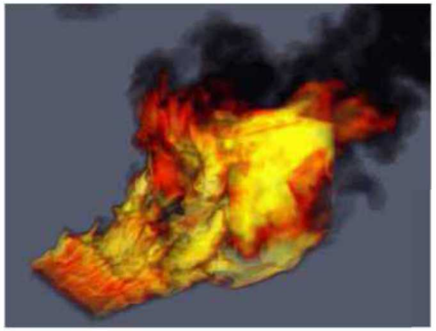
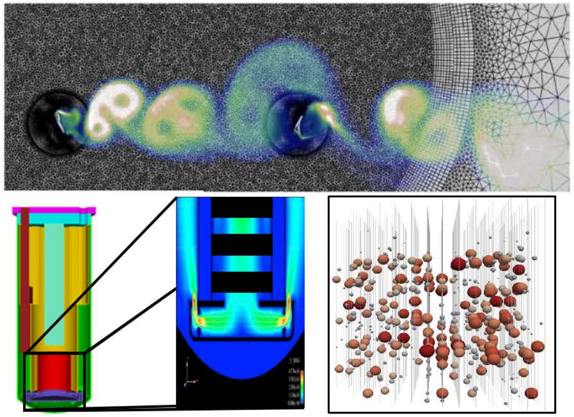
UQ & Optimization: DOE/DOD Mission Deployment

SAND2019-6928PE

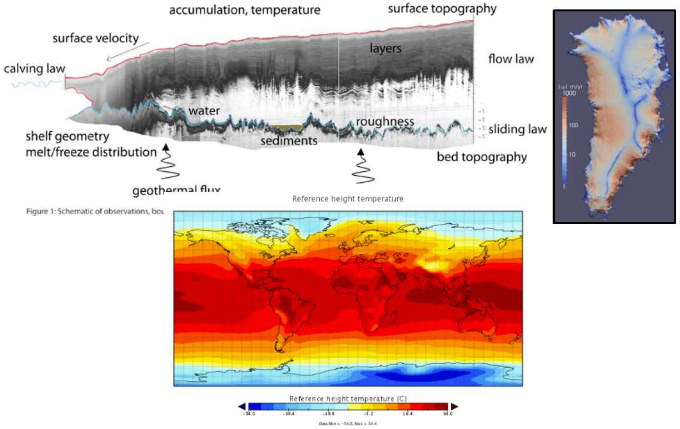
Stewardship (NNSA ASC)
Safety in abnormal environments



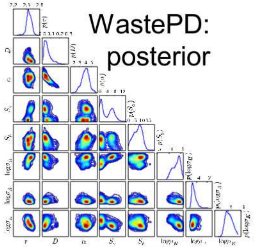
Energy (ASCR, EERE, NE)
Wind turbines, nuclear reactors

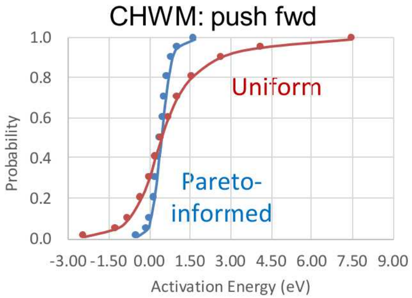


Climate (SciDAC, CSSEF, ACME)
Ice sheets, CISM, CESM, ISSM, CSDMS

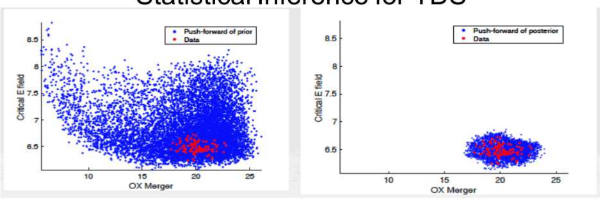


Addtnl. Office of Science:
(SciDAC, EFRC)
Comp. Matls: waste forms / hazardous matls (WastePD, CHWM)
MHD: Tokamak disruption (TDS)





Statistical Inference for TDS



Common theme across these applications:

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

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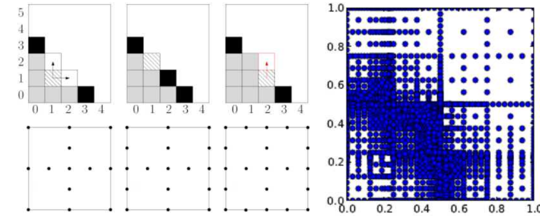
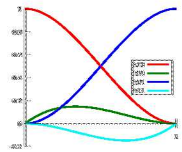
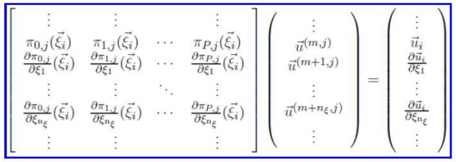
Research Thrusts for UQ

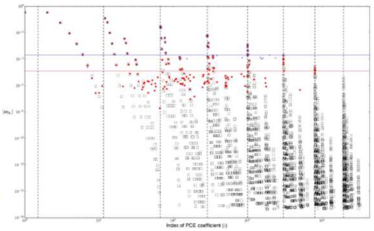
- *Focus:* Compute dominant uncertainty effects despite key challenges



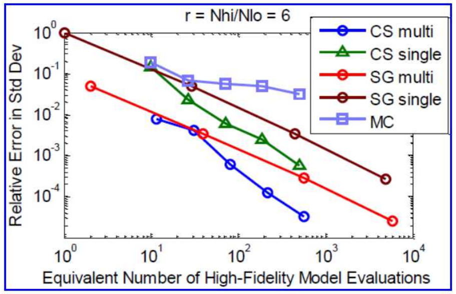
- Emphasize scalability and exploitation of special structure
  - *Adaptivity:* p- and h- refinement of stochastic expansions
  - *Adjoints:* gradient enhancement for PCE / SC / GP
  - *Sparsity:* compressed sensing
  - *Low Rank:* tensor / function train (w/ UMich)
  - *Dimension reduction:* active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







- Compound efficiencies
  - Multilevel-Multifidelity with sampling & CS/FT surrogates (new: ROM, NN)
  - Active subspaces: subspace quadrature, enhance MF control variates



- Address complexity w/ component-based approach
  - Emulator-based Bayesian inference, Mixed aleatory-epistemic UQ, Optimization under uncertainty (new: Optimal experimental design)
- Position UQ for next generation architectures
  - *Current (imperative):* multilevel parallelism (MPI + local async)
  - *Future (declarative):* exploit DAG + AMT for ensemble workflows (w/ Stanford)

"Science Pipeline" Metaphor

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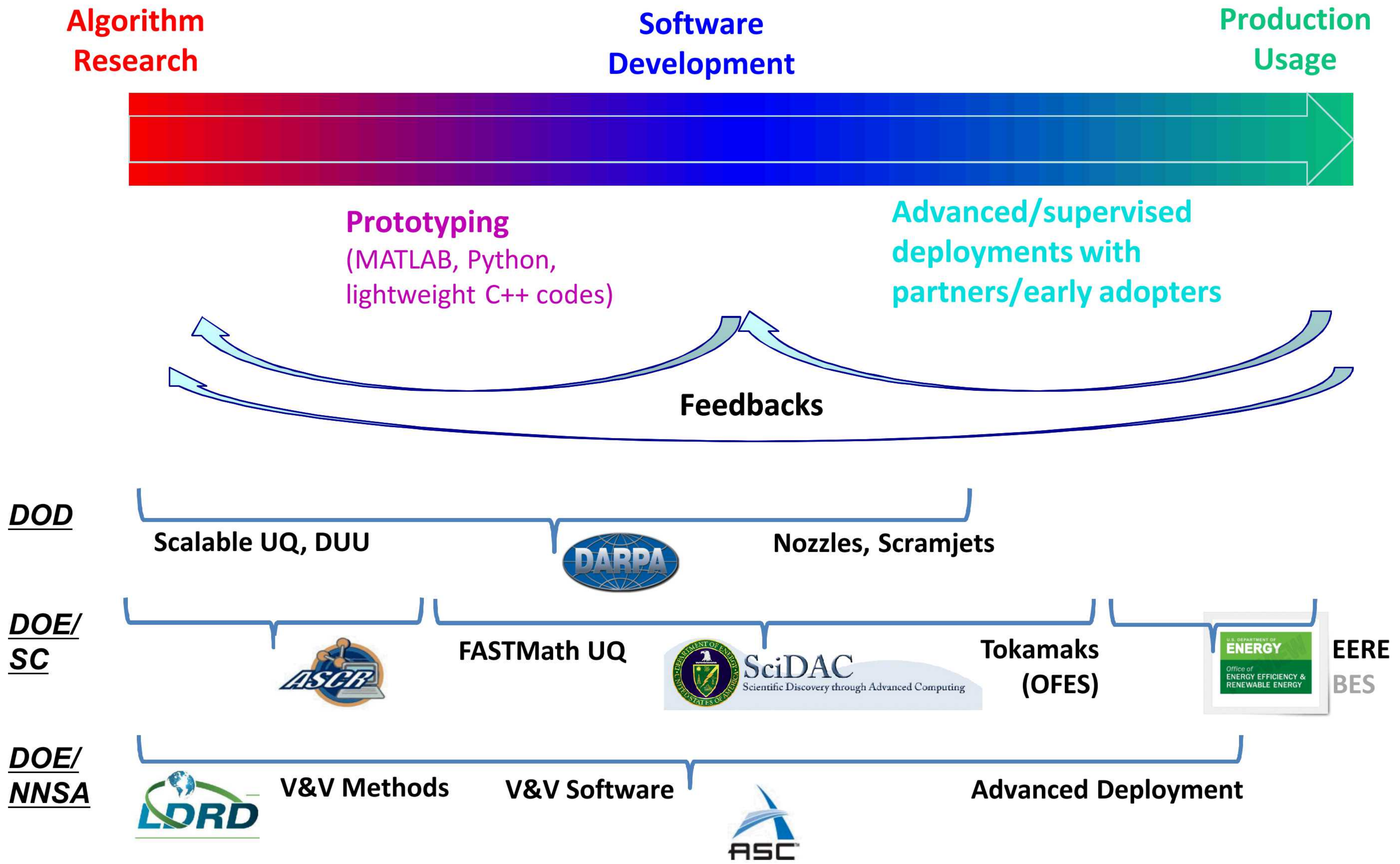
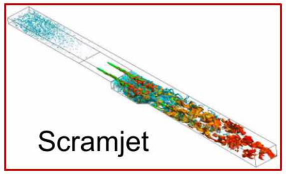
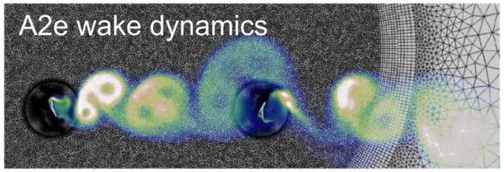


