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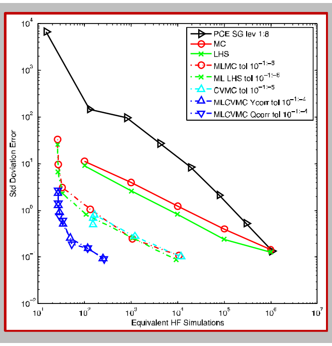
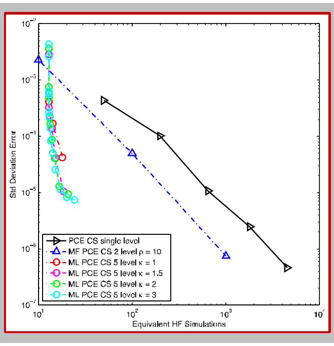
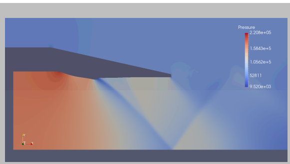
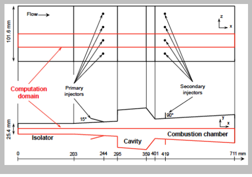


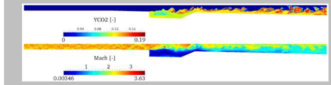


DAKOTA

Explore and predict with confidence







Multilevel-Multifidelity Approaches for Uncertainty Quantification and Design

Michael S. Eldred, Jason A. Monschke, John D. Jakeman, Gianluca Geraci
Sandia National Laboratories, Albuquerque, NM

SIAM CSE Conference, Atlanta, Feb 27—Mar 3, 2017

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Multiple Model Forms in UQ & Opt

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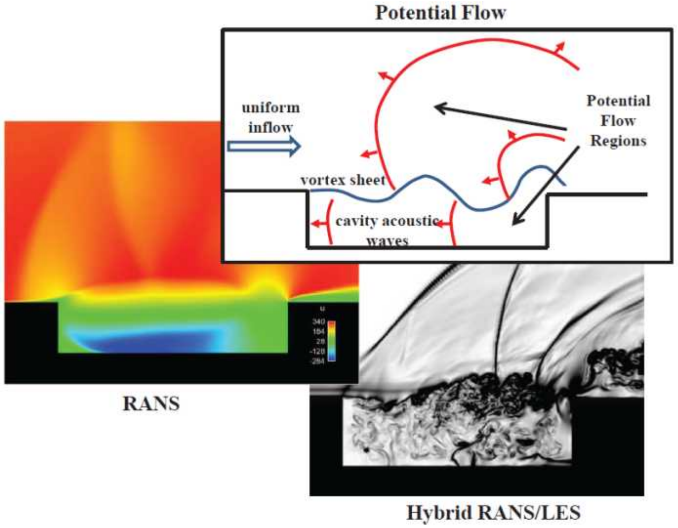
Discrete model choices for simulation of same physics

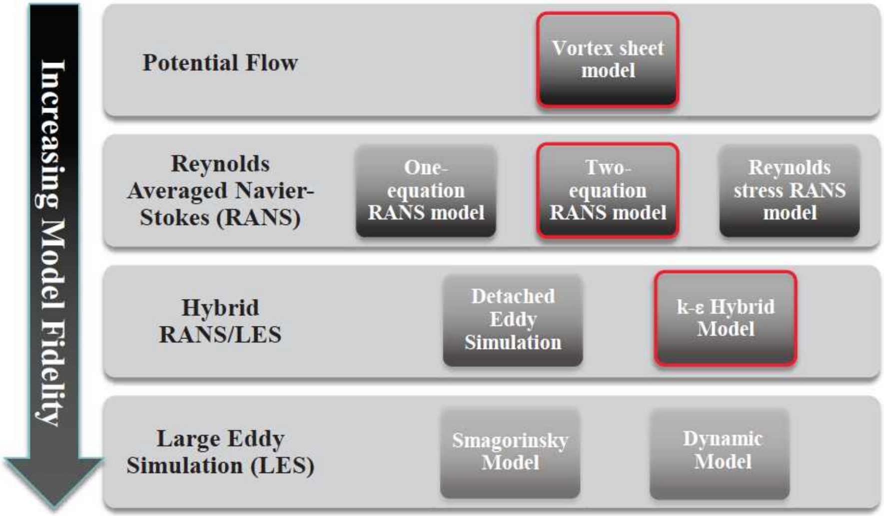
A clear hierarchy of fidelity (from low to high)

- 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

MF UQ with Spectral Stochastic Discrepancy Models

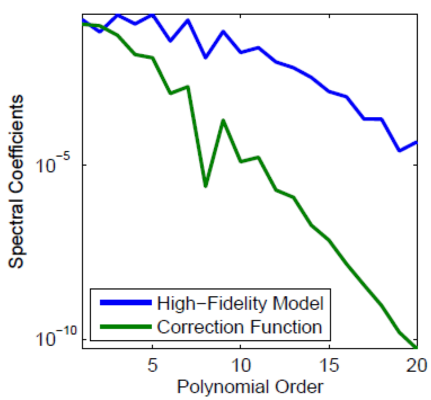
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity "design" codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

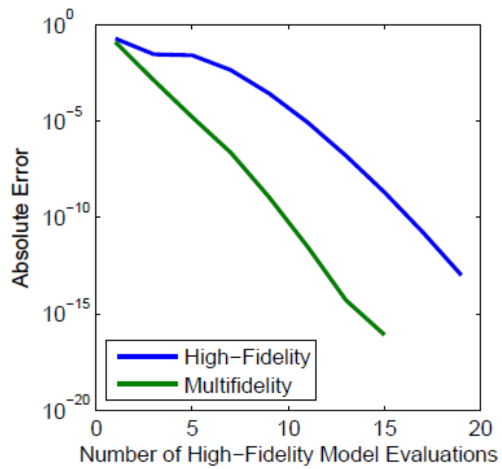
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

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

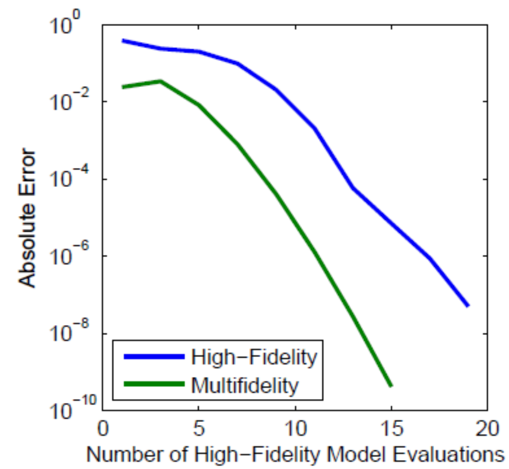
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2} \cos 0.5\xi \underbrace{- 0.5 e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

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





(a) Error in mean



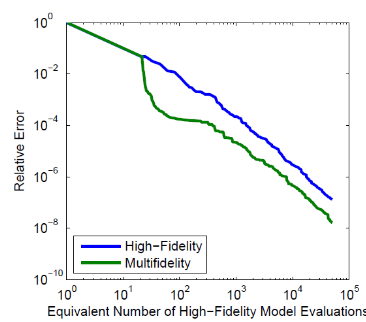
(b) Error in standard deviation

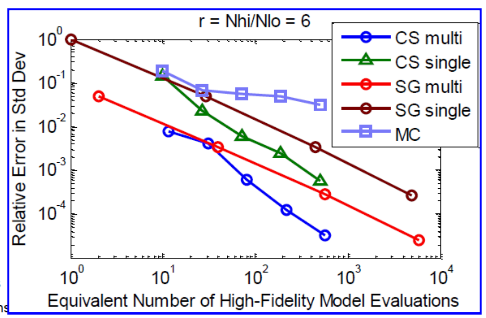
Adaptive sparse grid multifidelity algorithm:

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

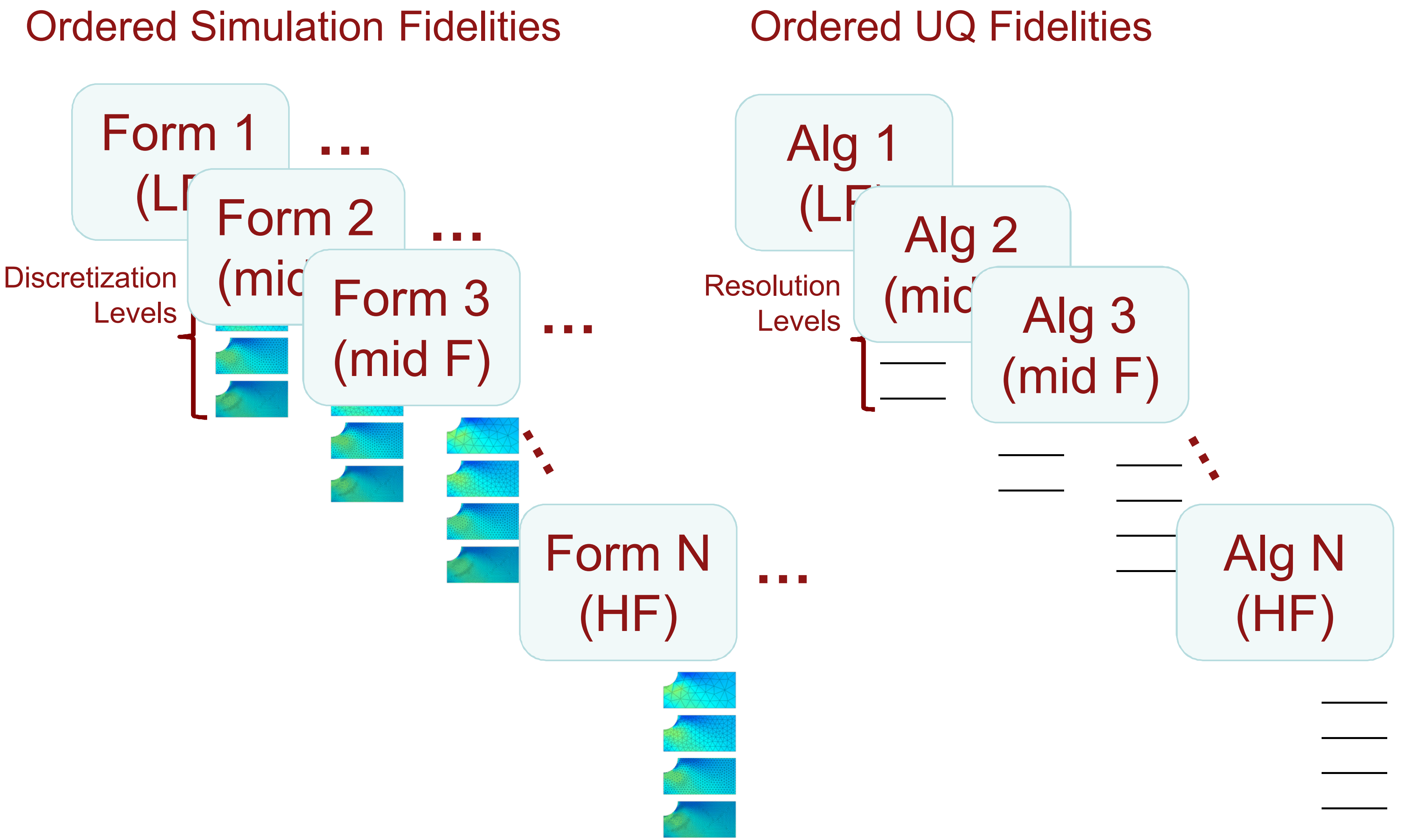
Compressed sensing multifidelity algorithm:

- Target sparsity within the model discrepancy





Generalized model management infrastructure



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

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

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

[Giles, 2008]

Control variate MC – targeting hierarchical model forms

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

[Ng & Willcox, 2014: G is LF model for Q]

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

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

1D steady state diffusion (elliptic PDE)

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

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

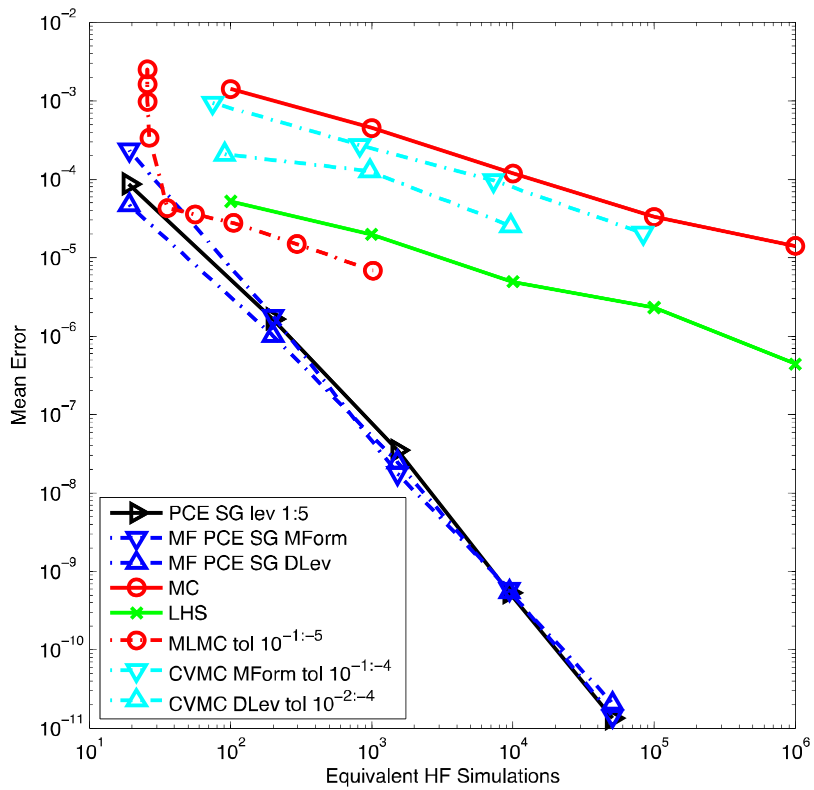
$$a(x;\boldsymbol{\xi}) = a_0(x) + \exp\left(\sigma \sum_{i=1}^{d} \sqrt{\lambda_i}\phi_i(x)\xi_i\right)$$

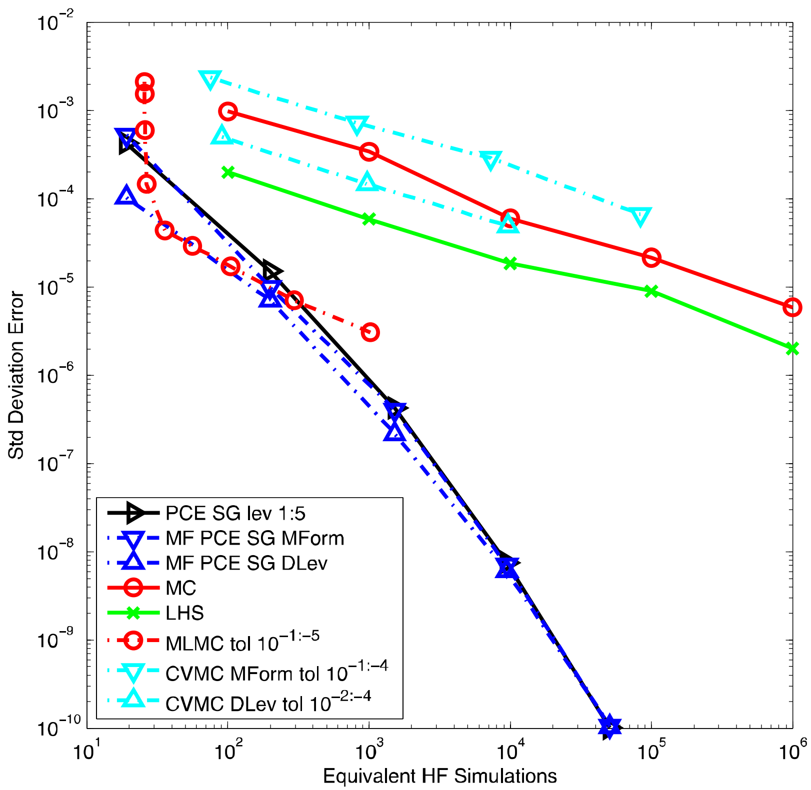
Model forms: covar. kernel + positivity (cosine/off, exp/on) for diffusivity RF

