CORR}}^{(m,d)}(x)$)
  if $d = D_m$ **then**
    $x_1^{(m,d)} = \arg\min_x f_{\text{corr}}^{(m,d)}(x)$
    return $x_1^{(m,d)}$
  else
    Partially solve: $x_1^{(m,d)} = \arg\min_x f_{\text{corr}}^{(m,d)}(x)$
    $x_1^{(m,d+1)} = R_{m,d}\left[x_1^{(m,d)}\right]$
    $f_{\text{corr}}^{(m,d+1)}(x) = \text{CORRECTION}(x_1^{(m,d)},\ R_{m,d},\ f_{\text{corr}}^{(m,d)}(x),\ f^{(m,d+1)}(x))$
    $x_2^{(m,d+1)} = \text{MLOPT}(m, d+1,\ x_1^{(m,d+1)},\ f_{\text{corr}}^{(m,d+1)}(x))$
    $e = P_{m,d}\left[x_2^{(m,d+1)} - x_1^{(m,d+1)}\right]$
    return result of linesearch along direction e
  end if
end procedure

MLMF 2: Trust Region Managed Multigrid

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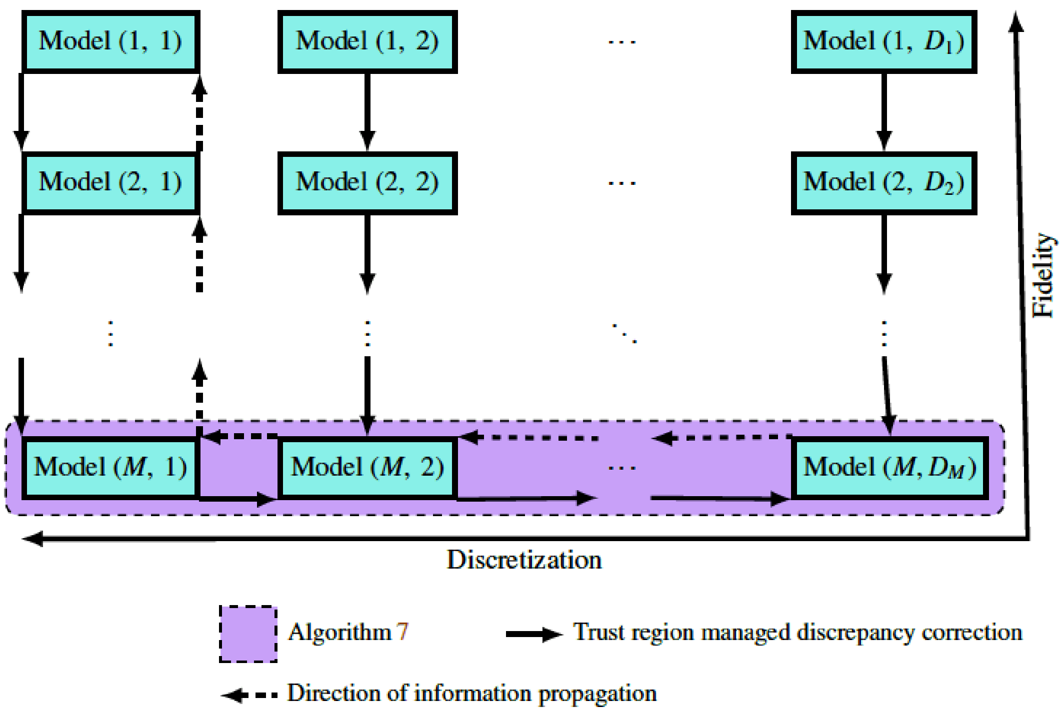
- **Outer iteration until convergence**
- **MLOPT: V cycle over discretizations for LF model**
- **RECTR: Update TR model form hierarchy for each *d***