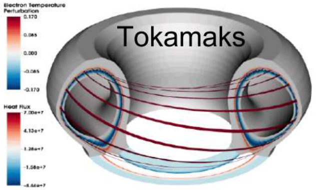
Research & Development in Multifidelity Methods

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

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



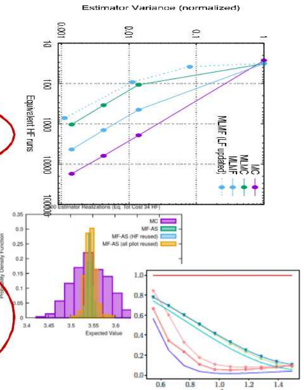




Emerging mission areas: abnormal thermal, Z-pinch MagLIF, quantum chemistry

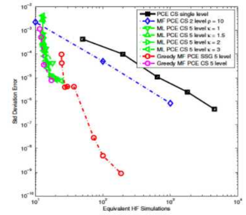
Monte Carlo UQ Methods

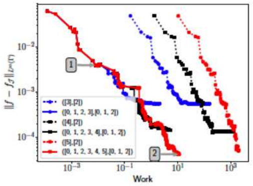
- *Production:* optimal resource allocation for multilevel, multifidelity, combined (DARPA SEQUOIA/ScramjetUQ)
- *Emerging:* active dimensions ('18 EE LDRD), generalized fmwk for approx control variates (ASC V&V Methods)
- *On the horizon:* control of time avg; learning latent var relationships (CIS LDRD); model tuning / selection (CIS LDRD, DOE BES)



Surrogate UQ Methods (PCE, SC)

- *Production (v6.10):* ML PCE w/ projection & regression; ML SC w/ nodal/hierarchical interp; greedy ML adaptation (DARPA SEQUOIA)
- *Emerging:* multi-index stochastic collocation, multilevel function train (ASC V&V Methods)
- *On the horizon:* new surrogates (ROM, deep NN) with error mgmt ('19 EE LDRD, DOE BES); unification of surrogate + sampling approaches (CIS LDRD)





Optimization Under Uncertainty

- *Production:* manage simulation and/or stochastic fidelity

- *Emerging:*
  Derivative-based methods (DARPA SEQUOIA)
  - Multigrid optimization (MG/Opt)
  - Recursive trust-region model mgmt.: extend TRMM to deep hierarchies

  Derivative-free methods (DARPA ScramjetUQ)
  - SNOWPAC (w/ MIT, TUM) w/ MLMC error estimates
- *On the horizon:* Gaussian process-based approaches: multifidelity EGO (FASTMath OUU); Optimal experimental design (OED) (A2e)

Key Challenge: existing ML/MF/MI performance is compelling on (elliptic) model problems, but significant generalization required for engineering applications with non-trivial model relationships

DARPA SEQUOIA: Hierarchy of Fidelity Levels

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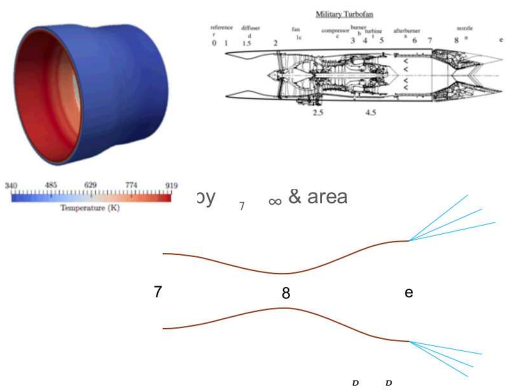
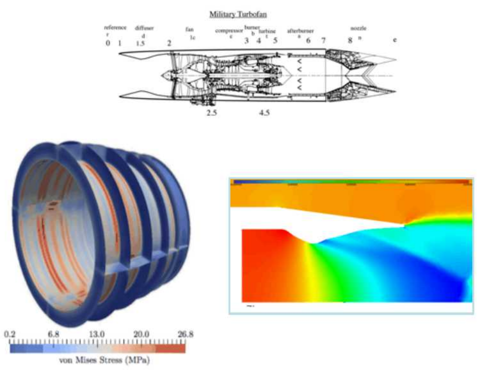
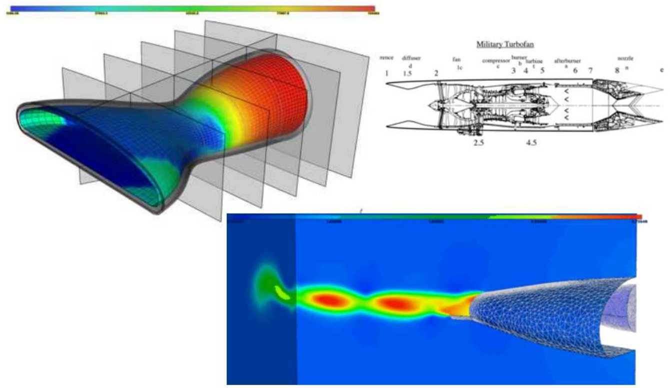






Low fidelity model

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

Medium fidelity model

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

High fidelity model

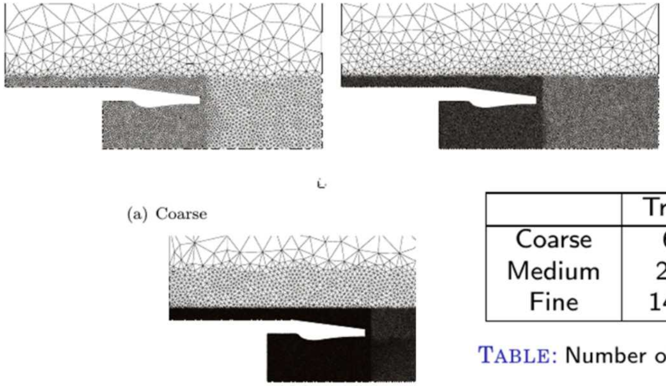
- 3D non-axisymmetric Euler/RANS CFD
- 1D heat transfer
- Full 3D FEM model
- 2 hours on 20 cores (3D RANS, coarse mesh)

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

Initial Deployment of MLCV MC to UCAV Nozzle UQ

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

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



(a) Coarse

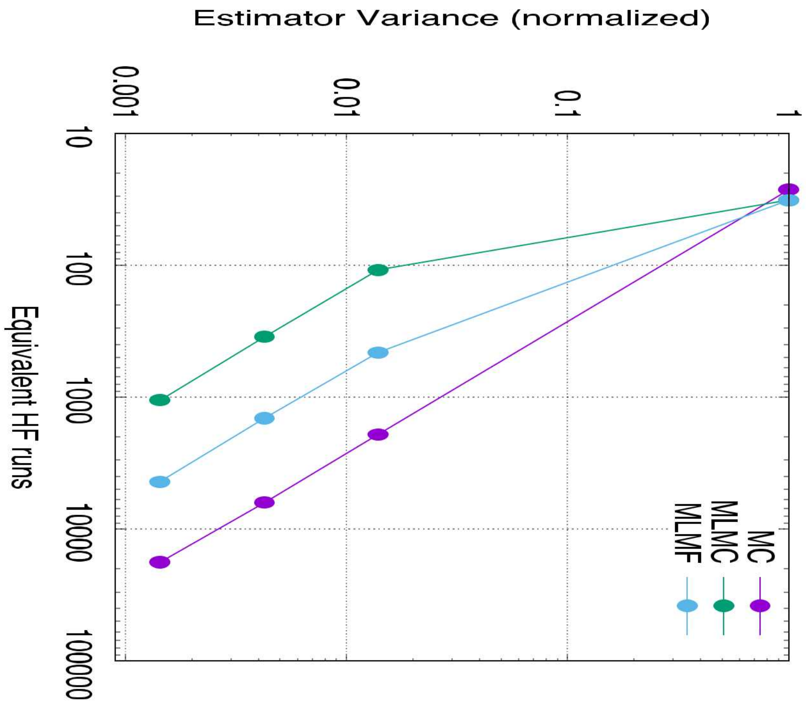
(c) Fine

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

TABLE: Number of triangles.