Discretization levels: 5 (poly degree for solution basis)

Dimensionality: 9 *QoI:* 3

Cost model: cubic in spatial, 10x kernel



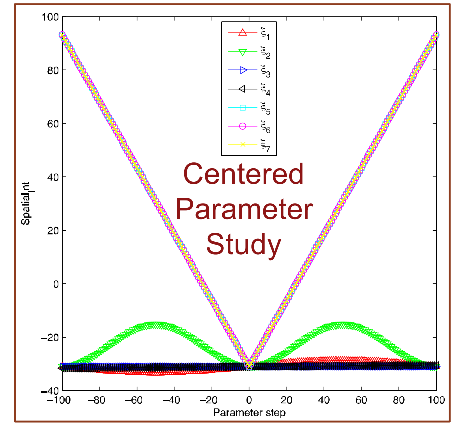


1D transient diffusion (parabolic PDE)

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

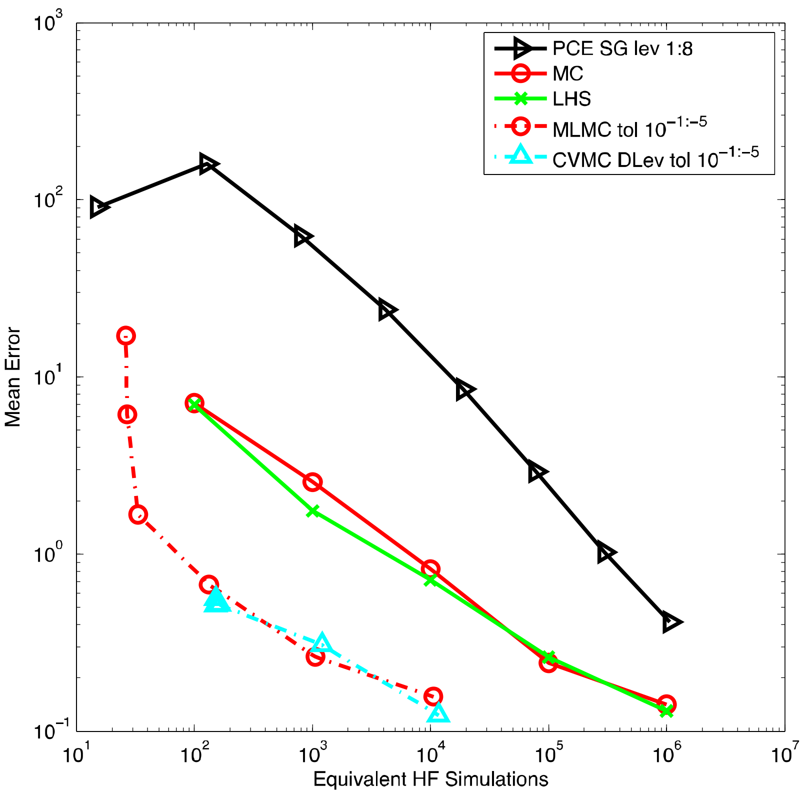
$$u(x,\xi,0) = u_0(x,\xi), \quad t \in [0,t_F] \quad \text{and} \quad \xi \in \Xi \subset \mathbb{R}^d$$

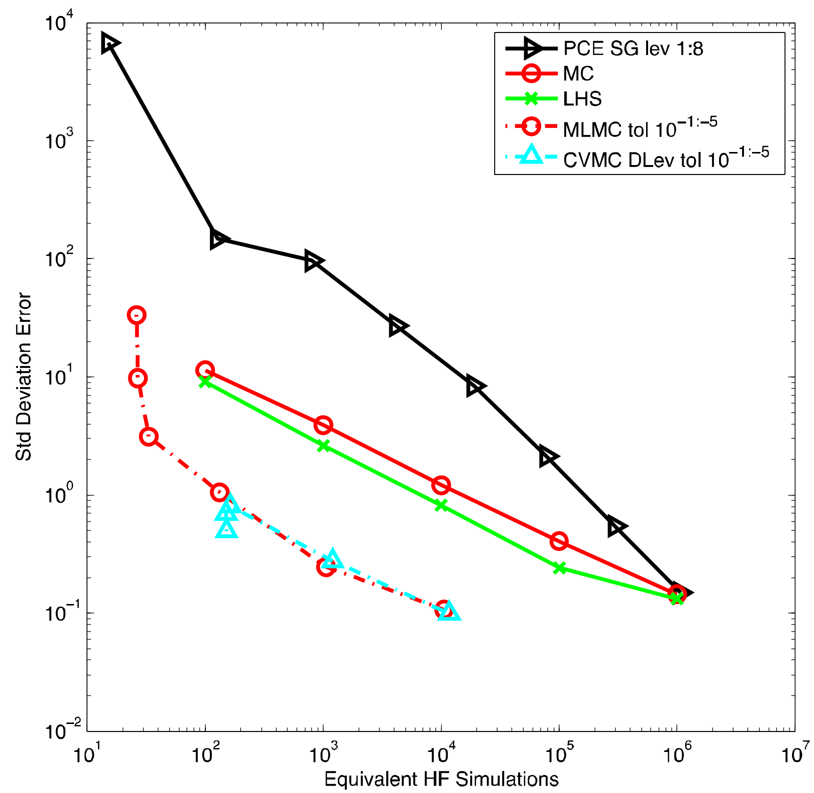
$$u(x,\xi,t)|_{\partial\Omega} = 0.$$



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

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





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-corr:

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

$$\Lambda_l = 1 - \rho_{HL}^2 \frac{1-r_l}{r_l}$$

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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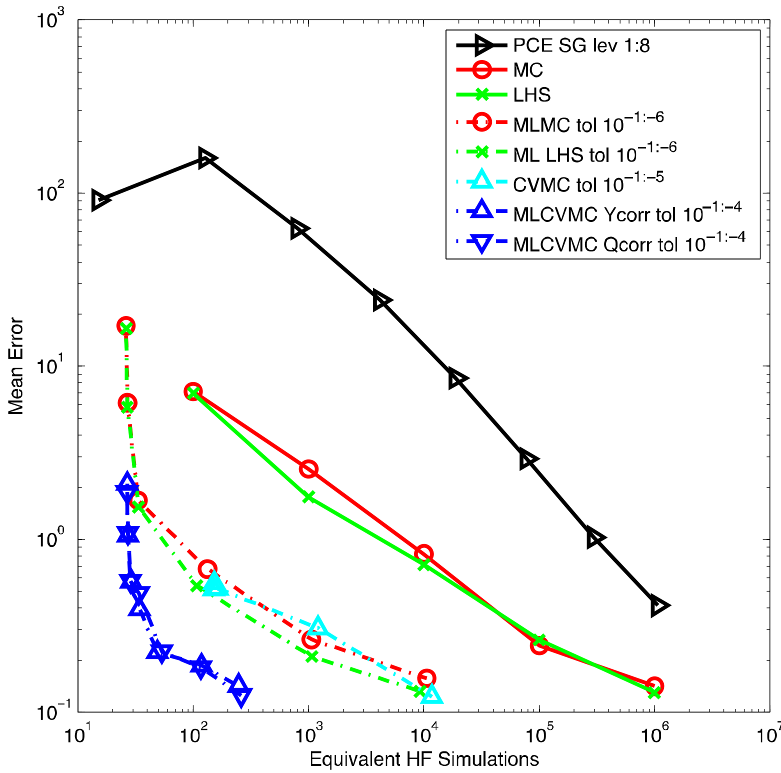
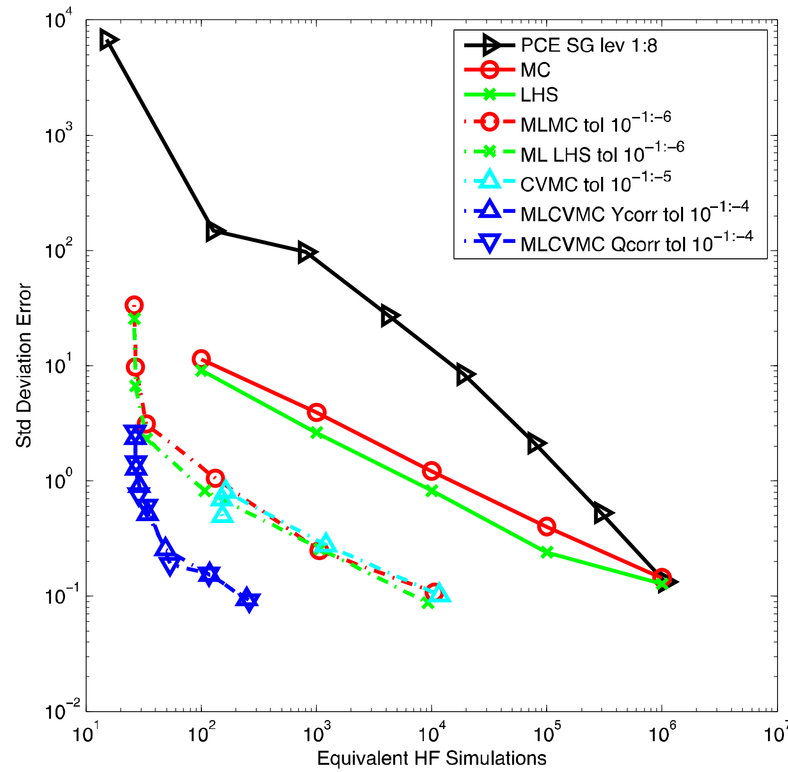
MLCV Y-corr: $$N_\ell^{HF,\star} = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L_{HF}}\left(\frac{\mathbb{V}ar\left(Y_\ell^{HF}\right)\mathcal{C}_\ell^{HF}}{1-\rho_{HL}^2}\Lambda_\ell\right)^{1/2}\right]\sqrt{\left(1-\rho_{HL}^2\right)\frac{\mathbb{V}ar\left(Y_\ell^{HF}\right)}{\mathcal{C}_\ell^{HF}}}$$

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

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





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

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

$$V[\hat{Q}] = \frac{\sigma_Q^2}{\gamma N^{\kappa}} \quad \Rightarrow \quad N_l = \sqrt[\kappa+1]{Var(Y_l) C_l} \sqrt[\kappa]{\frac{2}{\varepsilon^2 \gamma} \sum_{l=0}^{L} \sqrt[\kappa+1]{Var(Y_l) C_l^{\kappa}}}$$

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.

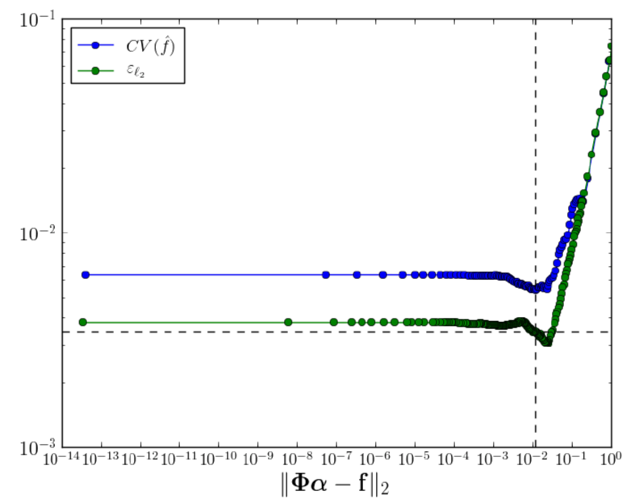
Note: γ does not affect *relative* sample allocation

- Given ε target and omitting $\gamma > 1$, N_l may overshoot (greater MSE reduction than targeted)

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

- For OLS/CS with cross validation, approximate $Var[\hat{Q}]$ from k-fold results
  - σ_Q^2 known from recovered PCE
  - Update κ across level pairs for each ML iteration

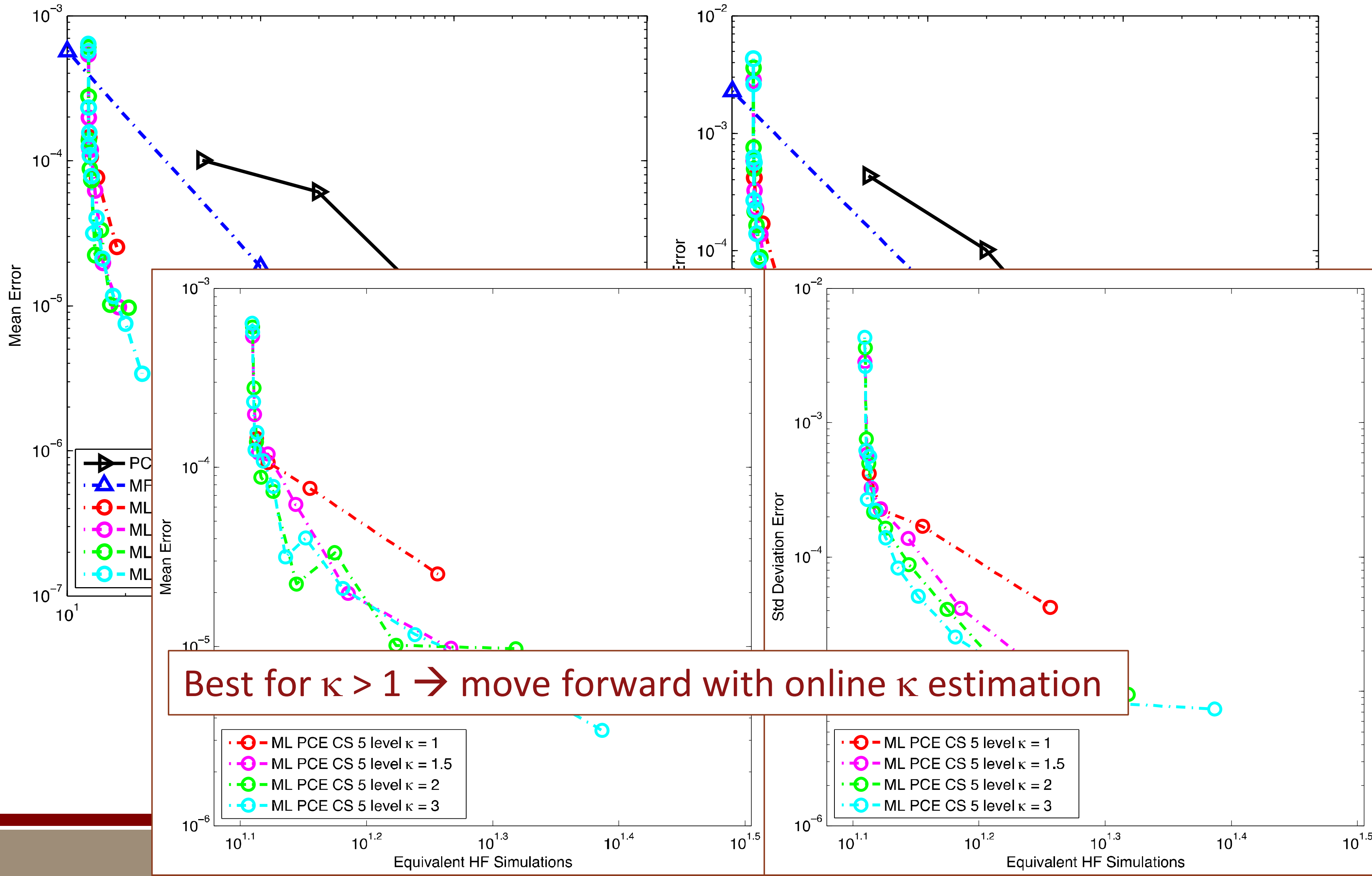
$$\kappa = \log \frac{\sigma_Q^2}{\gamma V[\hat{Q}]} / \log N$$