- **Partial optimization applied to every discretization for LF model**

Algorithm 8 Trust Region Managed Multigrid

procedure MLMFOPT2
  repeat
    $x_n = x_{n+1}$
    $x_{n+1} = \text{MLOPT}(M,\ 1,\ x_n,\ f^{(M,1)}(x))$
    for $d = 1$ to D_M **do**
      $\text{RECTR}(m = 1 : M,\ x_n^{(M,d)},\ x_{n+1}^{(M,d)},\ f_{\text{corr}}^{(m,d)}(x))$
    end for
  until convergence
  return x_{n+1}
end procedure

Algorithm 9 Recursive Trust Region Updating

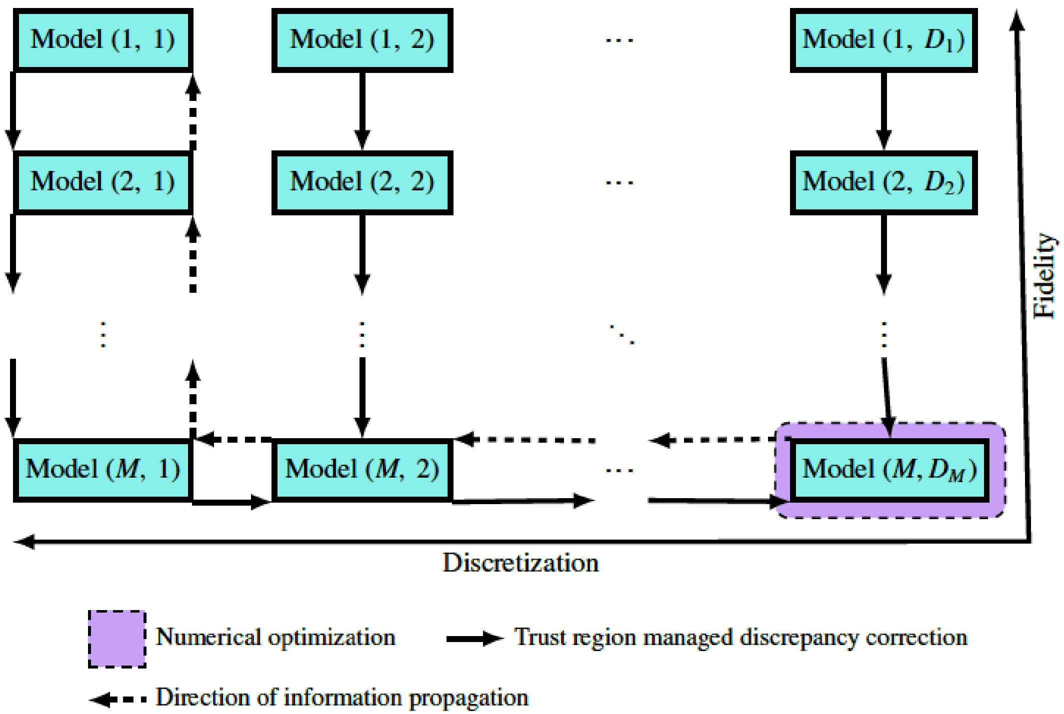
procedure $\text{RECTR}(r = 1:\text{LEN},\ x_c^r,\ x_*^r,\ f_{\text{CORR}}^r(x))$
  for r = len to 1 (bottom up: low to high || coarse to fine) **do**
    if State_r = new candidate x_*^r **then**
      Test for new center: $\text{TR}(x_c^r,\ x_*^r,\ f_{\text{corr}}^{r+1}(x),\ f_{\text{corr}}^r(x))$
    end if
    if State_r = new center x_c^r **then**
      Compute $f^{r-1}(x_c^r)$
      Compute $\text{CORRECTION}(x_c^r, R, f^{r-1}(x_c^r), f^r(x_c^r))$
      if $\text{Converged}(x_c^r,\ f_{\text{corr}}^{r-1}(x_c^r),\ L^{r-1},\ U^{r-1})$ **then**
        $x_*^{r-1} = x_c^r$ (new candidate)
      end if
    end if
  end for
  for r = 1 to len (top down: high to low || fine to coarse) **do**
    if State_r = new center x_c^r **then**
      Recompute $\text{CORRECTION}(x_c^r, R, f^{r-1}(x_c^r), f^r(x_c^r))$
    end if
    if parent corrected **then**
      Recur updated corrections for $f_{\text{corr}}^r(x_c^r)$
    end if
    Reset State_r
  end for
end procedure