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

TABLE: Computational cost.

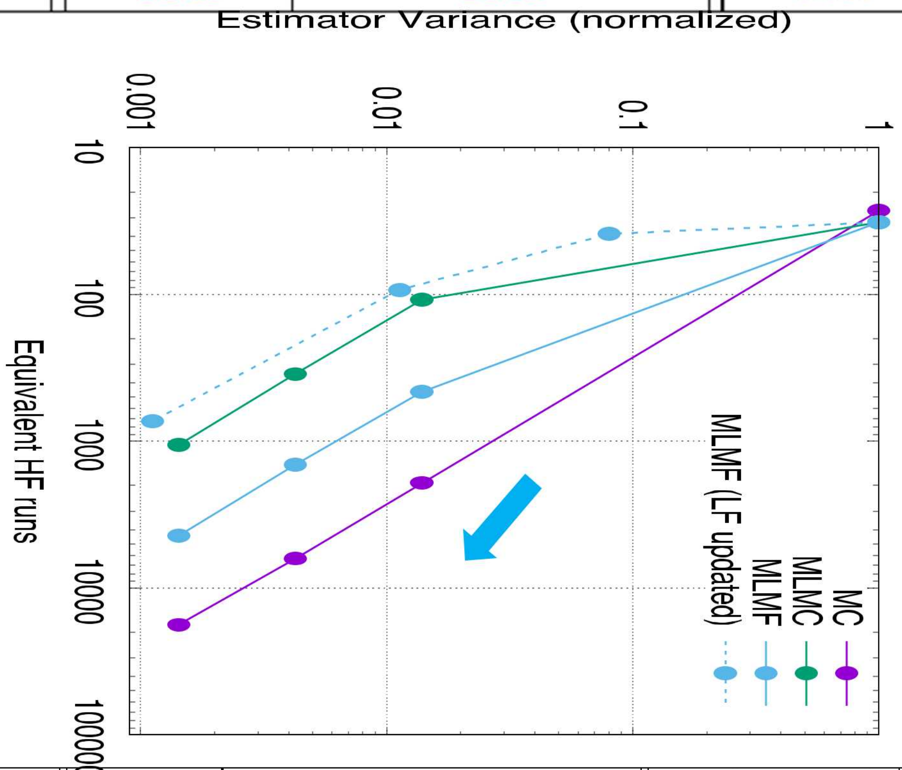


Optimal sample allocations based on relative cost, observed correlation between models, and observed variance distribution across levels

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

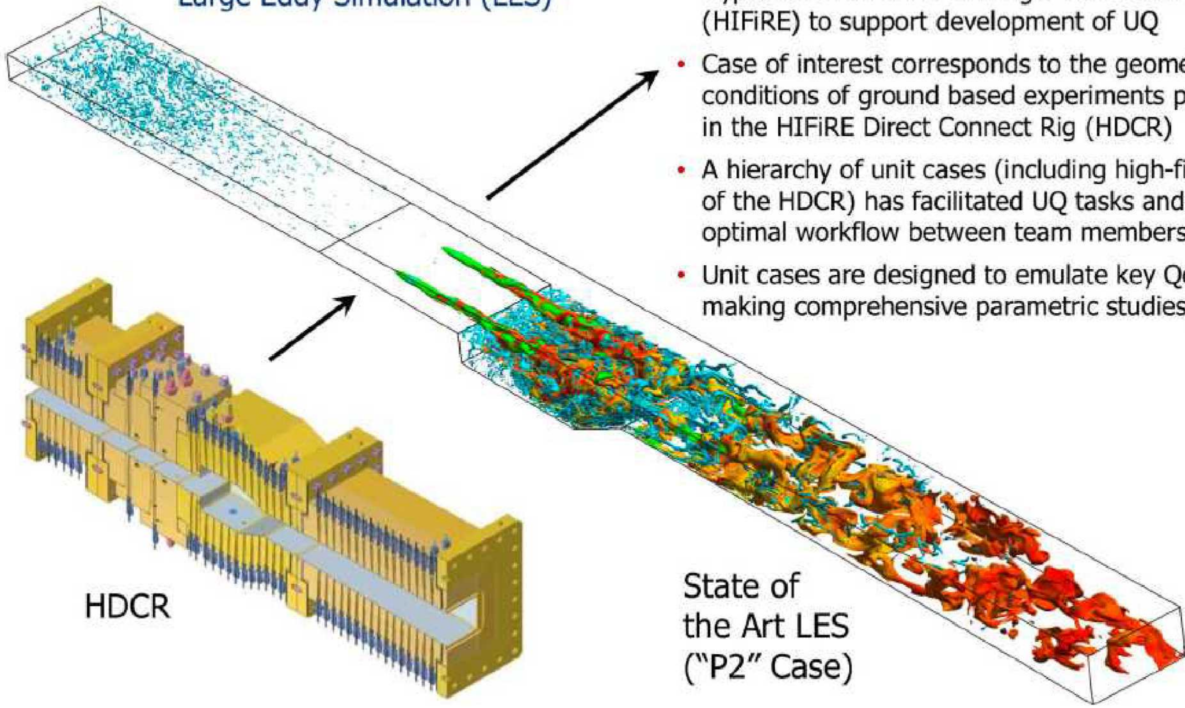
Updated Deployment of MLCV MC to UCAV Nozzle UQ

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

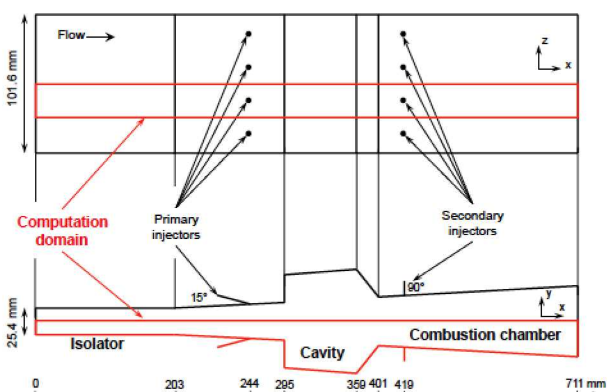


Accuracy ($\varepsilon^2/\varepsilon_0^2$)	LF	Medium Fidelity			LF (updated)	Medium Fidelity		
	Coarse	Coarse	Medium	Fine	Coarse	Coarse	Medium	Fine
0.1	N/A	N/A	N/A	N/A	404	20	20	20
0.01	21,143	1,757	20	20	3,091	177	31	20
0.003	69,580	5,775	36	20	N/A	N/A	N/A	N/A
0.001	212,828	17,715	109	34	32,433	1,773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

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

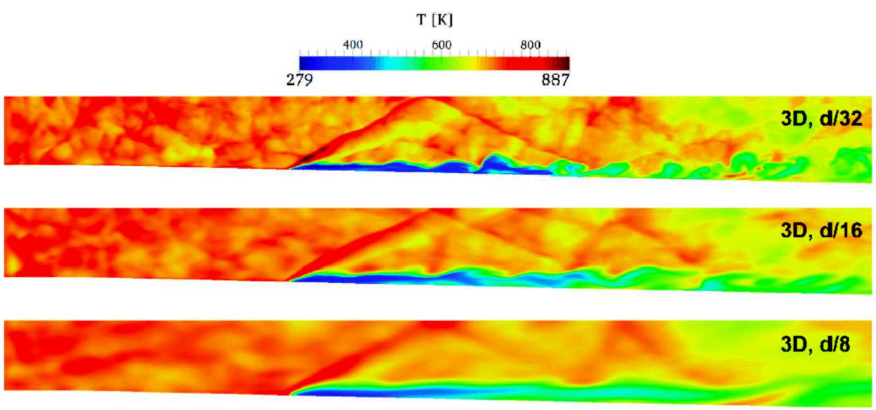


- Provided benchmark LES calculations of the Hypersonic International Flight Research Experiment (HIFiRE) to support development of UQ
- Case of interest corresponds to the geometry and conditions of ground based experiments performed in the HIFiRE Direct Connect Rig (HDCR)
- A hierarchy of unit cases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