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

Multilevel PCE Regression: SS diffusion

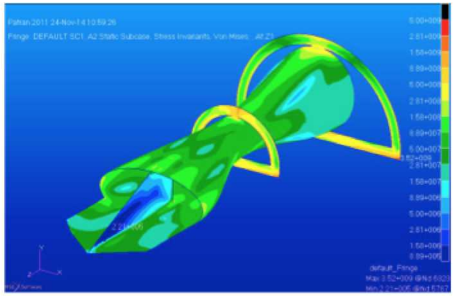
Single and multi-fidelity CS compared to multilevel CS



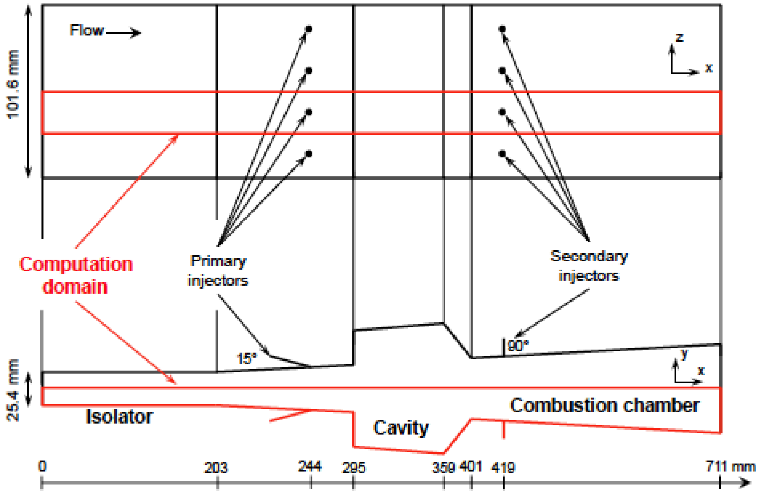
MLMF Deployment for DOE/DOD

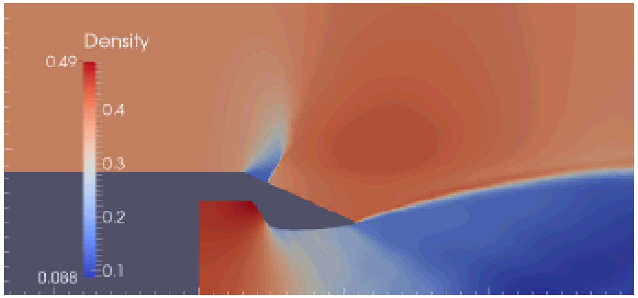
DARPA (EQUiPS)

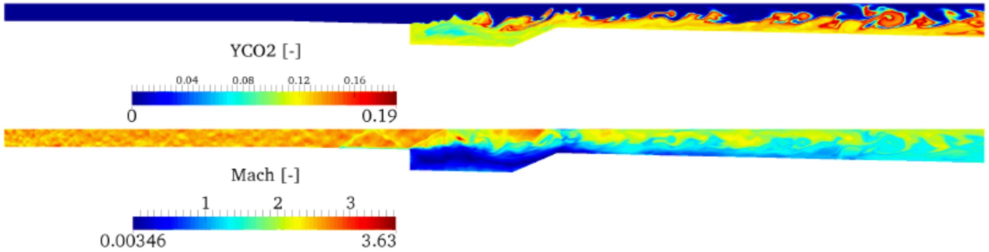
SEQUOIA
High perf UCAV nozzle



ScramjetUQ
HiFIRE hypersonic test facility







A2e HFM Wind (EERE)

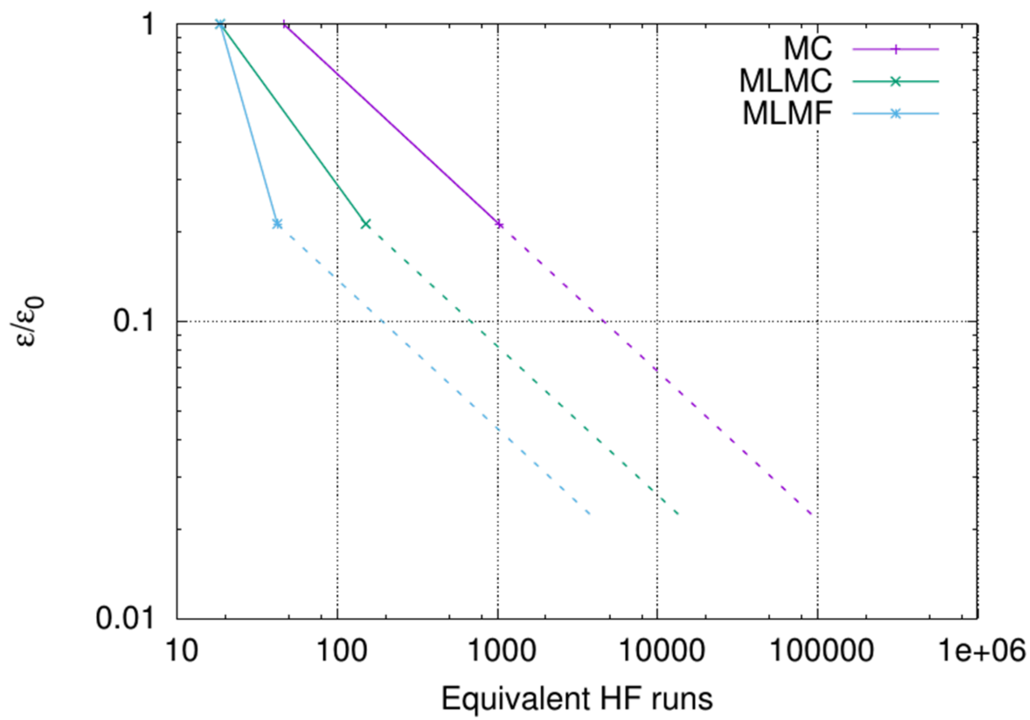
EFRC WastePD (SciDAC QUEST)

Example: Deployment of MLCV MC for DARPA

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, and observed variance distribution across levels

Impact: accurate stats for 3D LES in 24D using only 9 HF evals. (50 equiv HF)

Similar (in flight): MLMF OUU for scramjet; MLMF UQ and OUU for nozzle

Example: Deployment of MLCV MC for DARPA

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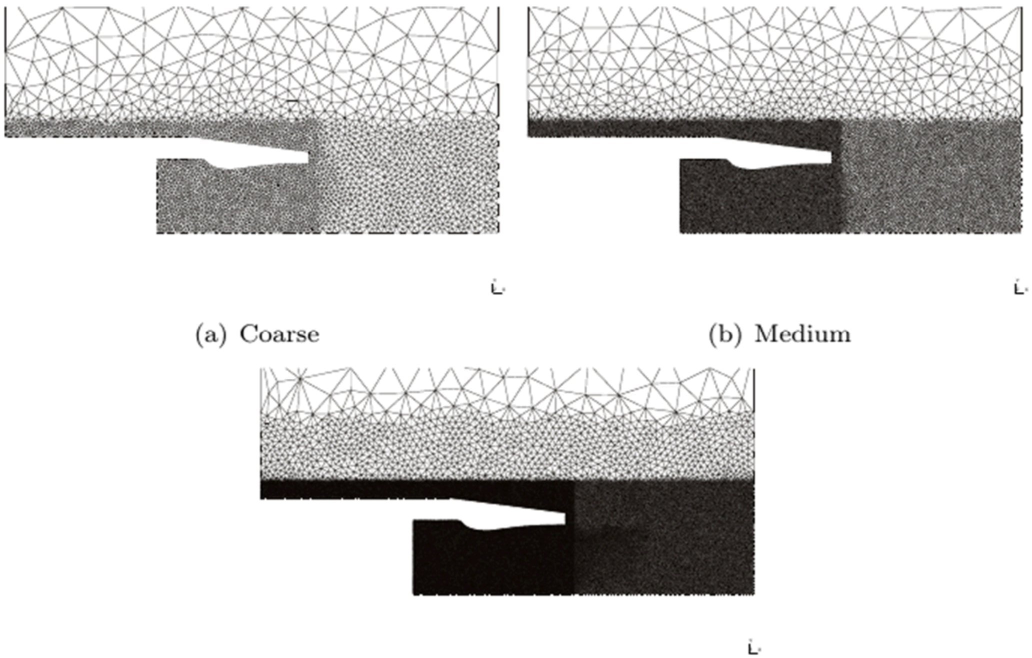
	correlation		Variance reduction [%]	
	Coarse	Fine	Coarse	Fine
$P_{0,mean}$	0.997	0.761	93	50
$P_{0,rms,mean}$	0.875	0.593	72	30
M_{mean}	0.975	0.649	89	36
TKE_{mean}	0.824	0.454	64	17
χ_{mean}	0.450	0.714	19	44

TABLE: Correlations and variance reduction.

	$P_{0,mean}$	$P_{0,rms,mean}$	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.

Deployment of MLCV MC to Nozzle UQ



(a) Coarse (b) Medium (c) Fine

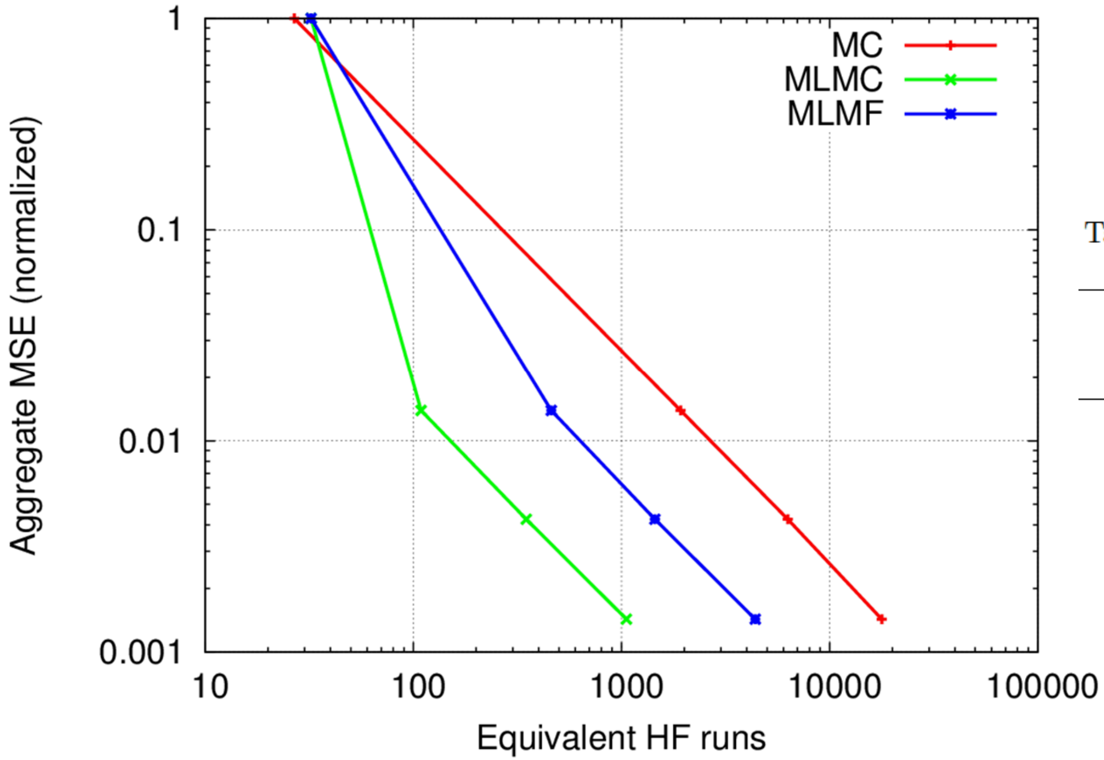
	Triangles
Coarse	6,119
Medium	29,025
Fine	142,124

TABLE: Number of triangles.

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

TABLE: Computational cost.

Deployment of MLCV MC to Nozzle UQ



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

QoI	correlation
Thrust	9.9865e-01
Mech. stresses	4.8106e-03
Thermal stresses	3.7389e-01

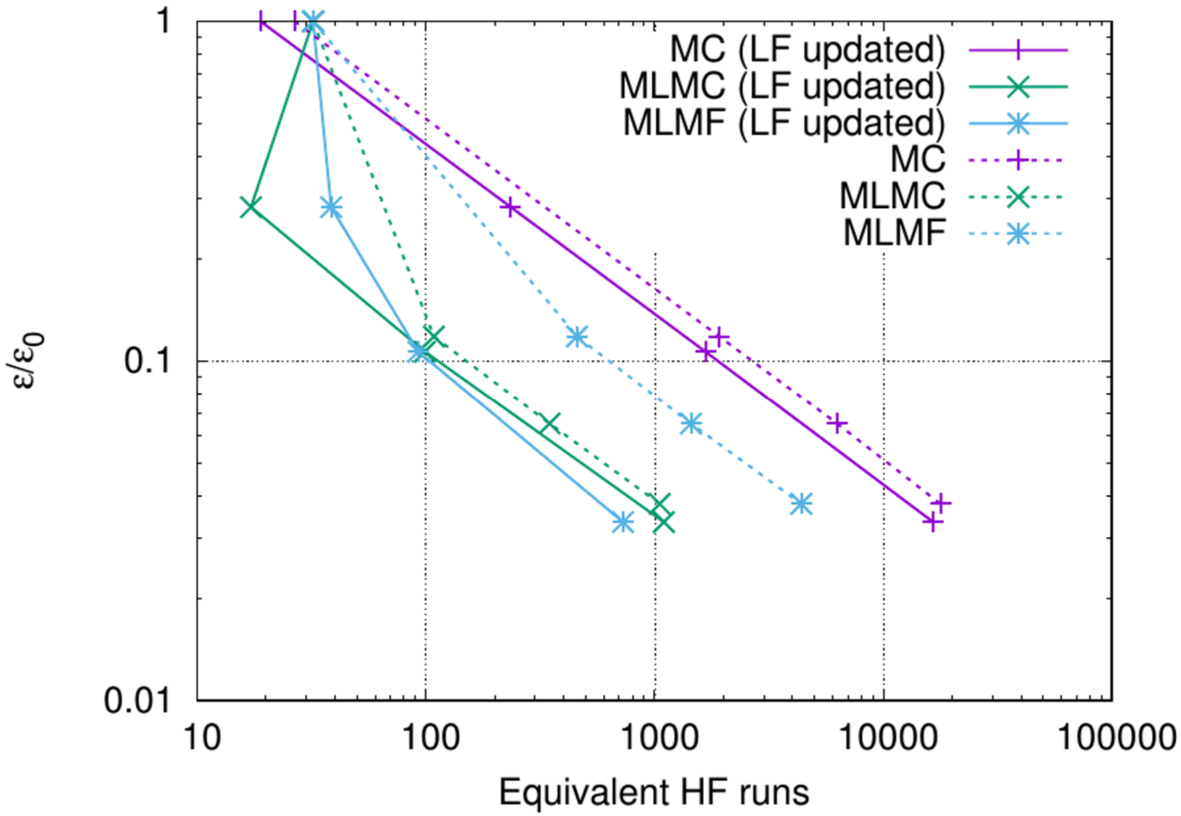
MLMC is effective across MF discretizations, CV is hampered by LF corr