MLMF 3: Nested TRMM

- **Outer iteration until convergence**
- **RECTR: Recur over discretizations for LF model**
- **RECTR: Update TR model form hierarchy for each *d***

Algorithm 10 Nested Trust Region Model Management

procedure MLMFOPT3
  repeat
    $x_n = x_{n+1}$
    $x_{n+1} = \arg\min_x f_{\text{corr}}^{(m,d)}(x)$
    RECTR($d = 1 : D_M,\ x_n^{(M,D_M)},\ x_{n+1}^{(M,D_M)},\ f_{\text{corr}}^{(m,d)}(x)$)
    for $d = 1$ to D_M **do**
      RECTR($m = 1 : M,\ x_n^{(M,d)},\ x_{n+1}^{(M,d)},\ f_{\text{corr}}^{(m,d)}(x)$)
    end for
  until convergence
  return x_{n+1}
end procedure



- **Optimization applied exclusively to LF model at coarse discretization**
- **Ordering of sweeps is not prescribed**

Computational Experiments

- Model Problem: Target solution profile for SS diffusion
- Model Problem: Minimize C_D for transonic airfoil
- Initial deployments for OUU in DARPA EQUiPS

Steady State Diffusion:
MG/Opt for Multilevel

ODE:

$$\frac{d}{dx}\left(a\frac{du}{dx}\right) = -f, \quad x \in (0,1)$$

$$u(0) = u(1) = 0$$

$$a = 2 + \cos(2\pi x)$$

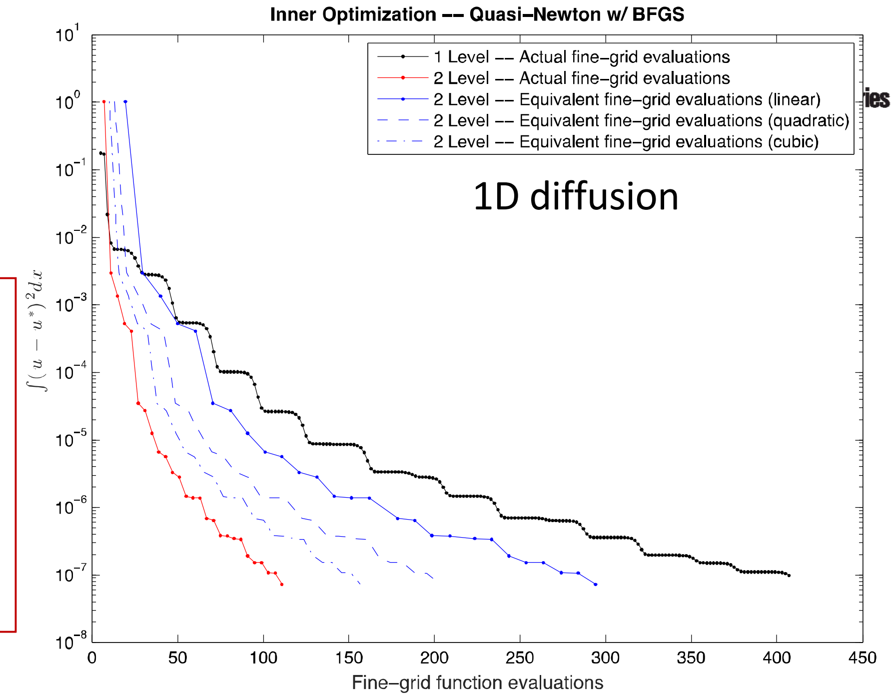
Optimization Problem:

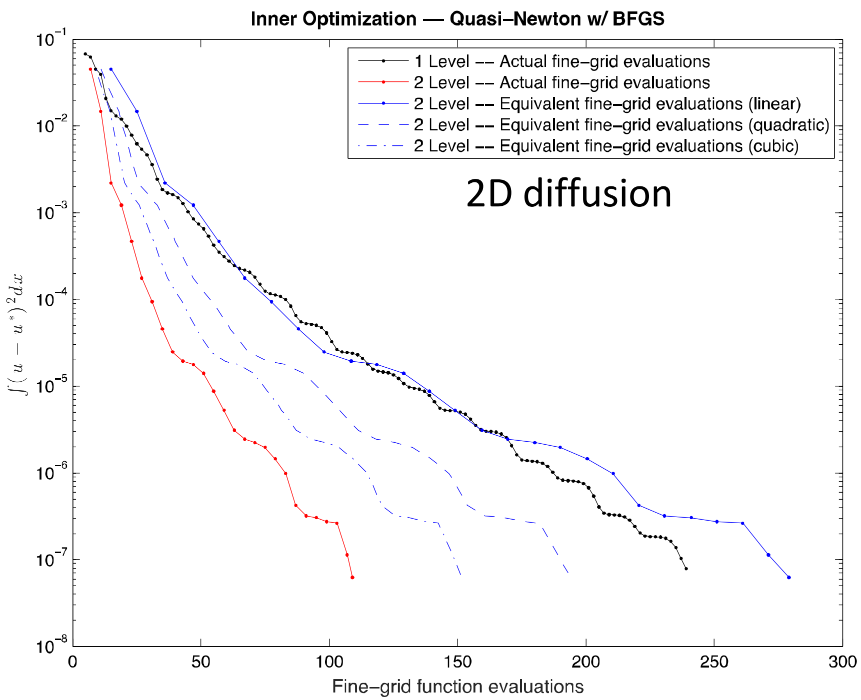
$$\underset{f}{\text{minimize}} \quad \int (u(f) - u^*)^2 dx$$

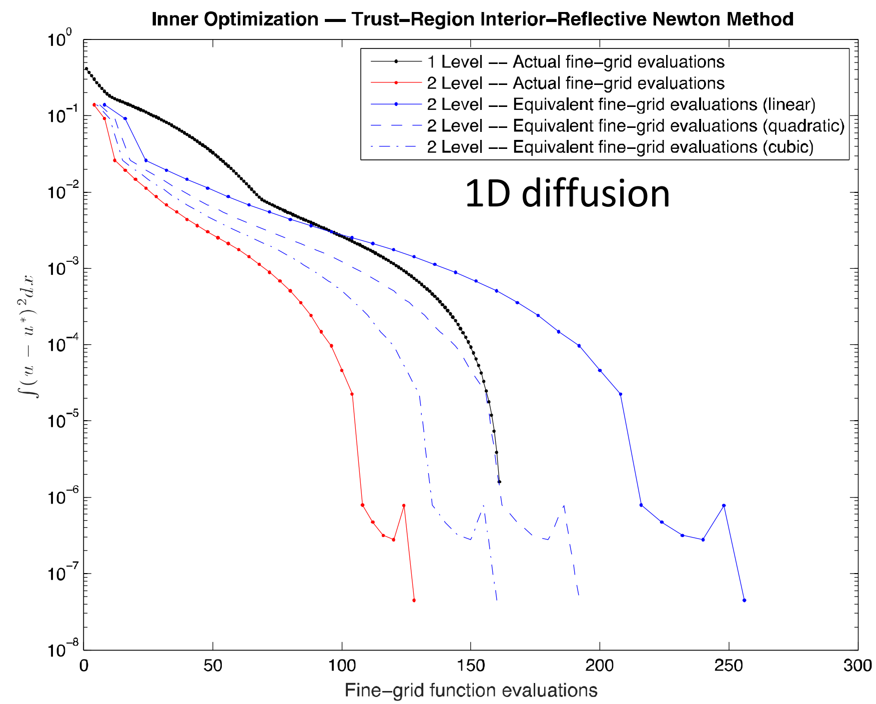
$$\text{subject to} \quad c(f, u(f)) = 0$$

$$u^* = \sin^2(2\pi x)$$

- **MATLAB Opt Solvers (2)**
- **Grid scalings (1D and 2D diffusion)**
- **Solver cost scalings (linear, quadratic, cubic)**