Model forms:
- 2D, 3D

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

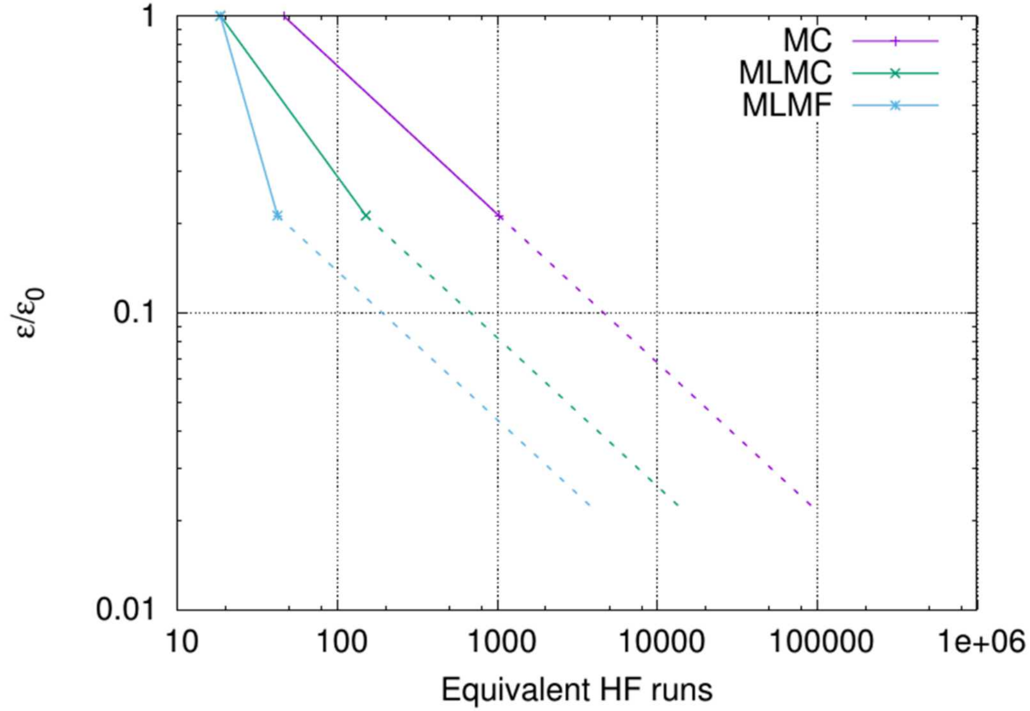


Initial Deployment of MLCV MC for Scramjet UQ

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

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

UQ Approach: MLCV algorithm described previously.



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

TABLE: Computational cost.

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

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

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

Updated Deployment of MLCV MC for Scramjet UQ

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

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

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

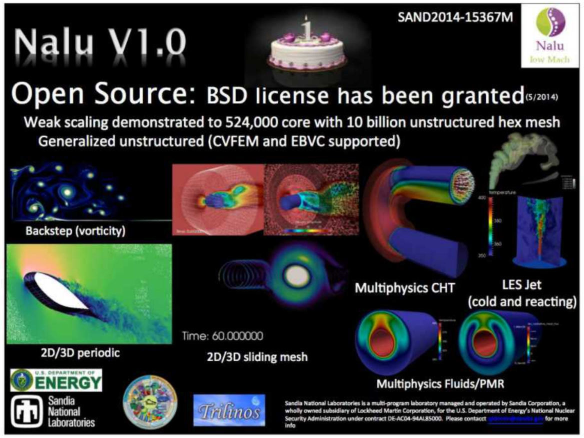
Observations from pilot sample: decay in variance across discretizations (LF d/8 and discrepancy d/16 – d/8) no longer observed for all QoI

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

Computational Approach

- Low Fidelity: **OpenFAST-AeroDyn-Turbsim** (https://github.com/OpenFAST)
  - Turbsim generates turbulent atmospheric boundary layer flow field, semi-empirical
  - AereoDyn models the aerodynamic forces on the rotor
  - OpenFAST models the structural and controls response of the rotor (same for Nalu)

- High Fidelity: **Nalu** (https://github.com/NaluCFD)
  - LES, Solves the Navier-Stokes equations in the low-Mach number approximation with the one-equation, constant coefficient, TKE model for SGS, unstructured massively parallel.
  - Actuator Line model of the rotor
  - Single, uniform mesh (no nesting)



Cost estimates for Nalu and OpenFAST simulations.

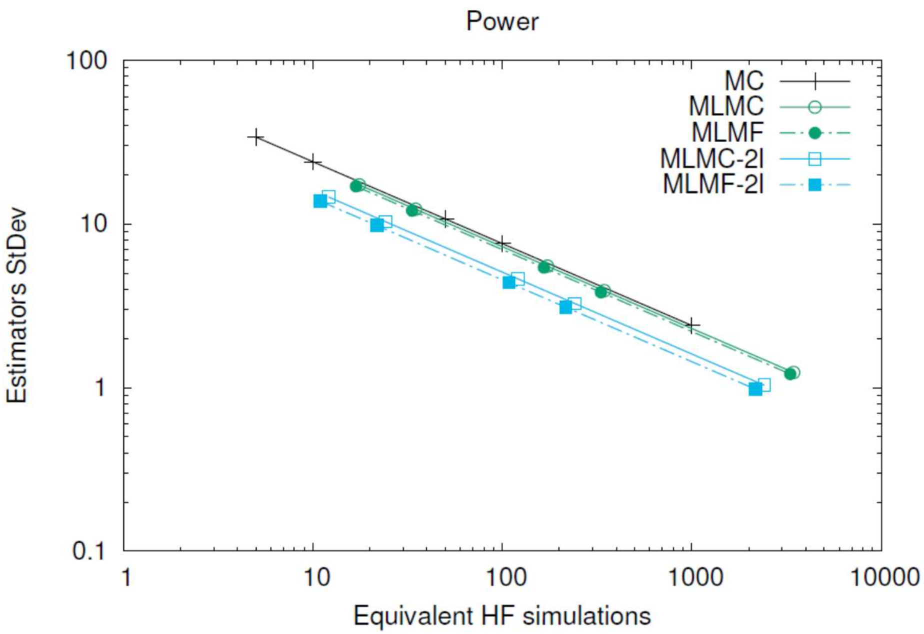
Case	Mesh size	Simulation time (seconds)	CPUs	Cost (CPU-hours)	Cost (relative)
OpenFAST		500	1	0.42	1
Coarse	100x50x50	2000	80	240	576
Medium	200x100x100	2000	160	960	2304
Fine	400x200x200	2000	400	6860	16500
Reference	800x200x200	2000	400	38400	91400

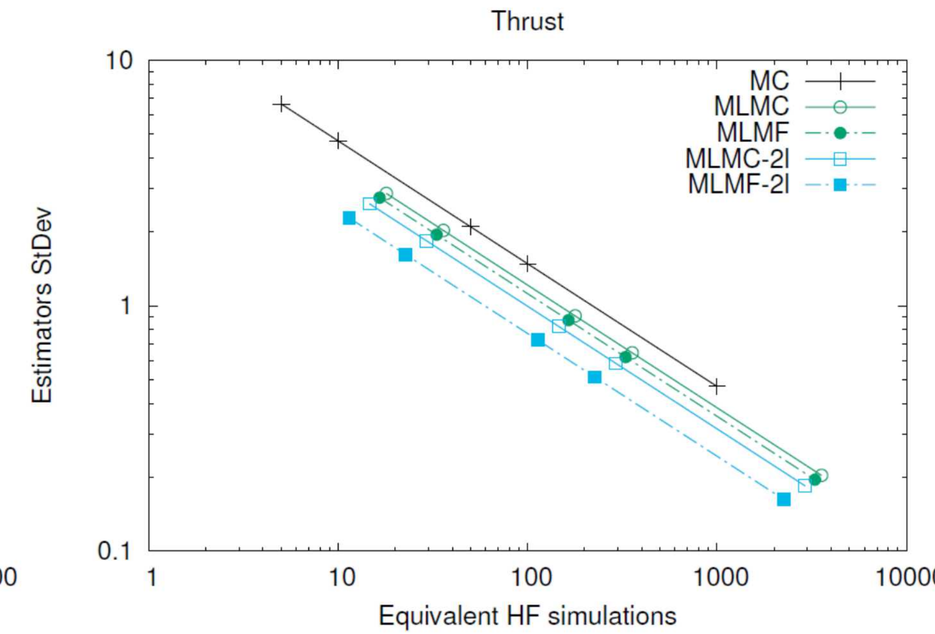
Domino, S. "Sierra Low Mach Module: Nalu Theory Manual 1.0", SAND2015-3107W, Sandia National Laboratories Unclassified Unlimited Release (UUR), 2015. https://github.com/NaluCFD/NaluDoc

Estimator Performance Extrapolation

Given the statistical properties estimated for power and thrust, we can extrapolate the behavior of several estimators:

- Standard MC estimator
- MLMC-3l: Multilevel $Q_0 + (Q_1 - Q_0) + (Q_2 - Q_1)$
- MLMF-3l: MLMC-3l with CV for Q_0
- MLMC-2l: Multilevel $Q_1 + (Q_2 - Q_1)$
- MLMF-2l: MLMC-2l with CV for Q_1

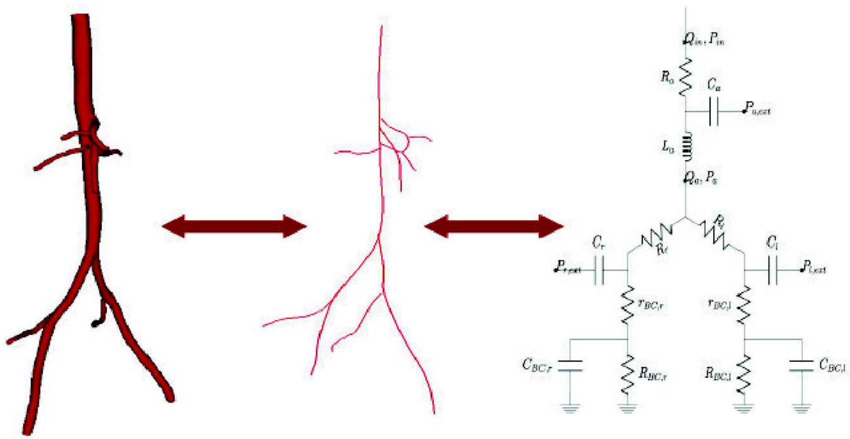




	Power			Thrust		
	MLMC	MLMF		MLMC	MLMF	
Level	Nalu	Nalu	OpenFAST	Nalu	Nalu	OpenFAST
0	161	137	2040	181	136	2887

Nalu LES for Q0 was too coarse and non-predictive

Multilevel – Multifidelity Sampling Methods
Cardiovascular flow

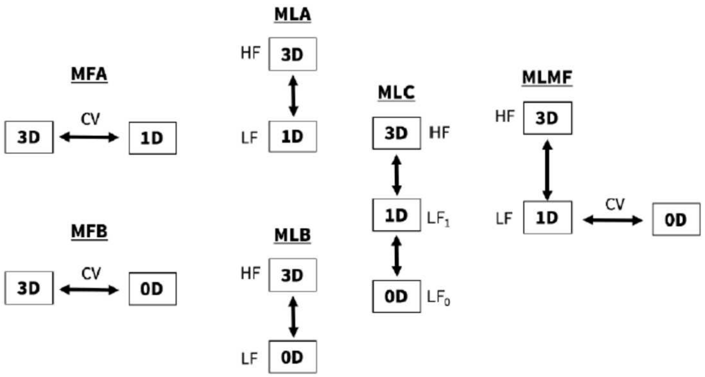


3D Model   1D Model   0D Model

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

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

Model relationships / graph topologies



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

Costs to achieve prescribed error tolerance

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

1D predictivity was insufficient and 0D contribution required control weighting

Multilevel – Multifidelity Challenges

Key Challenge: existing ML/MF/MI performance is compelling on (elliptic) model problems, but significant generalization required for engineering applications with non-trivial model relationships

- Do we really know the predictive value of each model a priori?
- Are the dependency relationships clear from the modeling source?
- Conversely, can there be a penalty in greater generality w/ more weights to estimate?

Research directions:

- *Generalize:* start from a fully-connected, weighted structure
  - Compute correlations across full model ensemble
- *Optimize:* learn latent relationships for an optimized graph representation
  - Estimate reduced weight set from finite simulation instances

Multilevel – Multifidelity Sampling Methods

Generalized framework for approx. control variates

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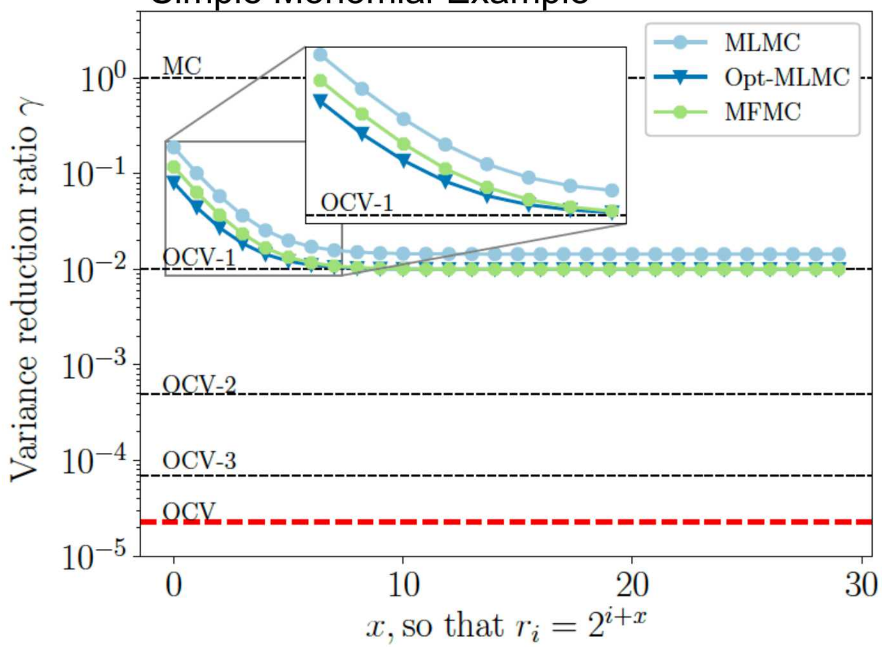
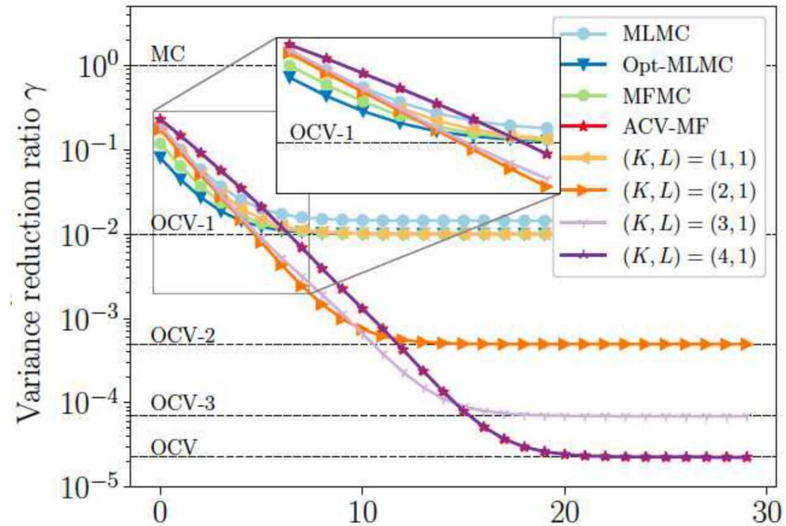
For M approximate models, look beyond (recursive) model pairings

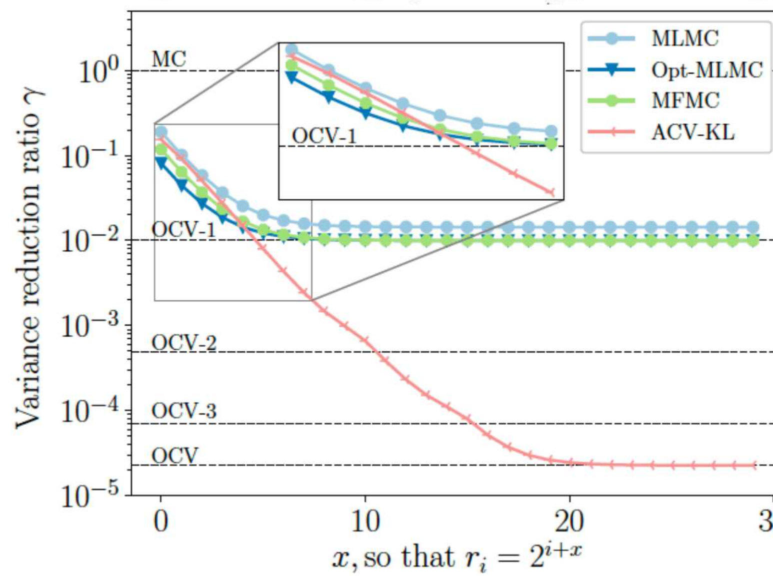
$$\hat{Q}^{\mathrm{CV}} = \hat{Q} + \sum_{i=1}^{M} \alpha_i \left(\hat{Q}_i - \mu_i \right)$$

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

Simple Monomial Example







A. Gorodetsky, G. Geraci, E., J. Jakeman “A Generalized Framework for Approximate Control Variates,” arxiv.org/abs/1811.04988