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

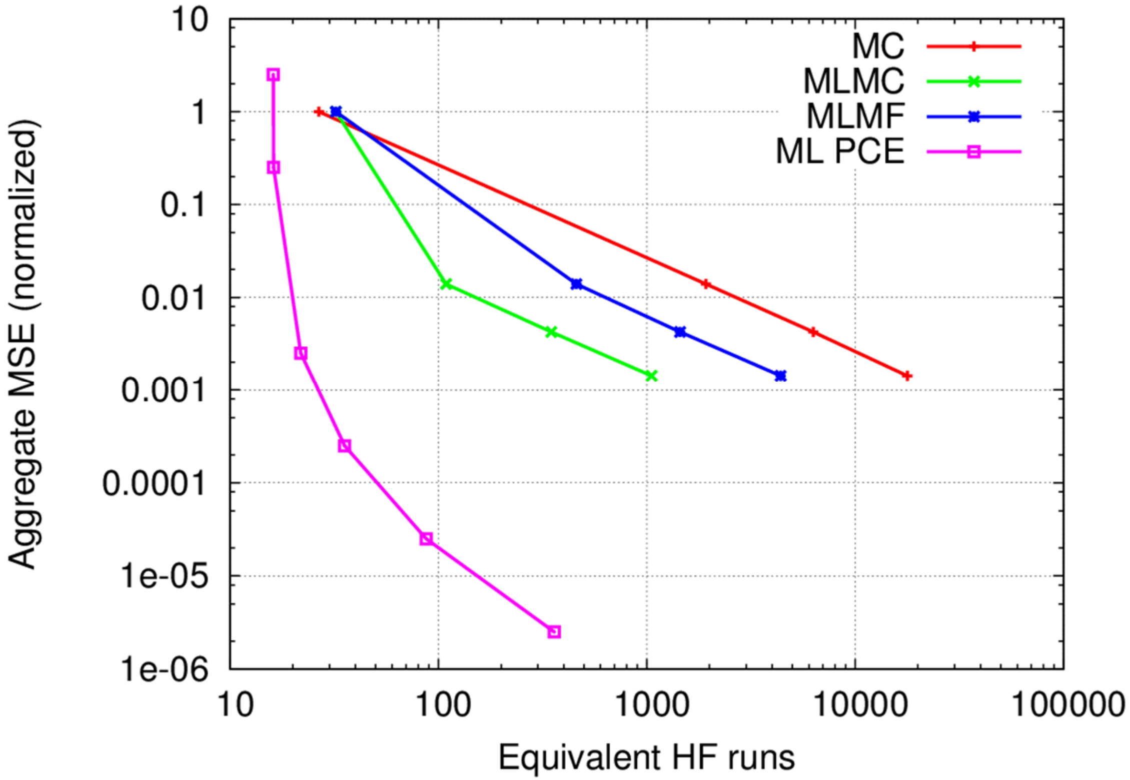
Deployment of MLCV MC to Nozzle UQ

	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

TABLE: Correlations and variance reduction for $\varepsilon^2/\varepsilon_0^2 = 0.001$.



Deployment of ML PCE to Nozzle UQ



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: MLMF PCE, allowing integration of multiple model forms

Multilevel-Multifidelity UQ Summary Points

SEQUOIA/ScramjetUQ multifidelity / multilevel deployments have a rich ensemble of model forms and discretization levels to explore

- Bringing several classes of approaches to bear, which are expected to exhibit differing levels of robustness & efficiency

Multilevel sampling fmwk for cost-optimized variance reduction is quite general

- MLCV MC applies LF control variate for each HF level
- ML LHS: behavior of estimator variance is similar and ML results in additional variance reduction that appears significant
  - In cases where LHS outperforms MC, ML LHS similarly outperforms MLMC
  - Naïve implementation: additional refinements using incremental approaches
- ML PCE: Adds optimal sample allocation to previous spectral stoch MF machinery. Initial prototype appears promising, but multiple verifications/refinements in progress
  - CS solver performance for large N, large candidate P (Vandermonde size)
  - CV and basis adaptation turned off for accelerated study of κ values
    → OMP may be overfitting, mutual coherence requires mitigation

In progress:

- Modified CV approach to improve correlations within MLCVMC
- Explore online estimation of the ML PCE variance conv. rate parameter (κ)
- Expand ML PCE to include CV across fidelities (MLCV PCE)

Optimization Foundational Components for ML and MF:

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

Trust-Region Model Management

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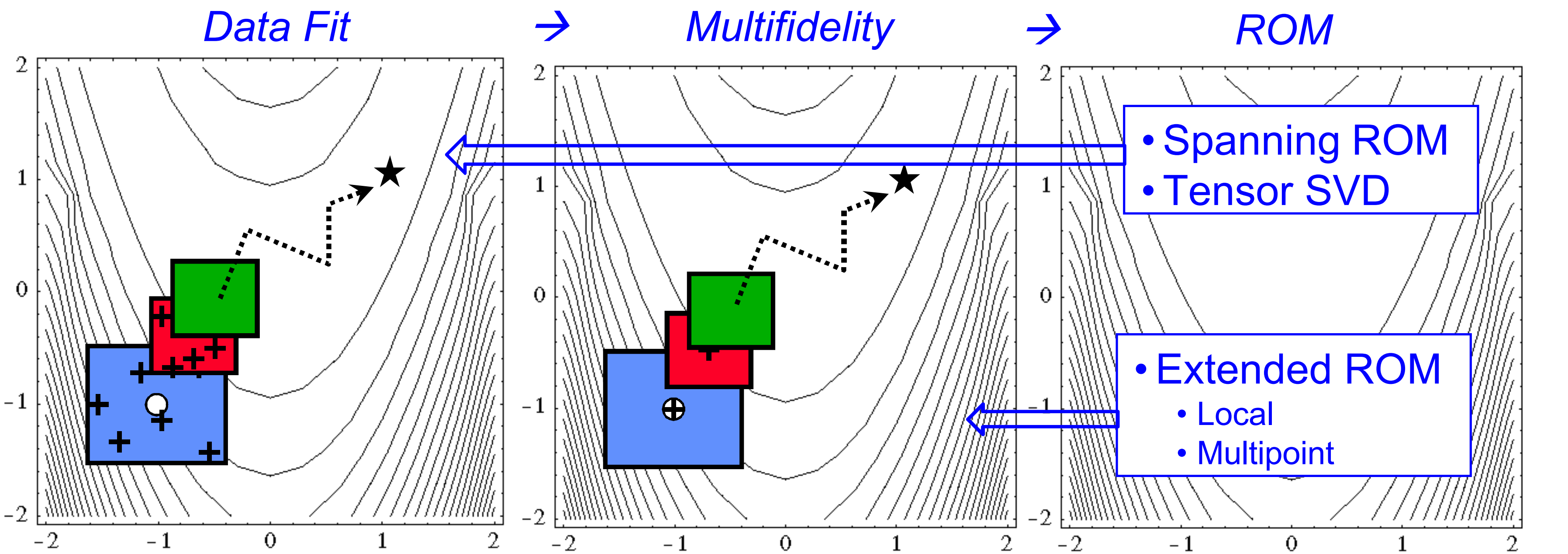


Data fit surrogates:

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

Data fits in SBO

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

Multifidelity surrogates:

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

Multifidelity SBO

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

ROM surrogates:

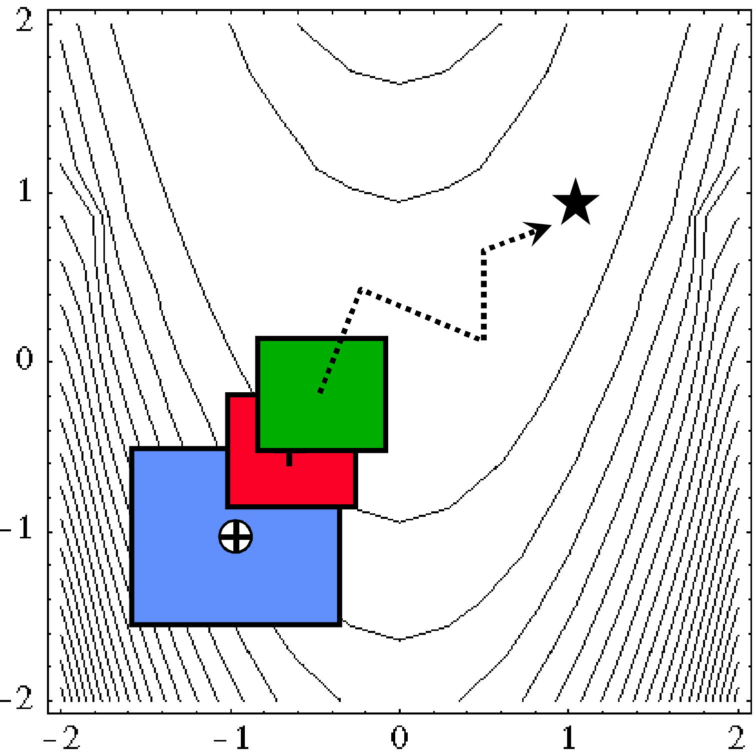
- Spectral decomposition (str. dynamics)
- POD/PCA w/ SVD (CFD, image analysis)

ROMs in SBO

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

TRMM – Multifidelity Case

Sequence of trust regions



Algorithm 2 Compute correction

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

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

if (correction order ≥ 0) **then**

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

end if

if (correction order ≥ 1) **then**

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

end if

if (correction order ≥ 2) **then**

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

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

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

end if

end procedure

Algorithm 3 Apply correction

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

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

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

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

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

Algorithm 4 Compute trust region updates

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

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

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

Multigrid optimization (MG/Opt)

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

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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

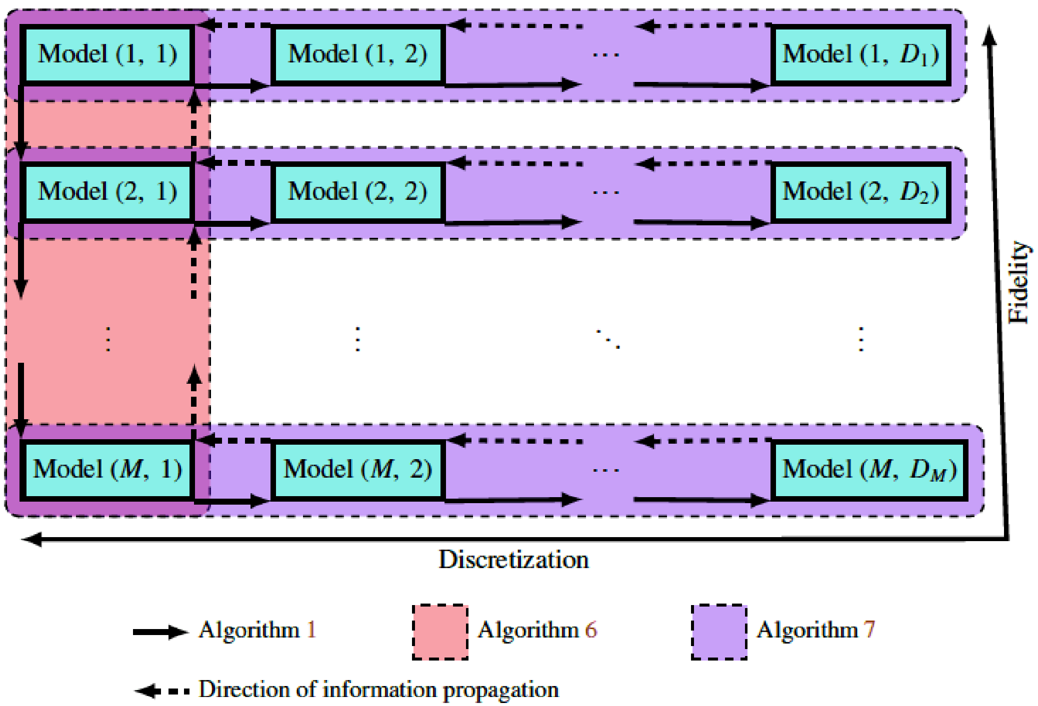
Algorithm 1 Multigrid Optimization

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

TRMM + MG/Opt for Multilevel-Multifidelity Hierarchies

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

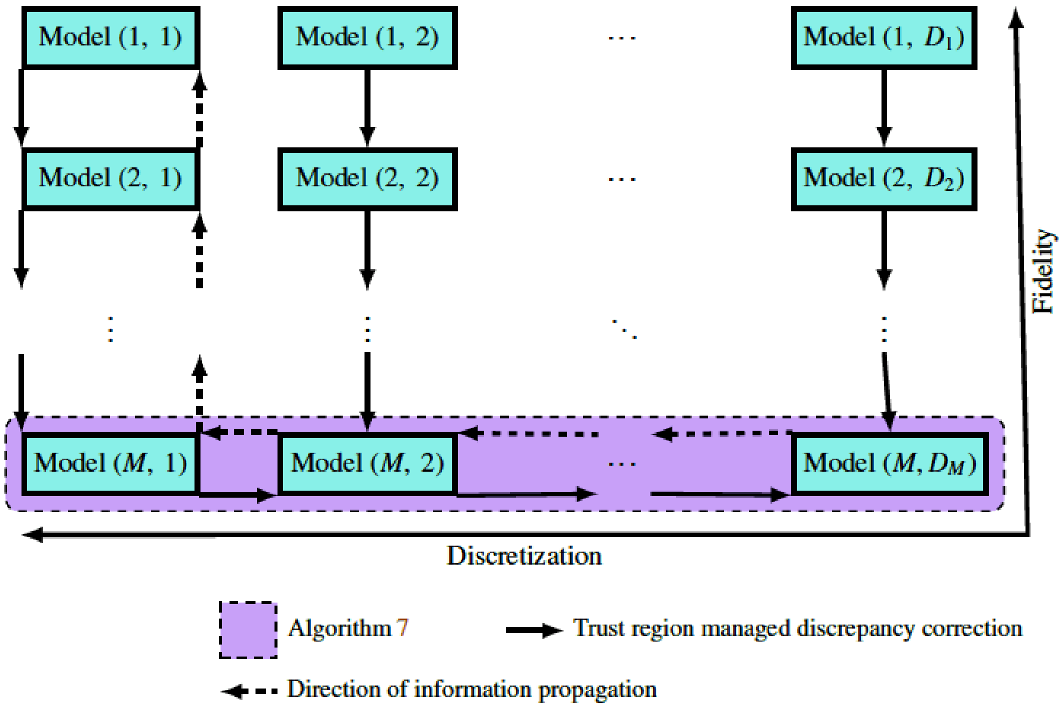
procedure MFOPT(m, $x_0^{(m,1)}$, $f_{\text{CORR}}^{(m,1)}(x)$)
  if $m = M$ **then**
    $x_1^{(m,1)} = \text{MLOPT}(k, 1, x_0^{(m,1)}, f_{\text{corr}}^{(m,1)}(x))$
    return $x_1^{(m,1)}$
  else
    Partially solve: $x_1^{(m,1)} = \text{MLOPT}(m, 1, x_0^{(m,1)}, f_{\text{corr}}^{(m,1)}(x))$
    $x_1^{(m+1,1)}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