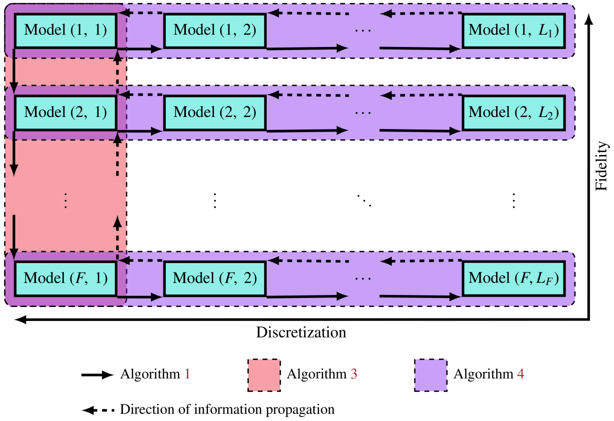


Steady State Diffusion:
Recursive MG/Opt and TRMM

$$c_{hi}(f, u(f)) = \frac{d}{dx}\left(a_{hi}\frac{du}{dx}\right) + f = 0, \quad x \in (0, 1),$$
$$u(0) = u(1) = 0,$$
$$a_{hi} = 2 + \cos(2\pi x) + 0.4\sin(6\pi x) \quad \textbf{HF}$$

MATLAB Prototypes

Initial formulation: nested multigrid



a) 1 fidelity and 1 level

	Fine
High-Fidelity	229

b) 1 fidelity and 2 levels

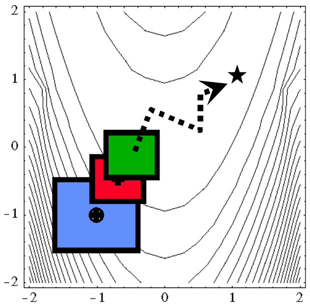
	Fine	Coarse
High-Fidelity	112	146

c) 2 fidelities and 2 levels

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

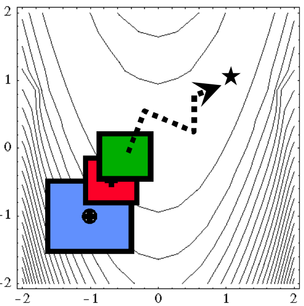
Dakota: NPSOL & TRMM

	LF evals	HF evals	Objective
Single-fidelity SQP	–	244	1.07e-07
Bi-Fidelity 1^{st}-order TRMM	7565	101	1.64e-07

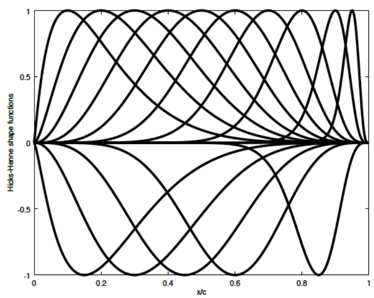


Transonic Airfoil Design: Minimize Drag, Preserve Lift

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & C_D(u(x)) \\ \text{subject to} \quad & C_L(u(x)) \geq \bar{C}_L \\ & c_{\text{RANS}}(x, u(x)) = 0 \\ & -0.01 \leq x \leq 0.01 \end{aligned}$$