Multilevel – Multifidelity Sampling Methods

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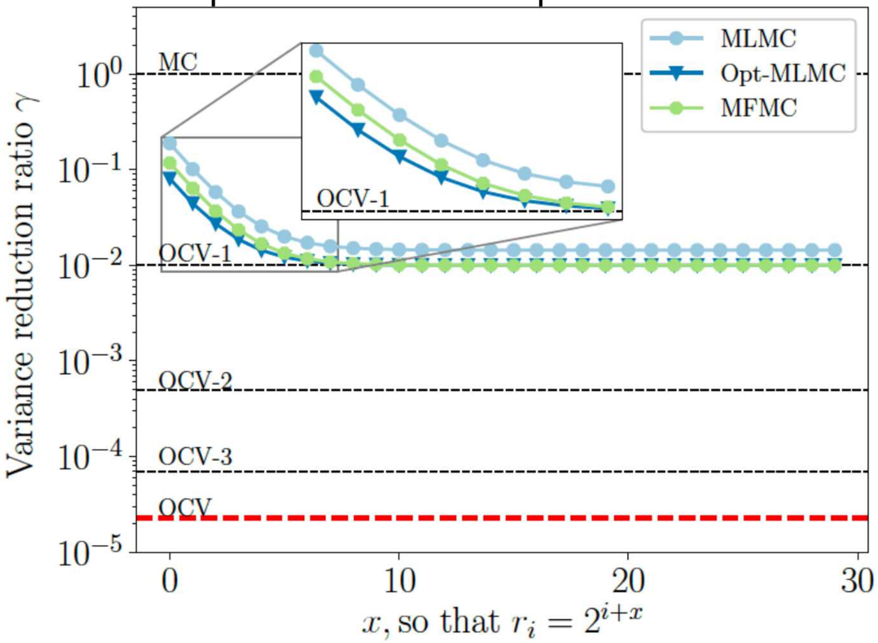
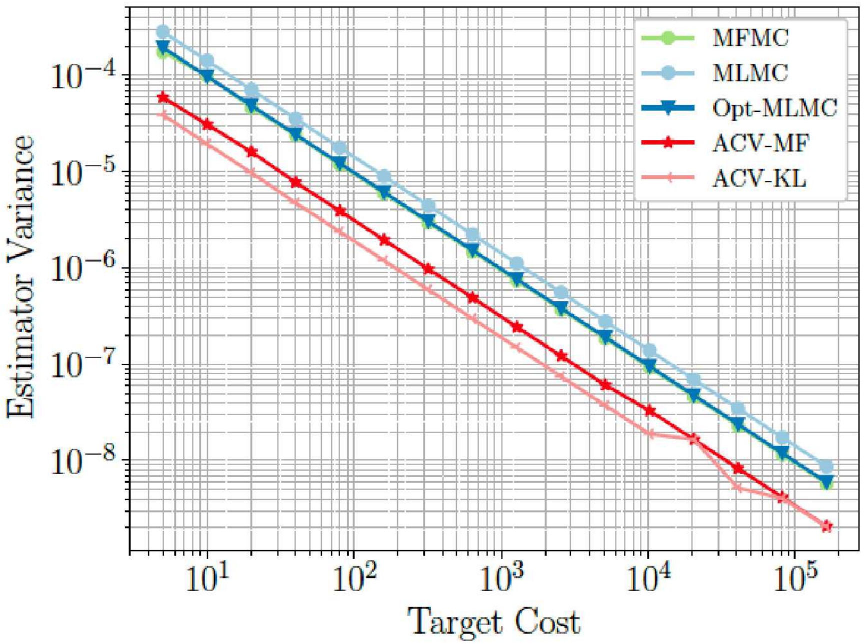
Simple Monomial Example



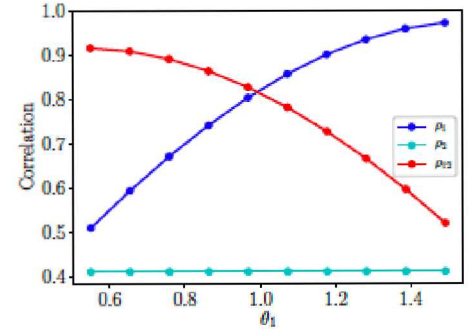


Generalized framework for approx. control variates

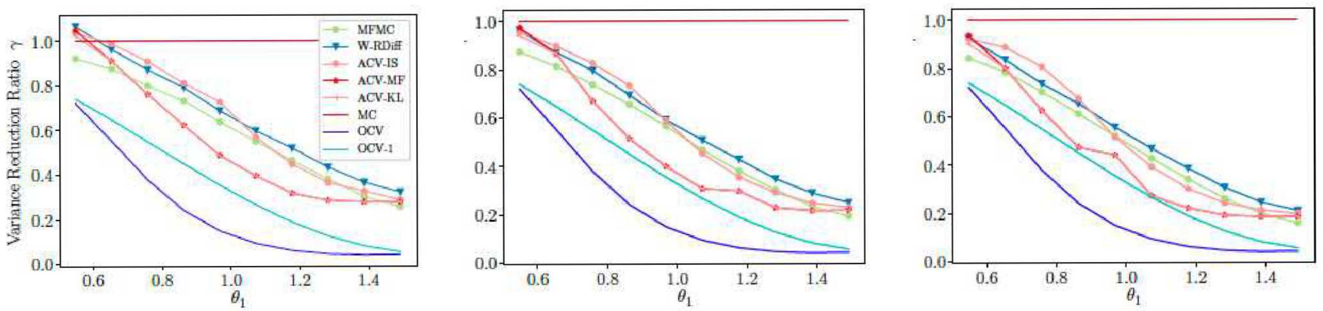
Tunable model problem

$$Q = A\left(\cos\theta\, x^5 + \sin\theta\, y^5\right), \quad Q_1 = A_1\left(\cos\theta_1\, x^3 + \sin\theta_1\, y^3\right), \quad Q_2 = A_2\left(\cos\theta_2\, x + \sin\theta_2\, y\right)$$

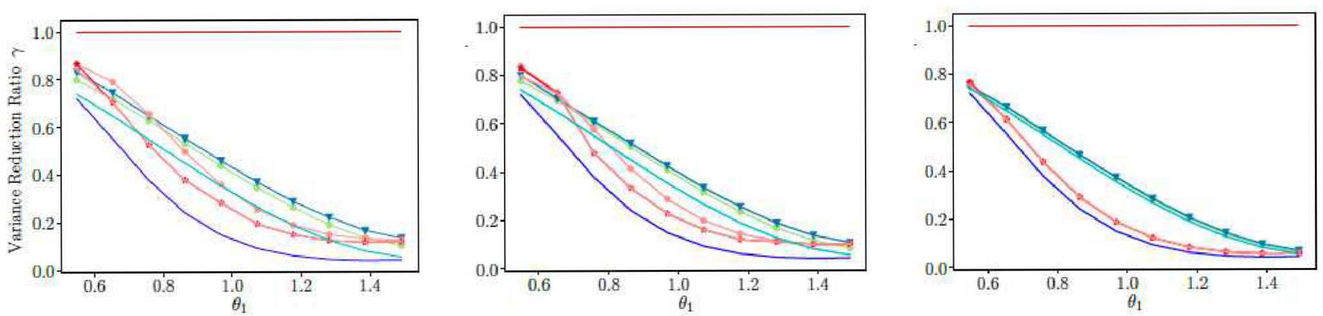
$$A = \sqrt{11},\ A_1 = \sqrt{7} \text{ and } A_2 = \sqrt{3} \qquad \theta = \pi/2,\ \theta_2 = \pi/6 \text{ and } \theta_2 < \theta_1 < \theta.$$



Exploiting the OCV vs. OCV-1 gap for different cost ratios



(a) $w = 10$ (b) $w = 15$ (c) $w = 20$



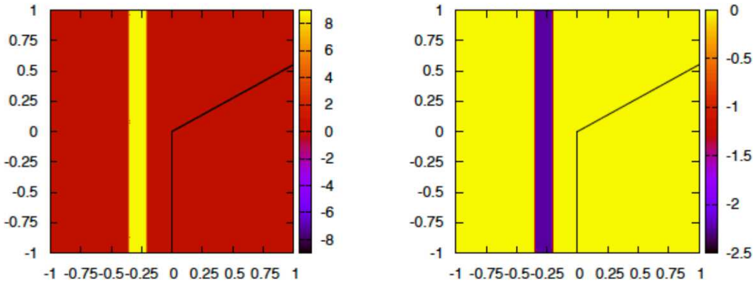
(d) $w = 50$ (e) $w = 100$ (f) $w = 1000$

A. Gorodetsky, G. Geraci, E., J. Jakeman "A Generalized Framework for Approximate Control Variates," arxiv.org/abs/1811.04988v3