- **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

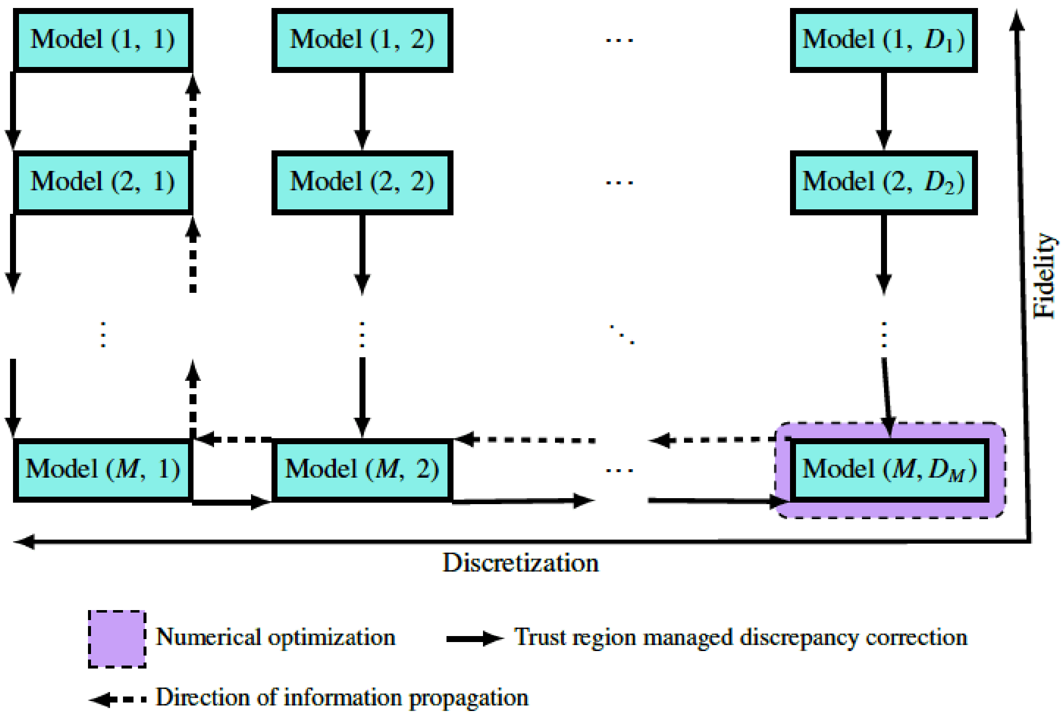
procedure MLMFOPT2
  repeat
    $x_n = x_{n+1}$
    $x_{n+1} =$ MLOPT$(M,\ 1,\ x_n,\ f^{(M,1)}(x))$
    for $d = 1$ to D_M **do**
      RECTR$(m = 1 : M,\ x_n^{(M,d)},\ x_{n+1}^{(M,d)},\ f_{\text{corr}}^{(m,d)}(x))$
    end for
  until convergence
  return x_{n+1}
end procedure

Algorithm 9 Recursive Trust Region Updating

procedure 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: 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

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

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

Computational Experiments with Model Problems

- Target solution profile for steady state diffusion
- Minimize C_D for transonic airfoil

Steady State Diffusion: Achieve Prescribed Solution Profile

HF

$$c_{\text{hi}}(f, u(f)) = \frac{d}{dx}\left(a_{\text{hi}}\frac{du}{dx}\right) + f = 0, \quad x \in (0,1),$$

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

$$a_{\text{hi}} = 2 + \cos(2\pi x) + \boxed{0.4\sin(6\pi x)}.$$

LF

$$c_{\text{low}}(f, u(f)) = \frac{d}{dx}\left(a_{\text{low}}\frac{du}{dx}\right) + f = 0, \quad x \in (0,1),$$

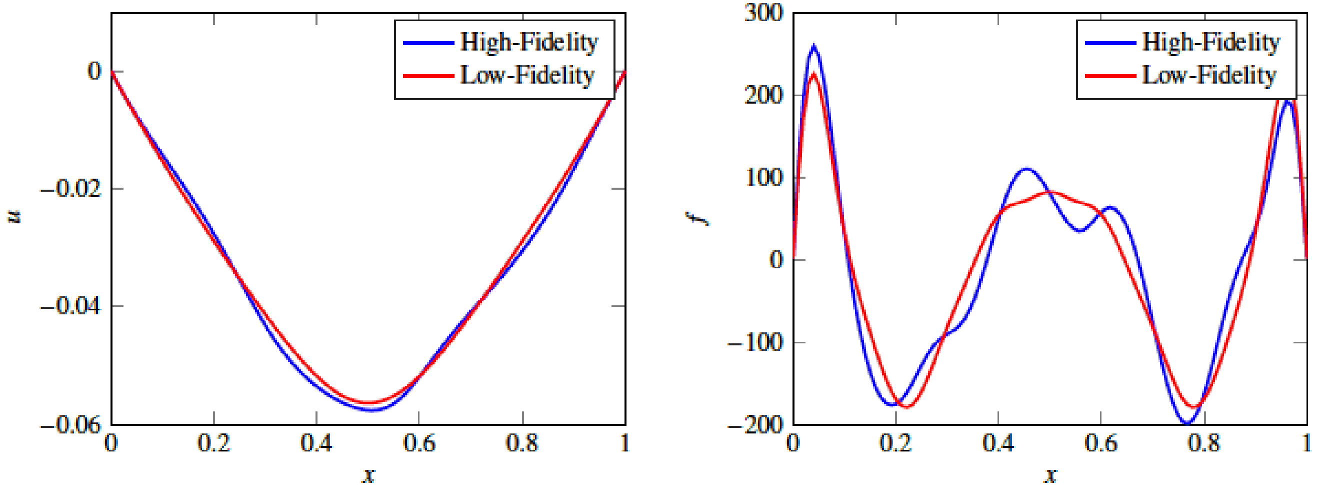
$$u(0) = u(1) = 0,$$

$$a_{\text{low}} = 2 + \cos(2\pi x).$$

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

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

$u^* = \sin^2(2\pi x)$ is the target solution

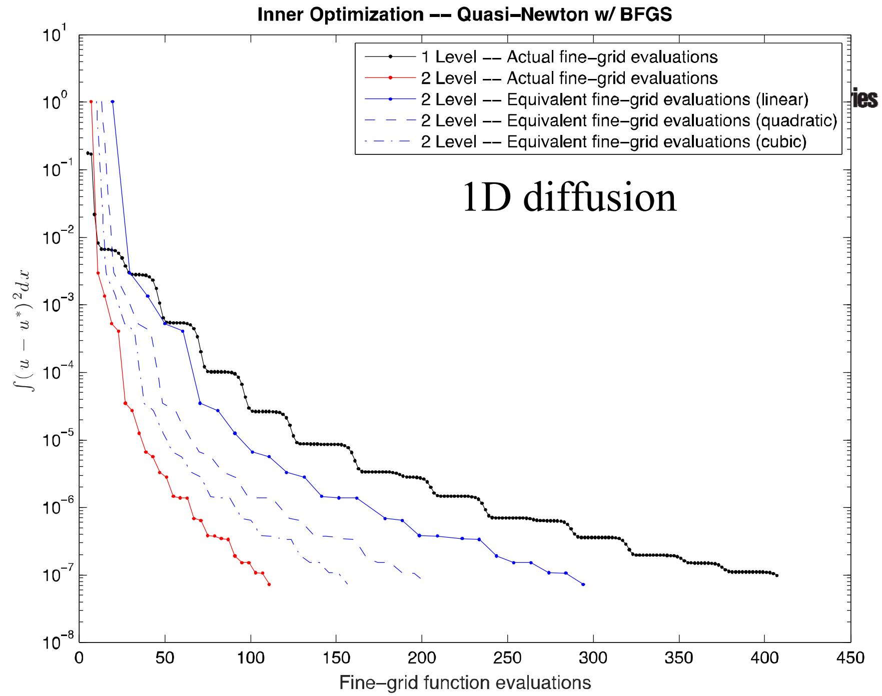


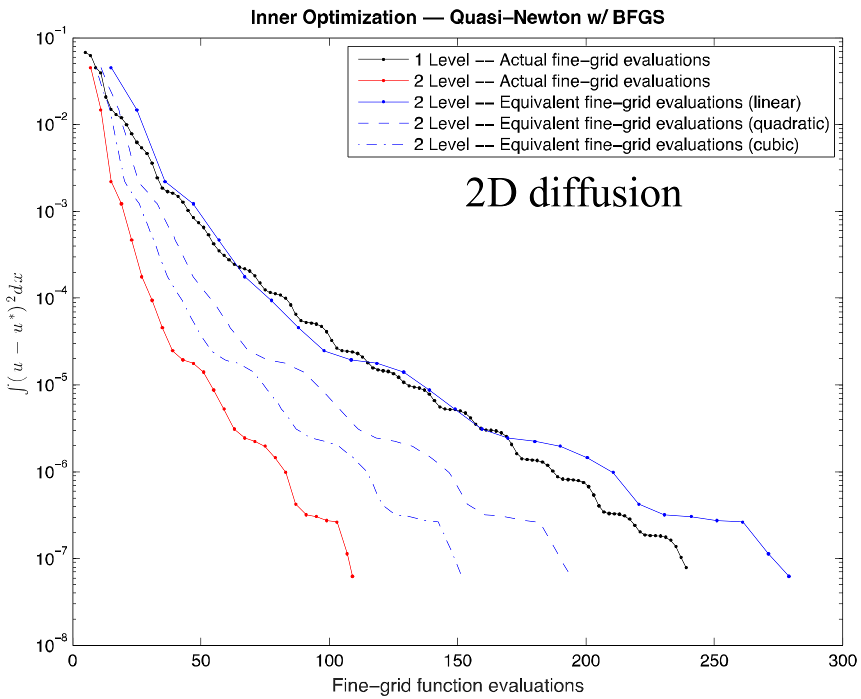
a) ODE solution at initial guess

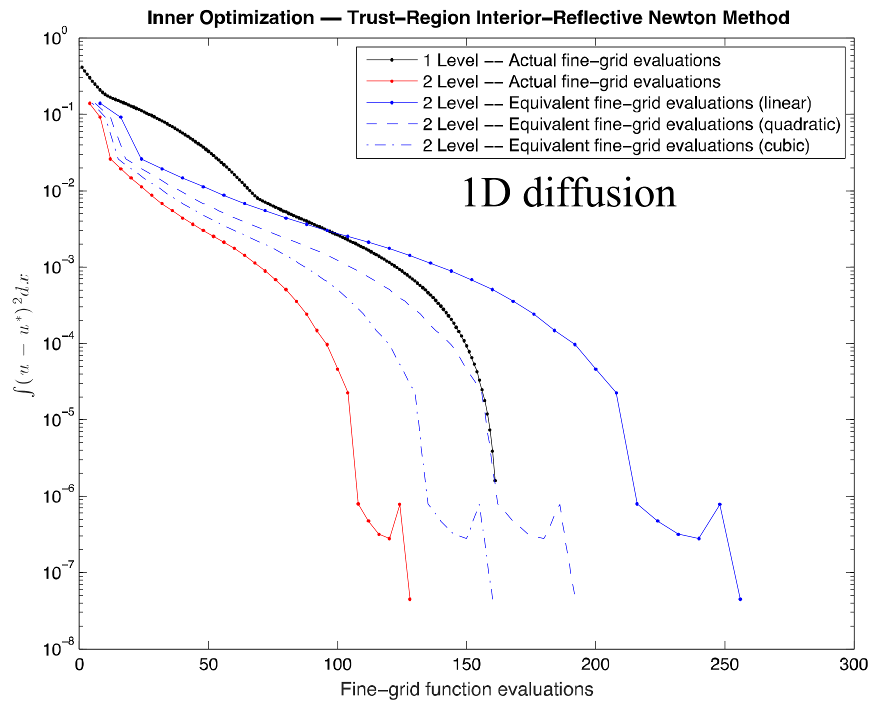
b) Optimal f for both fidelities

MG/Opt for Multilevel

- Coarse and fine discretizations (50, 100 pts) for LF model form
- Adjoint design gradients
- Prolongation/restriction via Lagrange interp.
- MATLAB Optimization Solvers (2)
- Grid scalings (1D and 2D diffusion)
- Solver cost scalings (linear, quadratic, cubic)







Steady State Diffusion

MATLAB Prototypes

a) 1 fidelity and 1 level

	Fine
High-Fidelity	229

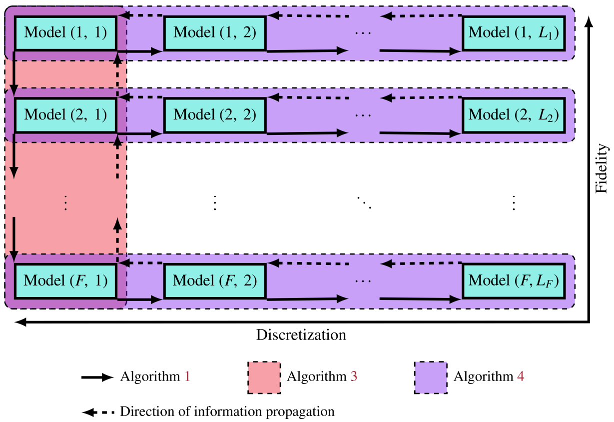
b) 1 fidelity and 2 levels

	Fine	Coarse
High-Fidelity	112	146

c) 2 fidelities and 2 levels

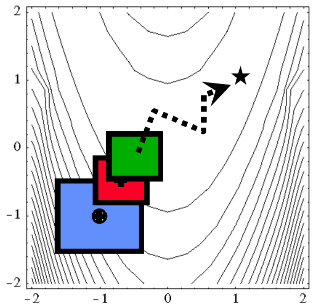
	Fine	Coarse
High-Fidelity	65	82
Low-Fidelity	26	29

Initial formulation: nested multigrid



Dakota: NPSOL & TRMM

	LF evals	HF evals	Objective
Single fidelity	–	244	1.07e-07
Bi-Fidelity 1^{st}-order	9163	80	1.56e-07



Transonic Airfoil Design

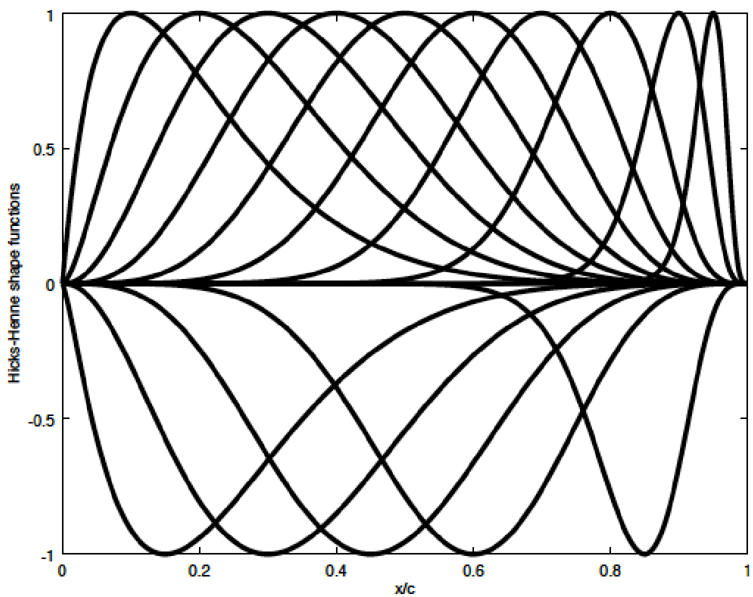
SU2 for transonic flow over a NACA 0012 airfoil
Mach number is 0.8