Design: Hicks Henne shape fns

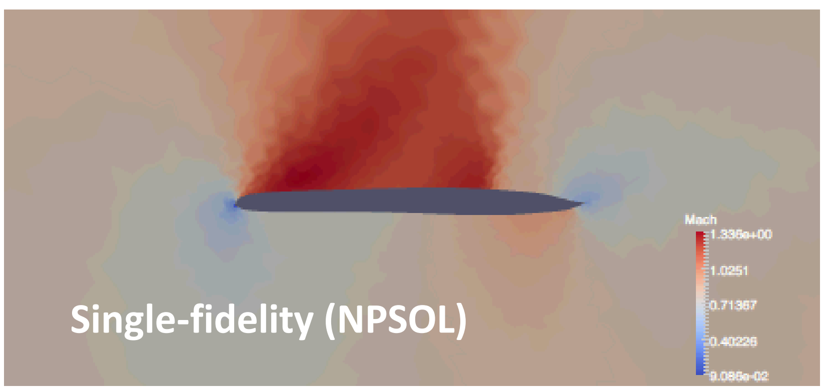


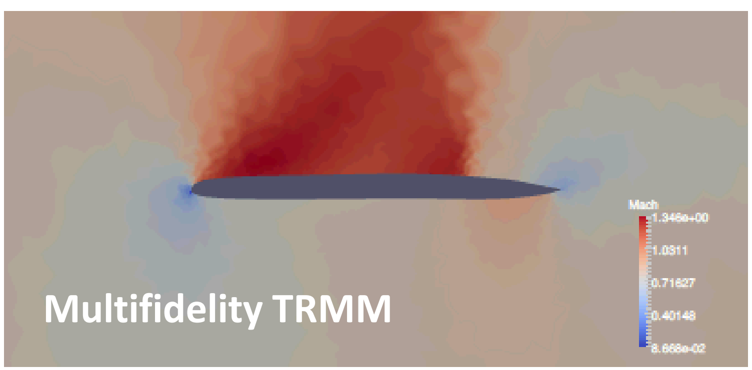
Algorithm 9 Recursive Trust Region Updating

procedure RECTR($r = 1$:LEN, x_c^r, x_*^r, $f_{\text{CORR}}^r(x)$)
  for r = len to 1 (bottom up: low to high || coarse to fine) **do**
    if State$_r$ = new candidate x_*^r **then**
      Test for new center: TR(x_c^r, x_*^r, $f_{\text{corr}}^{r+1}(x)$, $f_{\text{corr}}^r(x)$)
    end if
    if State$_r$ = new center x_c^r **then**
      Compute $f^{r-1}(x_c^r)$
      Compute CORRECTION($x_c^r, R, f^{r-1}(x_c^r), f^r(x_c^r)$)
      if Converged(x_c^r, $f_{\text{corr}}^{r-1}(x_c^r)$, L^{r-1}, U^{r-1}) **then**
        $x_*^{r-1} = x_c^r$ (new candidate)
      end if
    end if
  end for
  for r = 1 to len (top down: high to low || fine to coarse) **do**
    if State$_r$ = new center x_c^r **then**
      Recompute CORRECTION($x_c^r, R, f^{r-1}(x_c^r), f^r(x_c^r)$)
    end if
    if parent corrected **then**
      Recur updated corrections for $f_{\text{corr}}^r(x_c^r)$
    end if
    Reset State$_r$
  end for
end procedure

3-level Recursive TRMM for Euler

	Coarse evals	Medium evals	Fine evals	C_D	C_L
Reference NACA 0012	–	–	–	0.10345	0.80118
Single-fidelity SQP	–	–	806	0.064904	0.80118
Single-fidelity SLP	–	–	1190	0.065024	0.80199
Three-level 1^{st}-order TRMM	43630	4882	187	0.064968	0.80153





From optimization to DUU: DARPA Deployments

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UCAV
Nozzle

$$\underset{\mathbf{x}}{\text{minimize}} \quad \mathbb{V}[\ T\ ]$$
$$\text{subject to} \quad \mathbb{E}[\ W\ ] \leq \overline{W}$$
$$\mathbb{E}[\ T\ ] \geq \overline{T}$$
$$\mathbb{E}[\ ||T_w||\ ] \leq \overline{T}_w$$
$$\mathbb{E}[\ ||\sigma||\ ] \leq \overline{\sigma}$$