Generalized framework for approx. control variates

Two dimensional elasticity in heterogeneous media

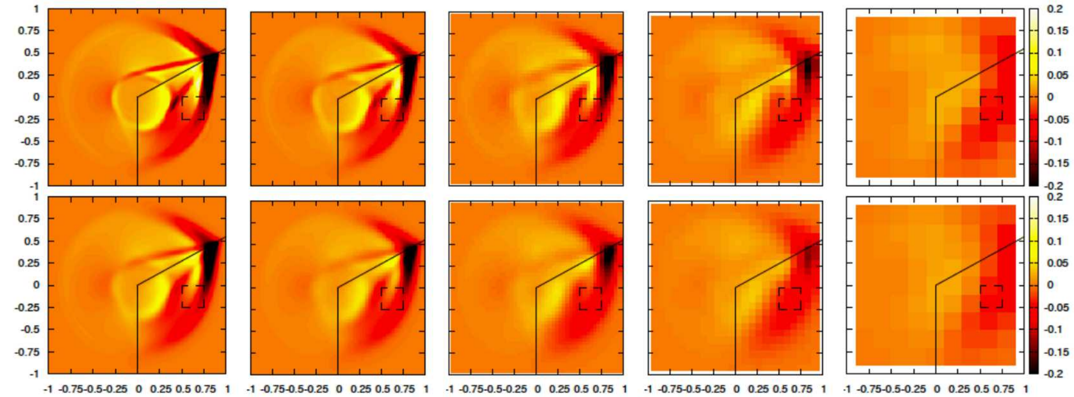
Hyperbolic system:
elastic wave propagation in 2D



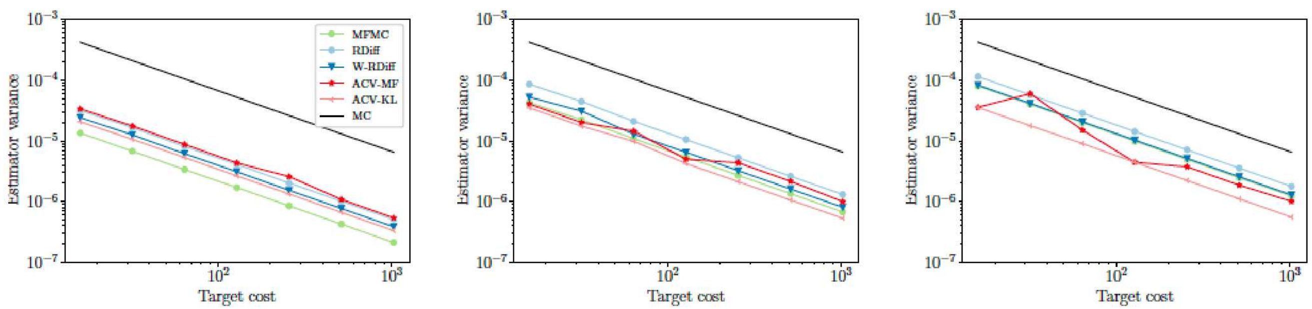
(a) Trace of the stress tensor. (b) Velocity *u* component.

$$q_t + Aq_x + Bq_y = 0$$

Shear stress contours for 2 fidelities x 5 discretizations



Well correlated discretization hierarchy → General multifidelity with model gaps



A. Gorodetsky, G. Geraci, E., J. Jakeman “A Generalized Framework for Approximate Control Variates,” arxiv.org/abs/1811.04988v3

Extra

Emphasis on Scalable Methods for High-fidelity UQ on HPC

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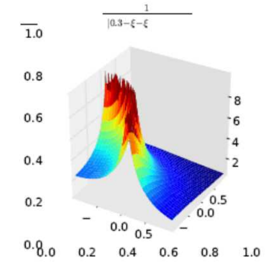
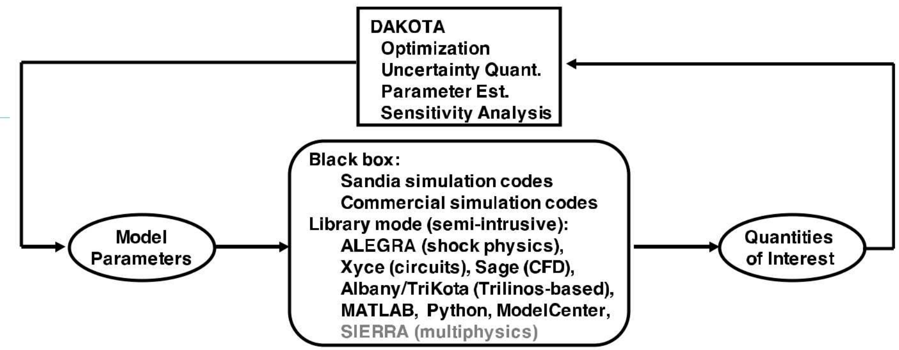


Compounding effects:

- 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)

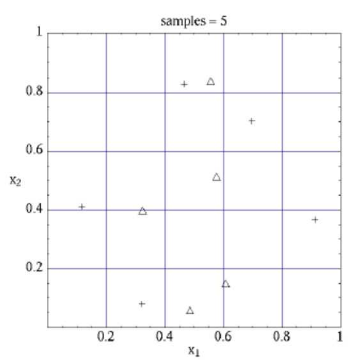
Steward Scalable Algorithms within DAKOTA

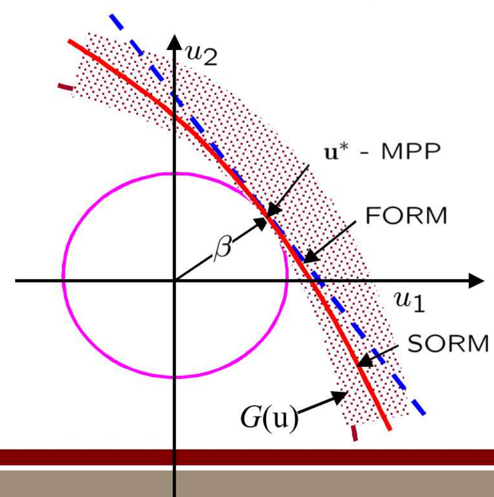
DAKOTA
Explore and predict with confidence

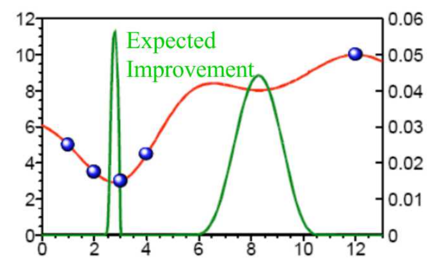


Core (Forward) UQ Capabilities:

- 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

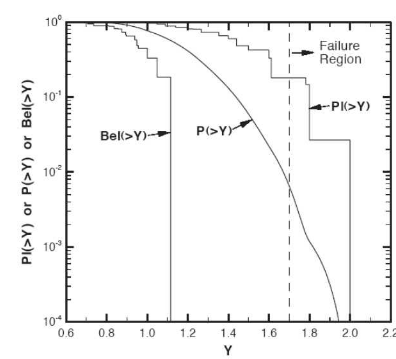






$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

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



Multiple Model Forms in UQ & Opt

Discrete model choices for simulation of same physics

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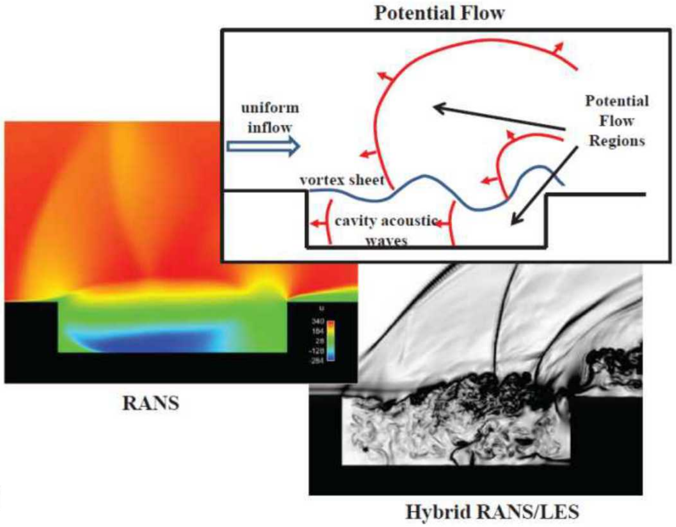
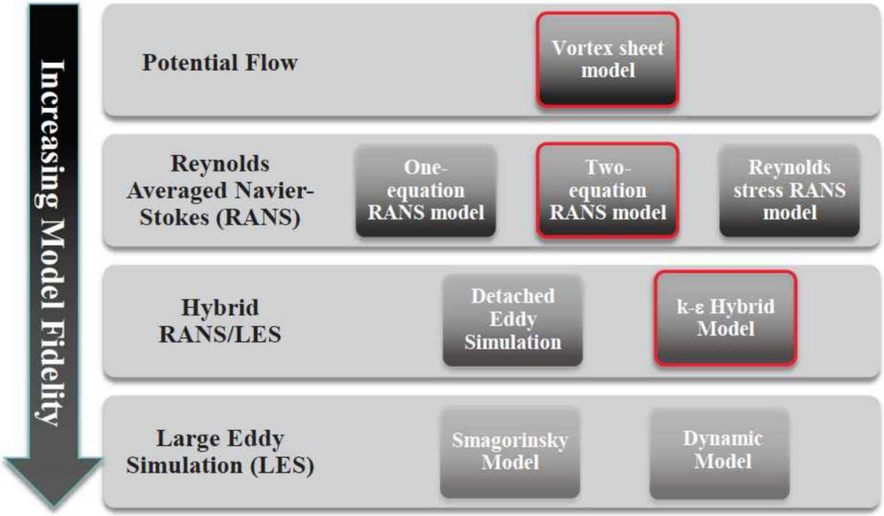
A clear hierarchy of fidelity (from low to high)
- Exploit less expensive models to render HF practical
    - *Multifidelity Opt, UQ, inference*
- Support general case of discrete model forms
    - Discrepancy does not go to 0 under refinement