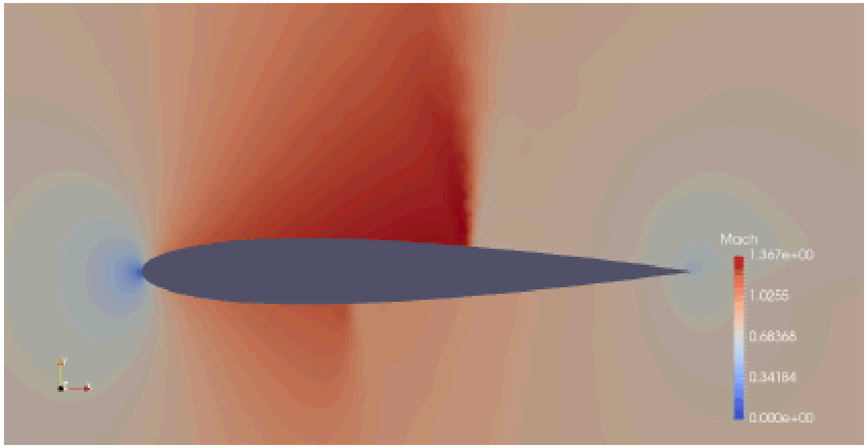
LF = Euler:

	Number of elements	Cost (sec)
Coarse	4,611	6
Medium	6,131	13
Fine	32,626	66

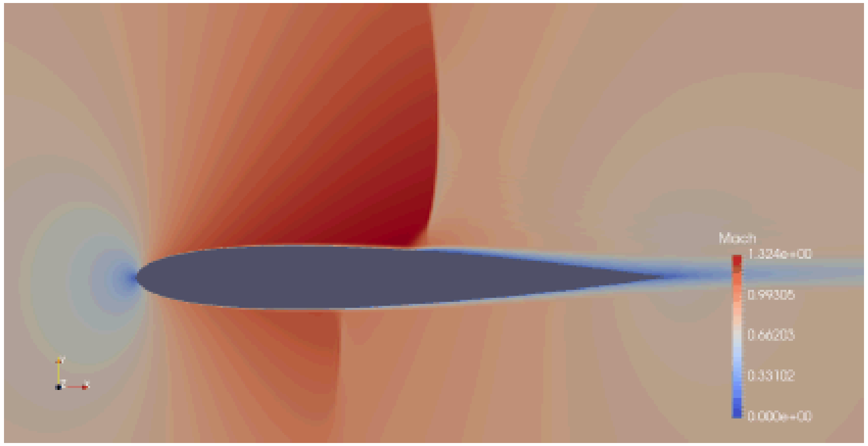
HF = RANS: viscous C-grid with 140,768 cells (coarse) or 319,859 cells (fine)

Design: Hicks Henne shape fns





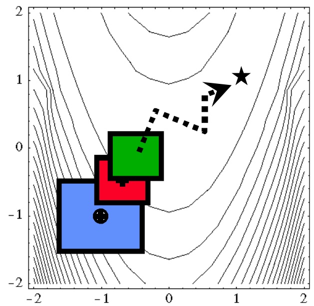
a) Euler fine grid, C_D = 0.0168 (baseline)



b) RANS-SA coarse grid, C_D = 0.0254 (baseline)

Transonic Airfoil Design: Minimize Drag, Preserve Lift

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

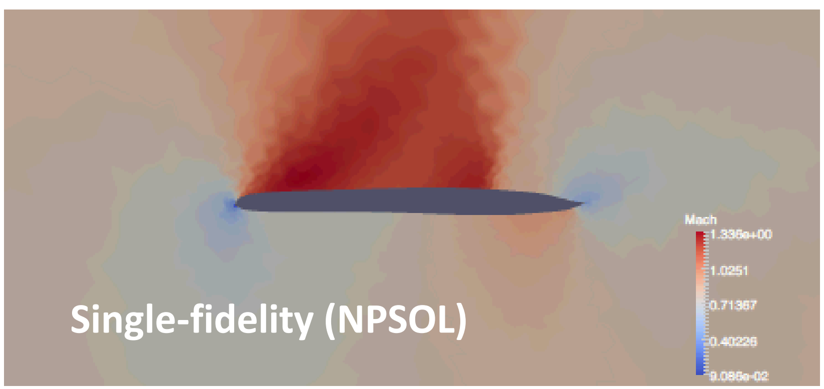


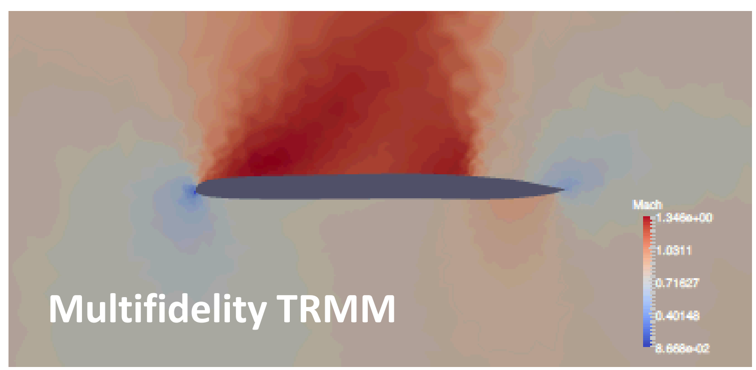
Algorithm 9 Recursive Trust Region Updating

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	–	–	–	0.1034	0.8012
Single fidelity	–	–	2697	0.06493	0.8012
TRMM 1st-order	29641	1874	197	0.06920	0.8475





Multifidelity DUU Deployment for Robust Design

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

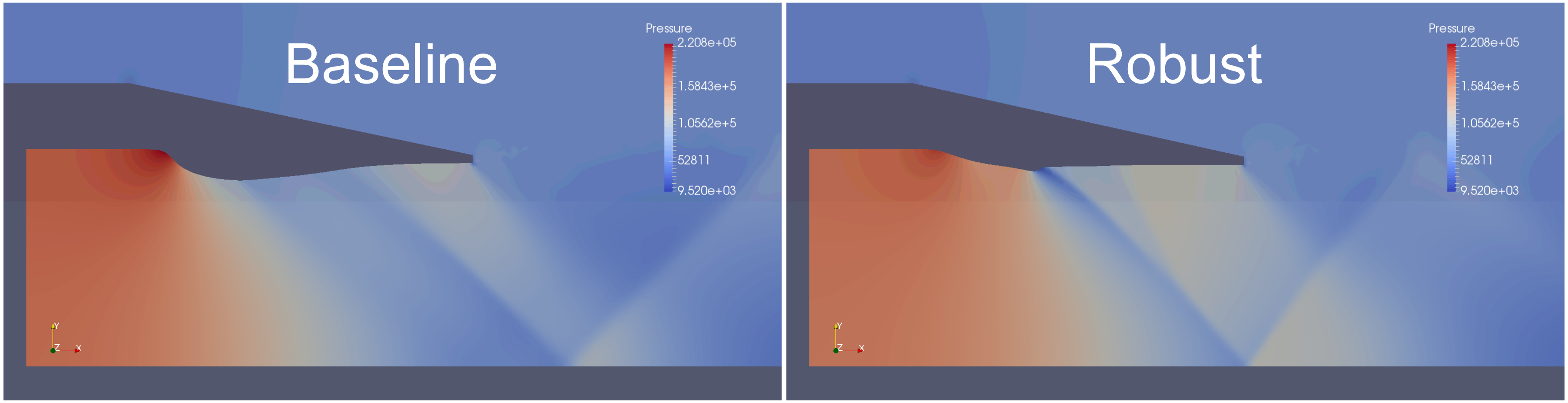
- 1st-order consistent TRMM w/ numerical grads
- 7 random vars
- 21 B-spline + 8 thickness design vars

Trust region cycles

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

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & \mathbb{V}[\ T\ ] \\ \text{subject to} \quad & \mathbb{E}[\ W\ ] \le \overline{W} \\ & \mathbb{E}[\ T\ ] \ge \overline{T} \\ & \mathbb{E}[\ \|T_w\|\ ] \le \overline{T}_w \\ & \mathbb{E}[\ \|\sigma\|\ ] \le \overline{\sigma} \end{aligned}$$

+bounds, linear cons.



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 recursive optimization schemes that exploit the full model ensemble

- MG/Opt and TRMM used as foundational algorithms for one hierarchy dimension
- Proposed MLMF approaches recurse across both multilevel + multifidelity dimensions:
  - Nested MG/Opt, Trust-region managed multigrid, Nested TRMM
- 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

MATLAB prototypes + Dakota production code being tested on model problems

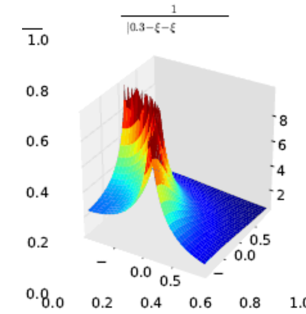
- Steady state diffusion targeting a prescribed solution profile
- Transonic airfoil optimization targeting minimal drag for prescribed lift
- Initial results point to benefits in interfacing optimizers exclusively at LF/coarse levels
  - MG/Opt tends to spread evaluations more evenly across its hierarchy
  - TRMM approach interfaces optimizers only with the least expensive model, relying on more expensive models only for validation and correction estimation
  - Prototype of MLMF 1 → Production implementations of MLMF 2 & 3

Extra Slides

Emphasis on Scalable Methods for High-fidelity UQ on HPC

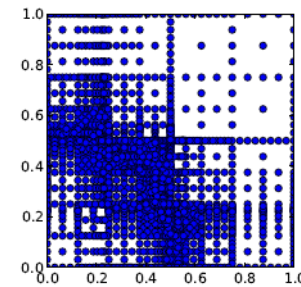
Key Challenges:

- Severe simulation budget constraints (e.g., a handful of HF runs)
- Moderate to high-dimensional in random variables: O(10^1) to O(10^2) [post KLE]
- Compounding effects:
  - Mixed aleatory-epistemic uncertainties (→ nested iteration)
  - Requirement to evaluate probability of rare events (e.g., safety criteria)
  - Nonsmooth responses (→ difficulty with fast converging spectral methods)



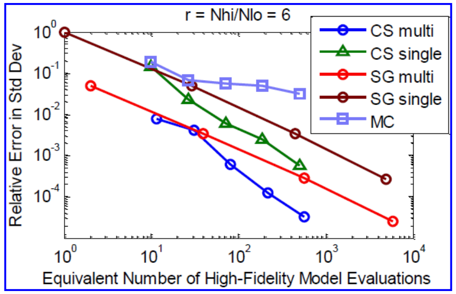
Core (Forward) UQ Capabilities:

- Sampling methods: MC, LHS, QMC, et al.
- Reliability methods: local (MV, AMV+, FORM, …), global (EGRA, GPAIS, POFDarts)
- Stochastic expansion methods: polynomial chaos, stochastic collocation
- Epistemic methods: interval estimation, Dempster-Shafer evidence



Research Thrusts:

- Compute dominant uncertainty effects despite key challenges above
- Emphasize scalability and exploitation of structure
  - Adaptivity, Adjoints, Sparsity, Dimension reduction
- Compound efficiency, address complexity w/ component-based approach
  - Multilevel-Multifidelity, Bayesian inference, Mixed A-E, OUU
- Position UQ for next generation architectures
  - Concurrent sub-iteration, fault-tolerance, AMT generalizations



Elliptic PDE with FEM

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

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

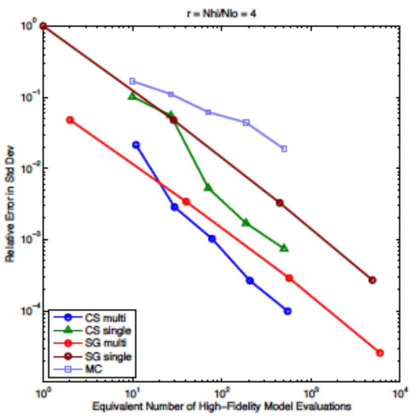
$$C_{\kappa\kappa}(x,x') = \exp\left[-\left(\frac{x-x'}{0.2}\right)^2\right]$$

QoI is u(0.5, ω).

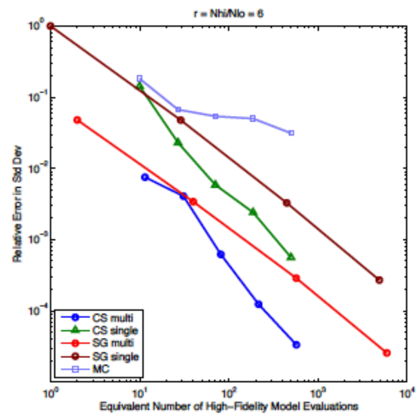
LF = coarse spatial grid with 50 states.

HF = fine spatial grid with 500 states.

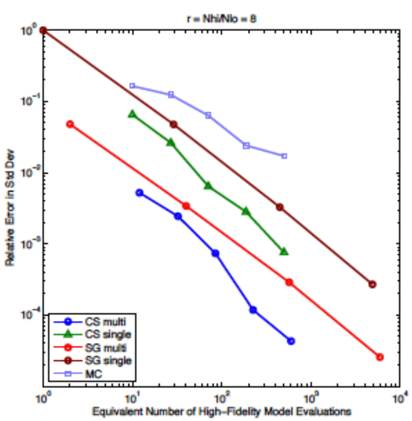
r_{work} = 40.



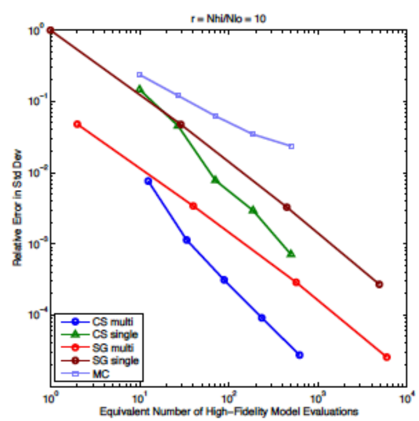
(a) $\rho_{\text{points}} = 4$



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



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



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

This is a particularly good case because it is multilevel, rather than general multifidelity. LF model is excellent predictor of HF results.

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

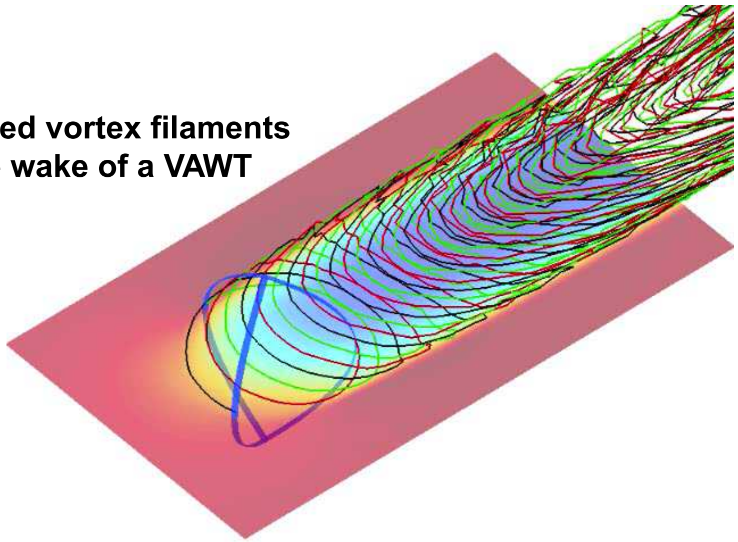
- lower complexity than HF model (sparse grid)
  → faster conv rate (affects exponent)
- lower variance than HF model
  → reduction in initial error (affects leading const)
- more sparse than HF model (CS)
  → fewer samples to recover coefficients

This existing multifidelity machinery is useful both as a benchmark and as a foundation for multilevel PCE approaches.