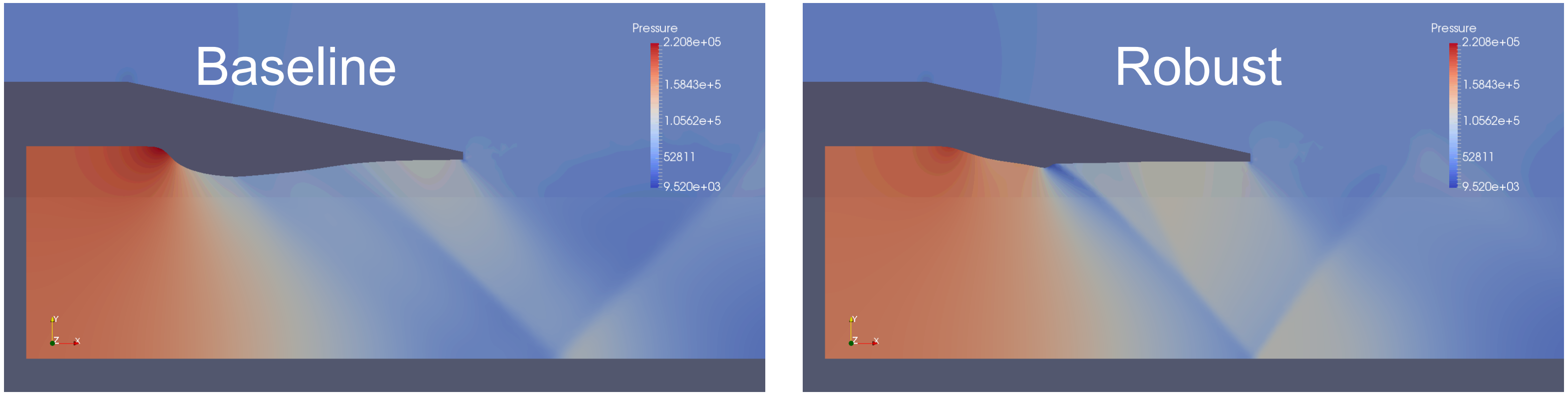
+bounds, linear cons.

LF statistics: L1 sparse grid w/ Euler COARSE
HF statistics: L1 sparse grid w/ Euler MEDIUM

- 1st-order consistent TRMM w/ numerical grads
- 7 rand vars, 29 des vars (21 B-spline, 8 thick)

Trust region cycles

- 5 iterations accepted by filter method
- Tuning of FDSS & solver conv. in progress



Scramjet (P1: Jet in cross flow)

$$\min_{z} \mathbb{E}_\theta[\mathbb{V}_y[\phi(z,\theta,y)]] + \alpha \cdot \mathbb{V}_\theta^{\frac{1}{2}}[\mathbb{V}_y[\phi(z,\theta,y)]], \quad \alpha \in \mathbb{R}$$
$$\text{s.t. } \mathbb{E}_\theta[\mathbb{E}_y[\chi(z,\theta,y)]] \leq \overline{\chi}, \quad \overline{\chi} \in \mathbb{R}$$

Vary UQ approach & simulation discretization:

- LF stats: L2 sparse grid combined exp, 2D d/8
- HF stats: L2 sparse grid uncertain exp, 2D d/16

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

Summary Remarks

The case for multilevel – multifidelity methods

- Push towards higher simulation fidelity can make opt, UQ, OUU untenable
- Multiple model fidelities and discretizations are often available that trade accuracy for reduced computational cost

Towards multilevel-multifidelity UQ tailored for smoothness and dimensionality

- Multilevel sampling fmwk for cost-optimized variance reduction is quite general
  - ML-MF MC accounts for LF control variate at each HF discretization level within multilevel MC
  - ML PCE with CS: Adds optimal sample allocation to previous MF PCE approach. Initial prototype appears promising, but multiple refinements (estimator var, ML FT, MLMF) in progress.

Towards recursive optimization schemes that exploit the full model ensemble

- Move beyond bi-fidelity: by exploiting richer model ensemble, computational effort can be pushed down the hierarchy, supporting case of only a handful of HF fine-grid evaluations
- MG/Opt and recursive TRMM used as foundational algorithms for one hierarchy dimension
- Proposed MLMF approaches recur across both multilevel + multifidelity dimensions:
  - Nested MG/Opt, Trust-region managed multigrid, Nested TRMM
- Initial results point to benefits in interfacing optimizers exclusively at LF/coarse levels
  - MG/Opt tends to spread evaluations more evenly across its hierarchy, whereas TRMM only interfaces optimizer with least expensive model (other models: validation, correction).
  - Prototype of Nested MG → Production implementations for TR-managed MG, Nested TRMM