Multifidelity UQ: VAWT Gust Response

Low fidelity

CACTUS: Code for Axial and Crossflow TUrbine Simulation

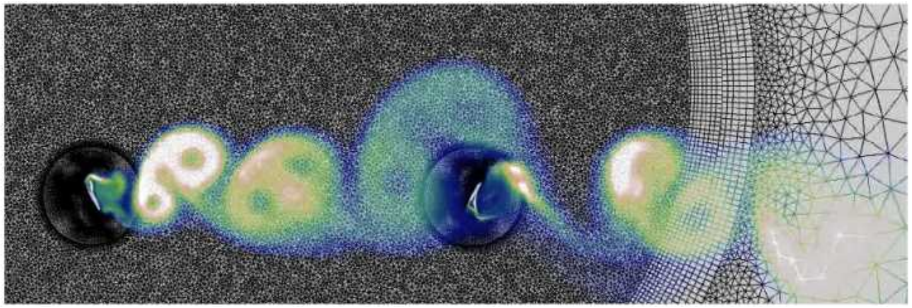


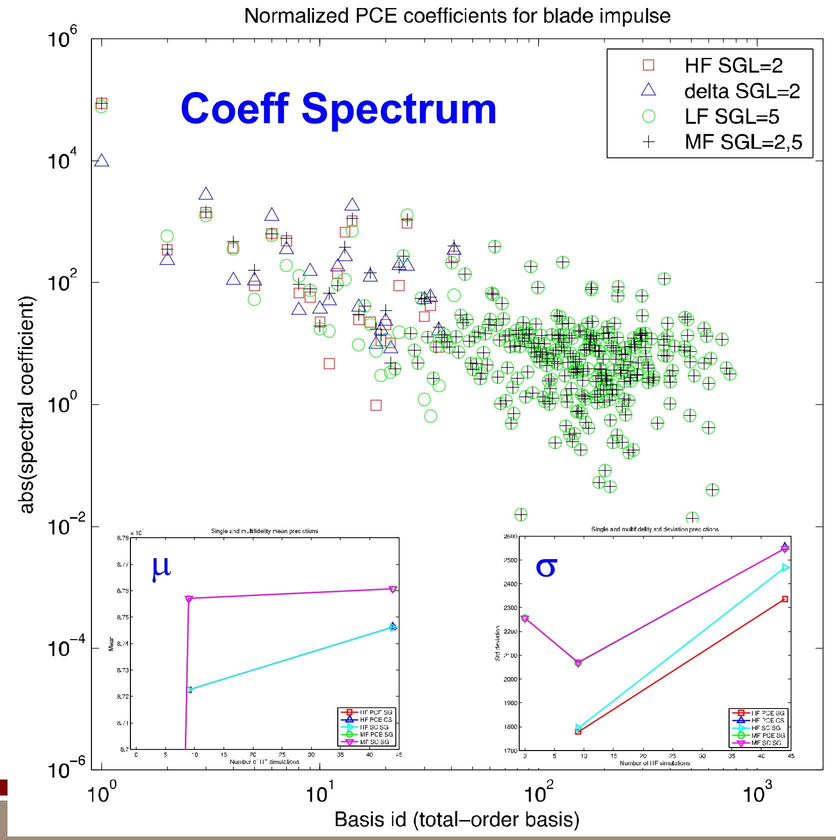
Computed vortex filaments in the wake of a VAWT

Vertical-axis Wind Turbine (VAWT)

High fidelity

DG formulation for LES

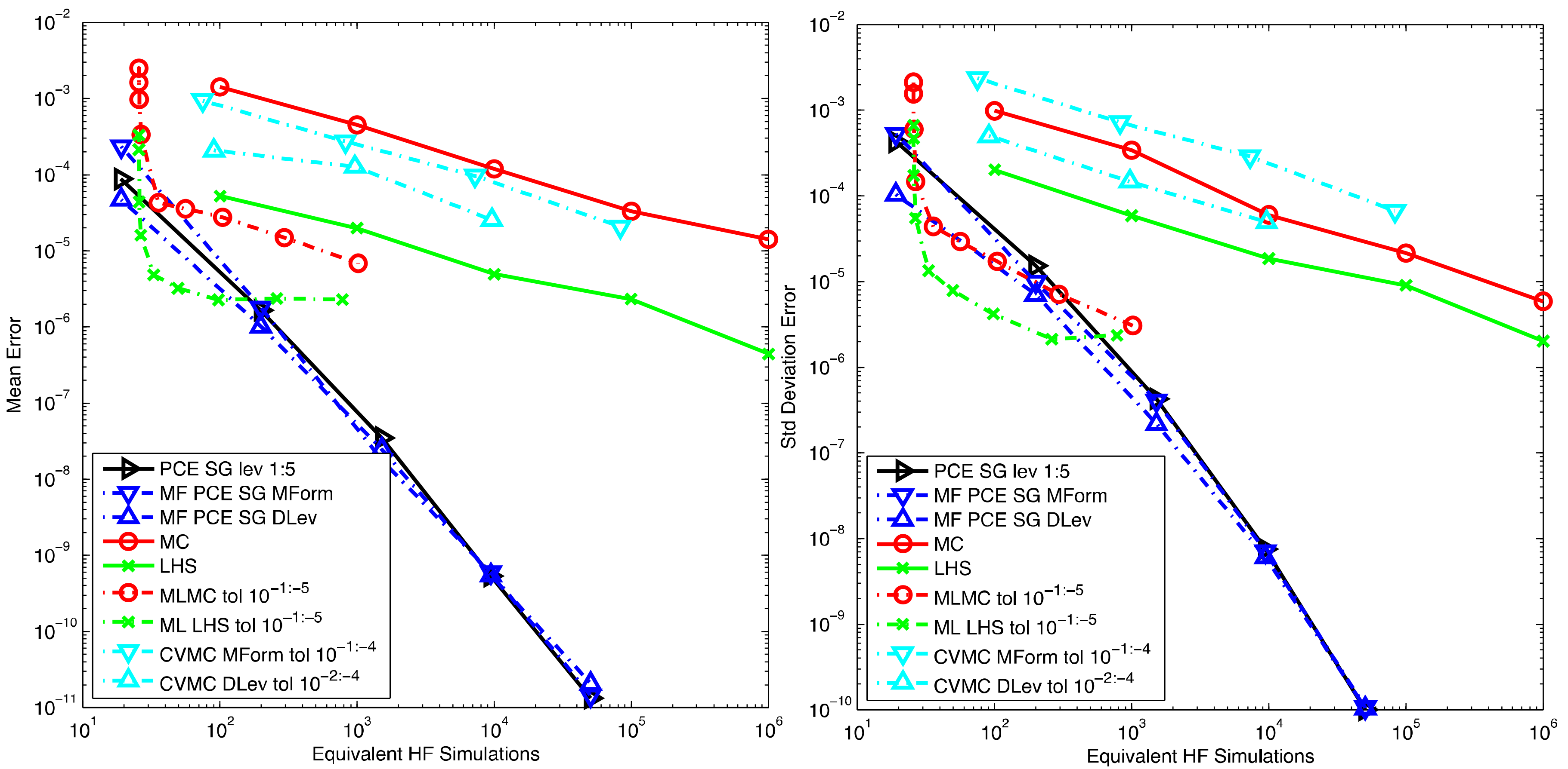




Multilevel LHS: 1D steady state diffusion

Pick $\kappa = \gamma = 1$ →
(same as MC)

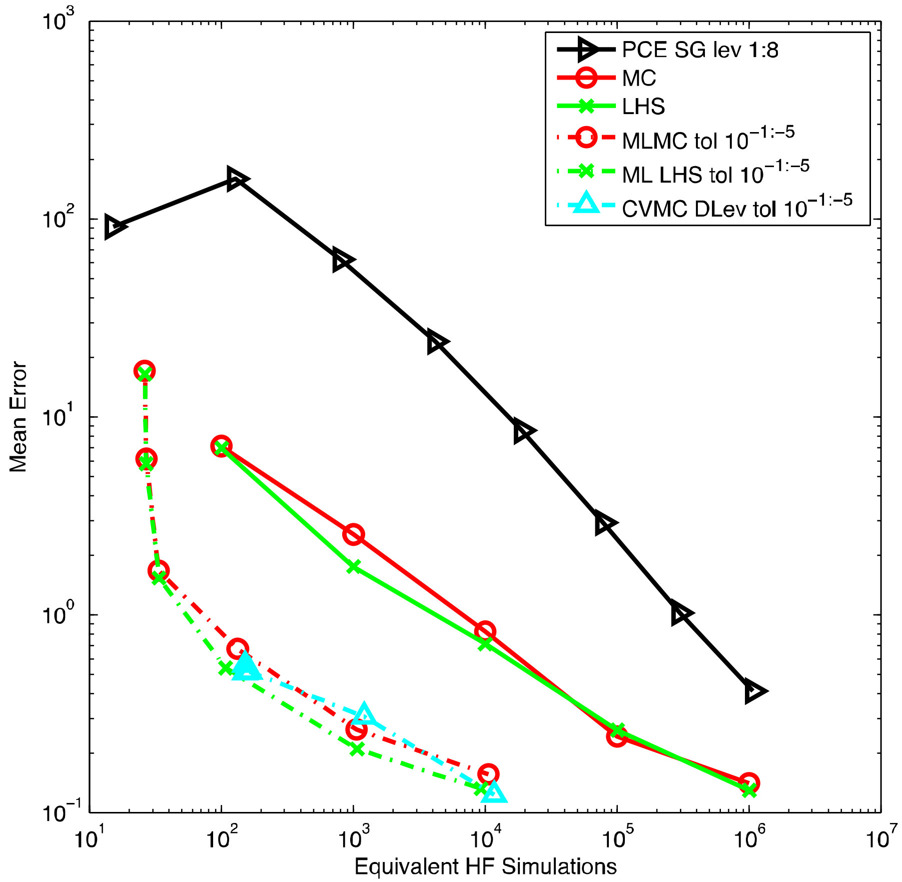
$$N_\ell = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L}\left(\mathbb{V}ar\left(Y_k\right)\mathcal{C}_k\right)^{1/2}\right]\sqrt{\frac{\mathbb{V}ar\left(Y_\ell\right)}{\mathcal{C}_\ell}}.$$

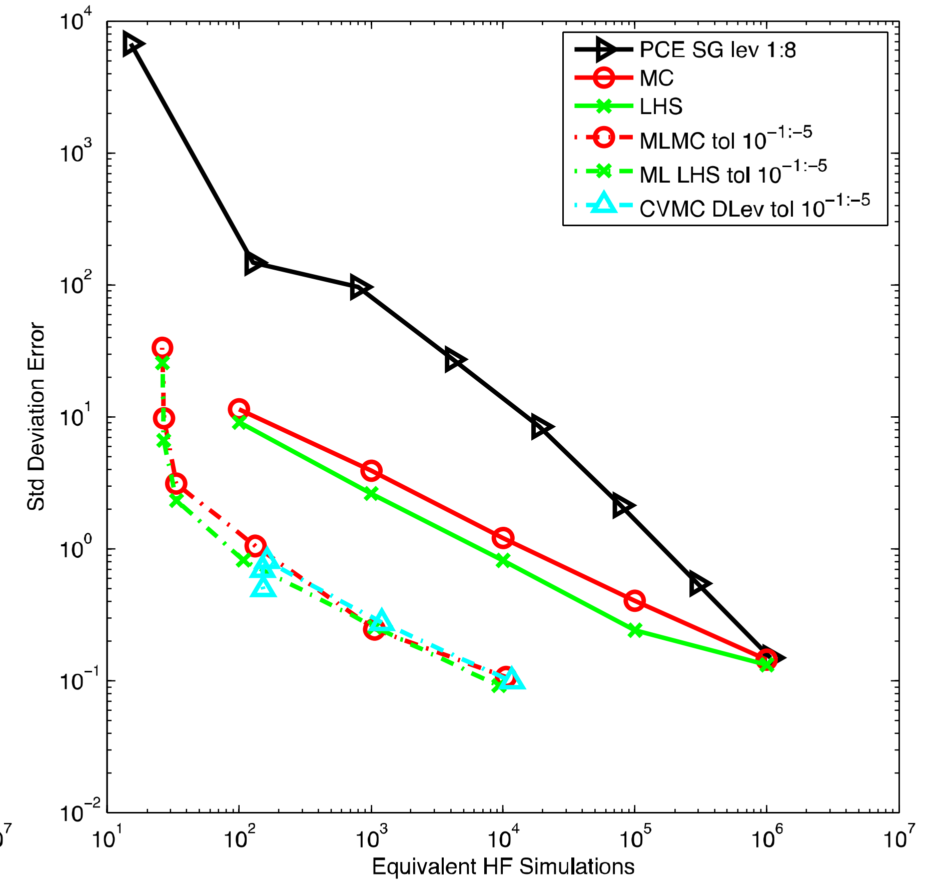


Multilevel LHS: 1D transient diffusion / heat equation

Pick $\kappa = \gamma = 1$ →
(same as MC)

$$N_\ell = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L}\left(\mathbb{V}ar\left(Y_k\right)\mathcal{C}_k\right)^{1/2}\right]\sqrt{\frac{\mathbb{V}ar\left(Y_\ell\right)}{\mathcal{C}_\ell}}.$$





Multilevel Control Variate MC: 1D steady state diffusion

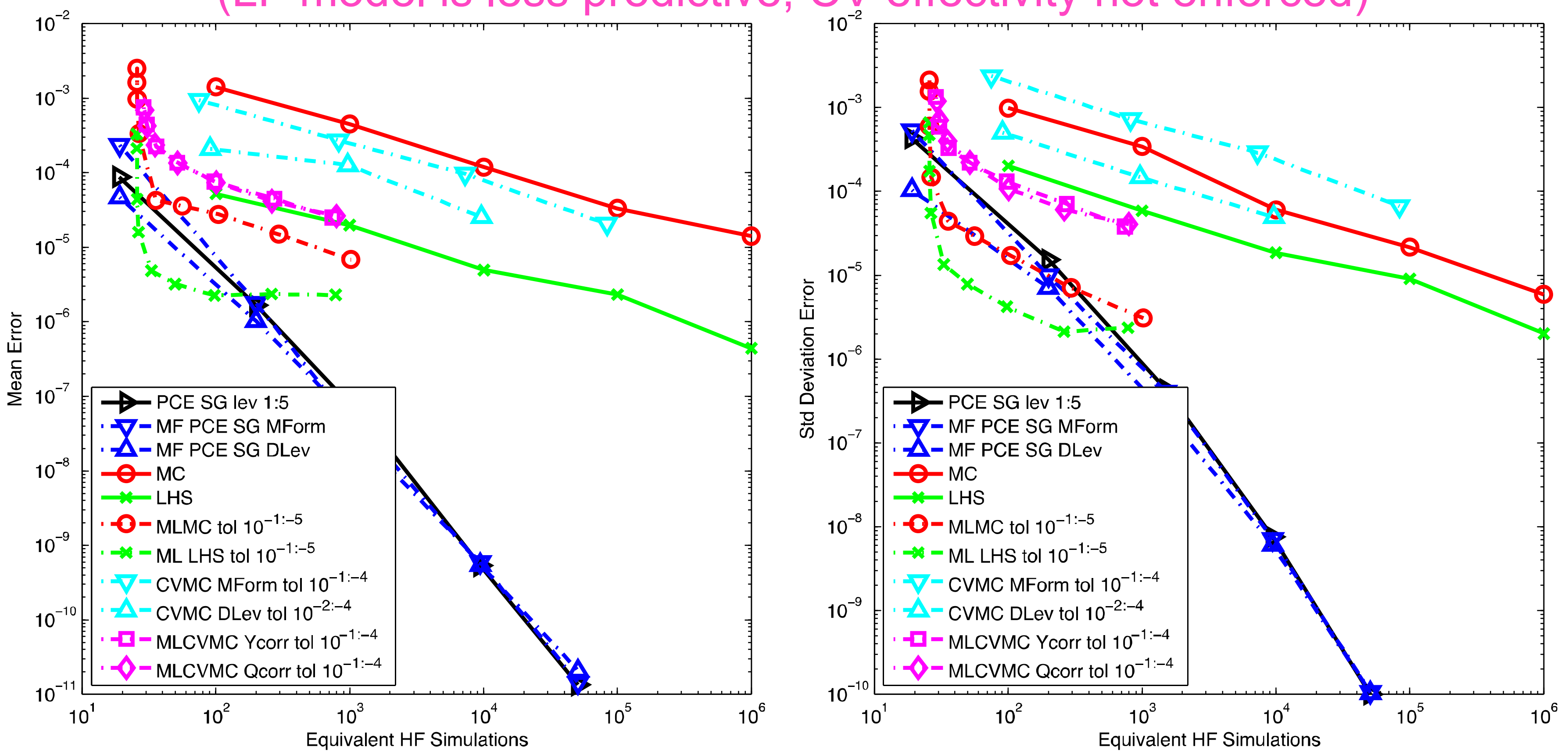
MLCV Y-corr:

$$N_\ell^{HF,\star} = \frac{2}{\varepsilon^2}\left[\sum_{k=0}^{L_{HF}} \left(\frac{\mathbb{V}ar\left(Y_\ell^{HF}\right) C_\ell^{HF}}{1-\rho_{HL}^2}\Lambda_\ell\right)^{1/2}\right]\sqrt{\left(1-\rho_{HL}^2\right)\frac{\mathbb{V}ar\left(Y_\ell^{HF}\right)}{C_\ell^{HF}}}$$

MLCV Q-corr:

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

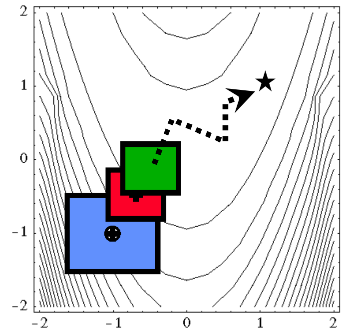
MLCV MC (magenta) less effective for this problem
(LF model is less predictive; CV effectivity not enforced)



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)

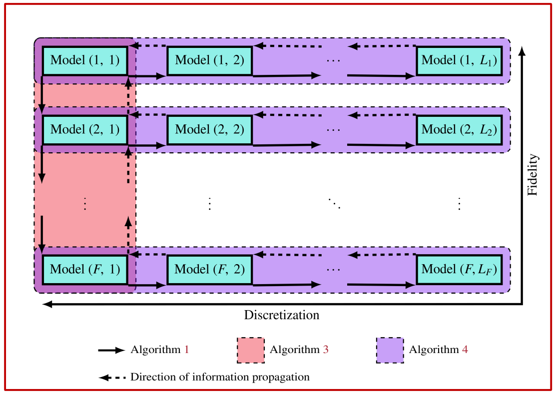
- targets *hierarchy of discretization levels*
- multigrid V cycle to hierarchy of *optimization solves*
- coarse optim. generates search direction for fine optim.
  - corrections + line search globalization → provable convergence

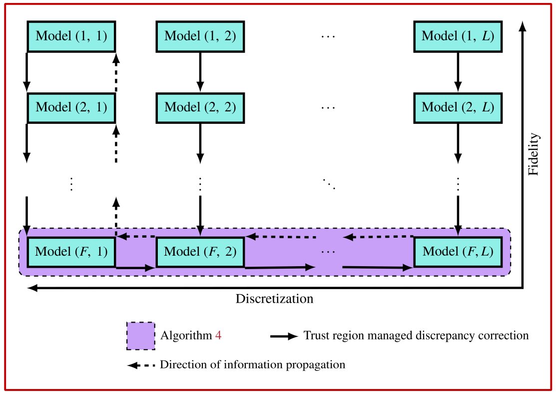
Algorithm 1 Multigrid Optimization

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

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





Model Problem (Q2)

ODE:

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

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

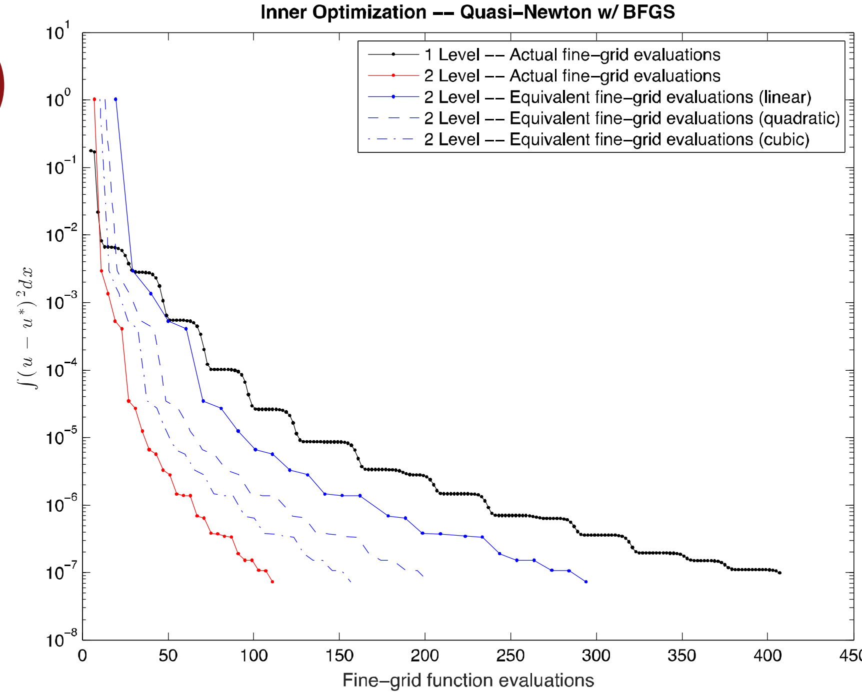
$$a = 2 + \cos(2\pi x)$$

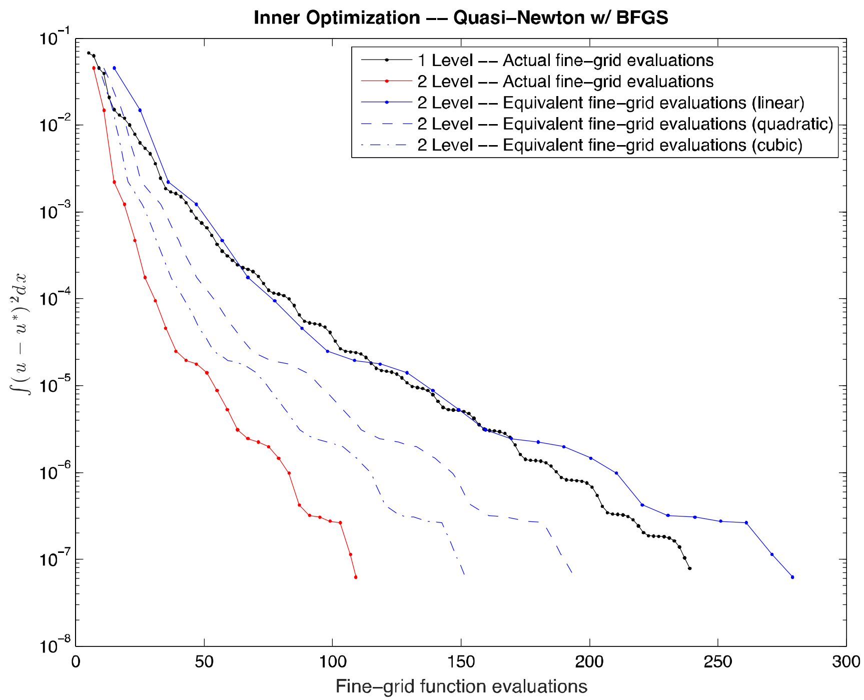
Optimization Problem:

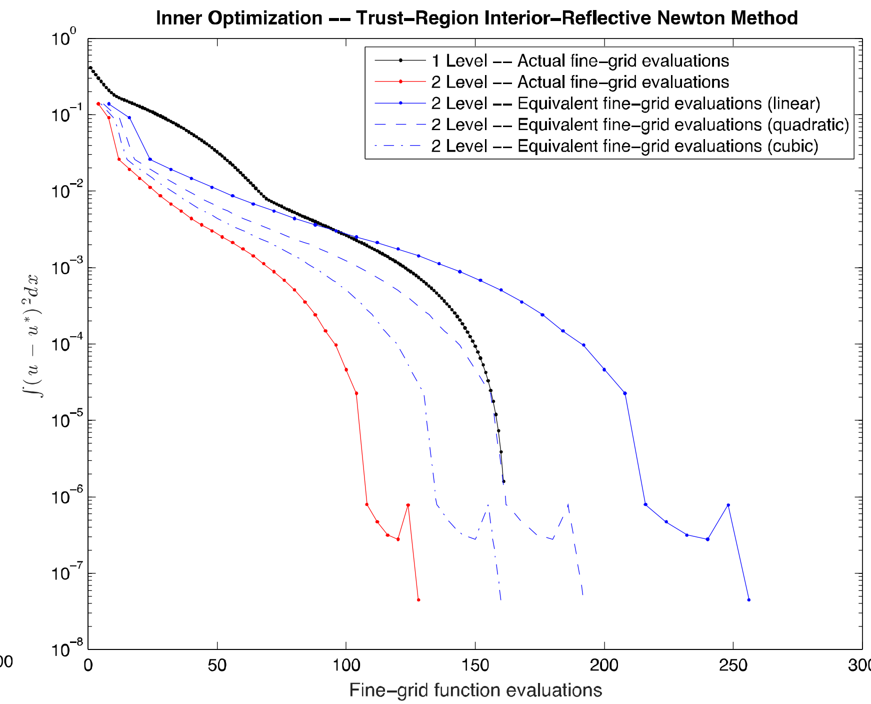
$$\text{minimize} \quad \int (u(f) - u^*)^2 dx$$

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

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

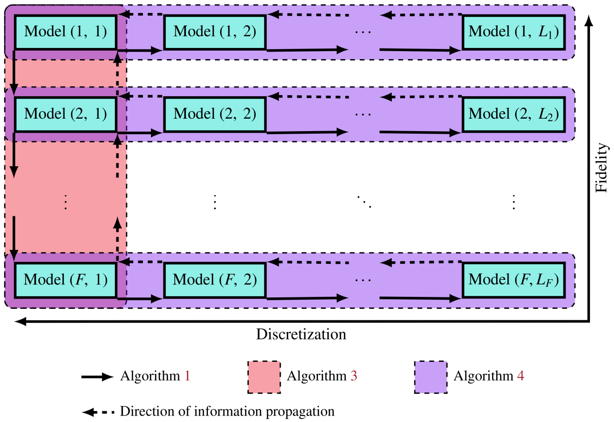






Multilevel-Multifidelity Optimization – Initial Results

Initial formulation: nested multigrid

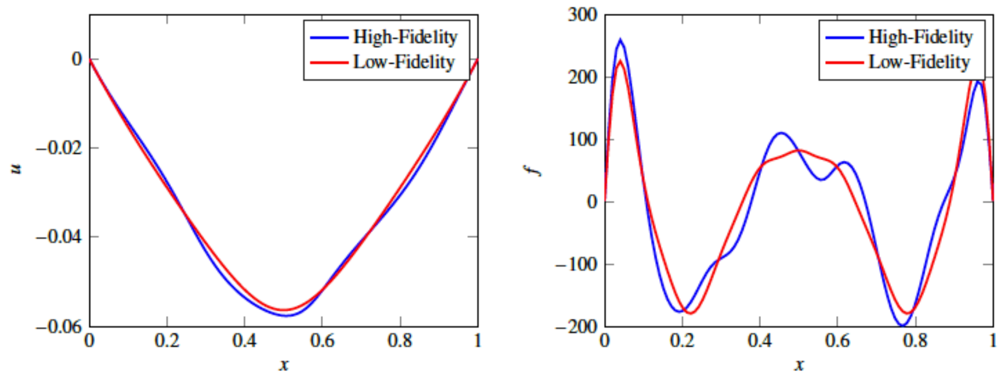


$$c_{\text{hi}}(f, u(f)) = \frac{d}{dx}\left(a_{\text{hi}} \frac{du}{dx}\right) + f = 0, \quad x \in (0,1),$$
$$u(0) = u(1) = 0,$$
$$a_{\text{hi}} = 2 + \cos(2\pi x) + 0.4 \sin(6\pi x).$$

$$c_{\text{low}}(f, u(f)) = \frac{d}{dx}\left(a_{\text{low}} \frac{du}{dx}\right) + f = 0, \quad x \in (0,1),$$
$$u(0) = u(1) = 0,$$
$$a_{\text{low}} = 2 + \cos(2\pi x).$$

$$\underset{f}{\text{minimize}} \quad \int (u(f) - u^*)^2 dx$$
$$\text{subject to} \quad c_{\text{hi}}(f, u(f)) = 0$$

$u^* = \sin^2(2\pi x)$ is the target solution



a) ODE solution at initial guess

b) Optimal f for both fidelities

a) 1 fidelity and 1 level

	Fine
High-Fidelity	229

b) 1 fidelity and 2 levels

	Fine	Coarse
High-Fidelity	112	146

c) 2 fidelities and 2 levels

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

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

Transonic Airfoil Design: Minimize Drag

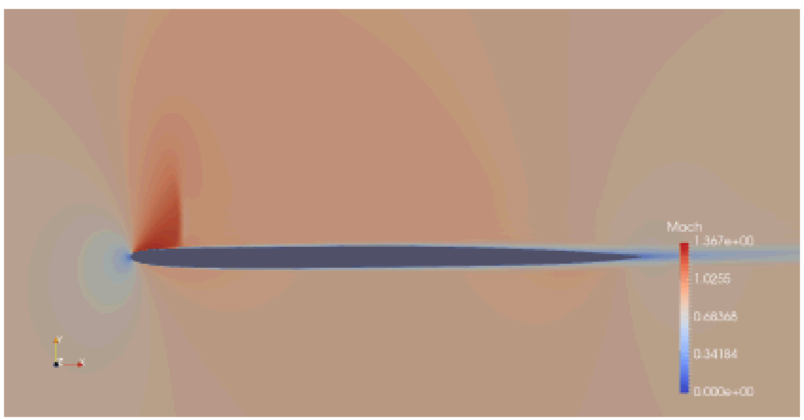
Sandia National Laboratories

MG/Opt (unconstrained)

$$\underset{x}{\text{minimize}} \quad C_D(u(x))$$
$$\text{subject to} \quad c_{\text{RANS}}(x, u(x)) = 0$$

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



d) RANS-SA coarse grid, C_D = 0.0111 (optimized)

High-Fidelity, Coarse	11
Low-Fidelity, Fine	23