An ensemble of peer models lacking clear preference structure / cost separation: e.g., SGS models
- *With data:* model selection, inadequacy characterization
    - Criteria: predictivity, discrepancy complexity
- *Without (adequate) data:* epistemic model form uncertainty propagation
    - Intrusive, nonintrusive
- *Within MF context:* CV correlation



Discretization levels / resolution controls
- Exploit special structure: discrepancy → 0 at order of spatial/temporal convergence

Combinations for multiphysics, multiscale

Simple demonstration of key ML-MF concepts
Monte Carlo Sampling: MSE for mean estimator

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

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

Monte Carlo:

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

two sources of error:

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

Looking at the Mean Square Error:

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

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

Simple demonstration of key ML-MF concepts
Multilevel MC: decomposition of estimator variance

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

Ingredients:

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

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

- Multilevel Monte Carlo estimator

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

- The Mean Square Error is

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

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

Simple demonstration of key ML-MF concepts

Multilevel MC: optimal resource allocation

Let us consider the numerical cost of the estimator

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

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

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

Balance ML estimator variance (stochastic error) and residual bias (deterministic error)
→ don't over-resolve one at the expense of the other

Level independent

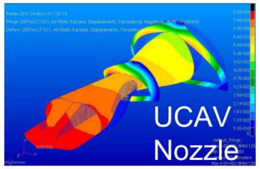
Level dependent

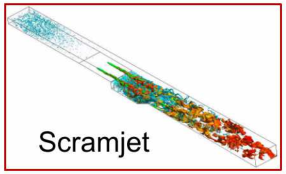
Optimal sample profile

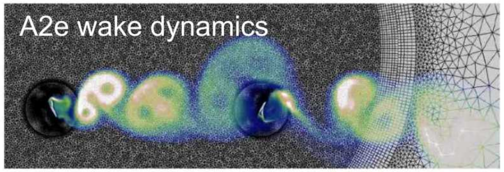
Research & Development in Multifidelity Methods

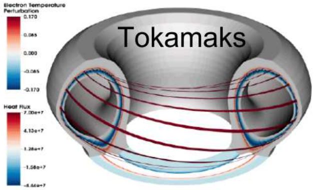
Recurring R&D theme: couple scalable algorithms with exploiting a (multi-dimensional) model hierarchy

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





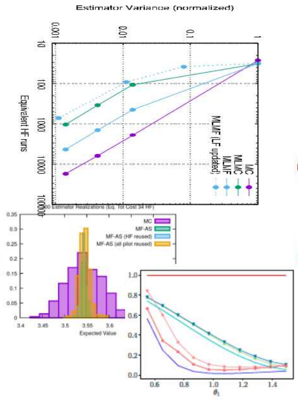




Emerging mission areas: abnormal thermal, Z-pinch MagLIF, quantum chemistry

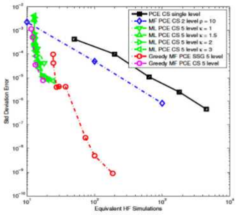
Monte Carlo UQ Methods

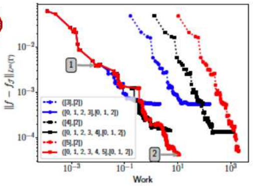
- *Production:* optimal resource allocation for multilevel, multifidelity, combined (DARPA SEQUOIA/ScramjetUQ)
- *Emerging:* active dimensions ('18 EE LDRD), generalized fmwk for approx control variates (ASC V&V Methods)
- *On the horizon:* control of time avg; learning latent var relationships (CIS LDRD); model tuning / selection (CIS LDRD, DOE BES)



Surrogate UQ Methods (PCE, SC)

- *Production (v6.10):* ML PCE w/ projection & regression; ML SC w/ nodal/hierarchical interp; greedy ML adaptation (DARPA SEQUOIA)
- *Emerging:* multi-index stochastic collocation, multilevel function train (ASC V&V Methods)
- *On the horizon:* new surrogates (ROM, deep NN) with error mgmt ('19 EE LDRD, DOE BES); unification of surrogate + sampling approaches (CIS LDRD)





Optimization Under Uncertainty

- *Production:* manage simulation and/or stochastic fidelity

- *Emerging:*
  Derivative-based methods (DARPA SEQUOIA)
  - Multigrid optimization (MG/Opt)
  - Recursive trust-region model mgmt.: extend TRMM to deep hierarchies

  Derivative-free methods (DARPA ScramjetUQ)
  - SNOWPAC (w/ MIT, TUM) w/ MLMC error estimates
- *On the horizon:* Gaussian process-based approaches: multifidelity EGO (FASTMath OUU)

Surrogate approaches: Greedy multilevel refinement

$$\hat{Q}_L \approx \hat{Q}_0 + \sum_{l=1}^{L} \hat{\Delta}_L, \text{ for } \Delta_l \equiv Q_l - Q_{l-1}$$

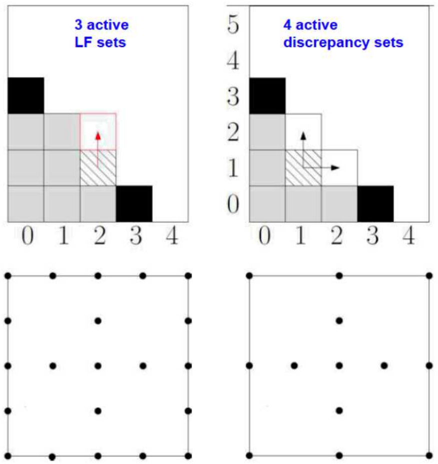
Compete refinement candidates across model levels: max induced change / cost

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

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

Level candidate generators:

- *Uniform refinement:* 1 exp order / grid level candidate per model level
  - Tensor / sparse grids: projection PCE, nodal/hierarchical SC
  - Regression PCE: least squares / compressed sensing
- *Anisotropic refinement:* 1 exp order / grid level candidate per model level
  - Tensor / sparse grids
- *Index-set refinement:* many candidates per level
  - Generalized sparse grids: projection PCE, nodal/hierarch SC
  - Regression PCE
- *Adapted candidate basis:* ~3 frontier advancements per model level
  - Regression PCE (Jakeman, E., Sargsyan, "Enhancing ℓ1-minimization estimates of polynomial chaos expansions using basis selection," *J. Comp. Phys.,* Vol. 289, May 2015.)



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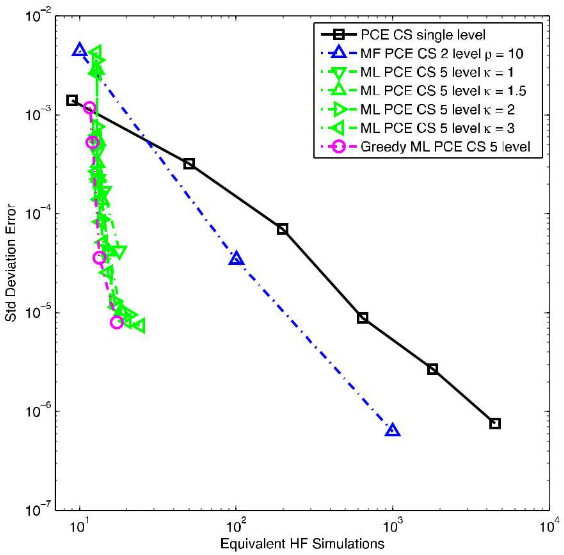
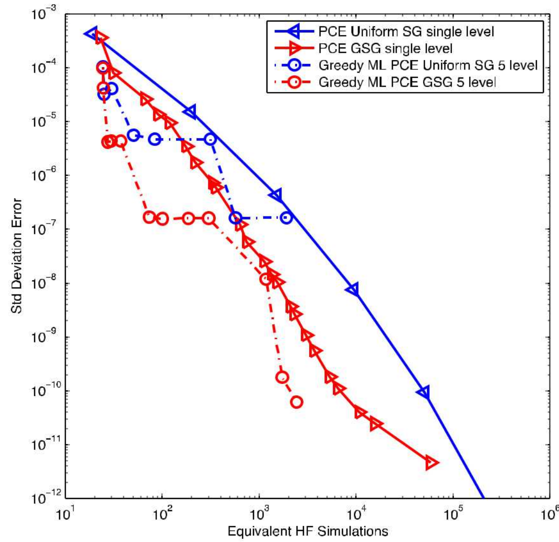
Multilevel / Multi-index PCE: greedy competition across models

Greedy ML PCE: uniform CS



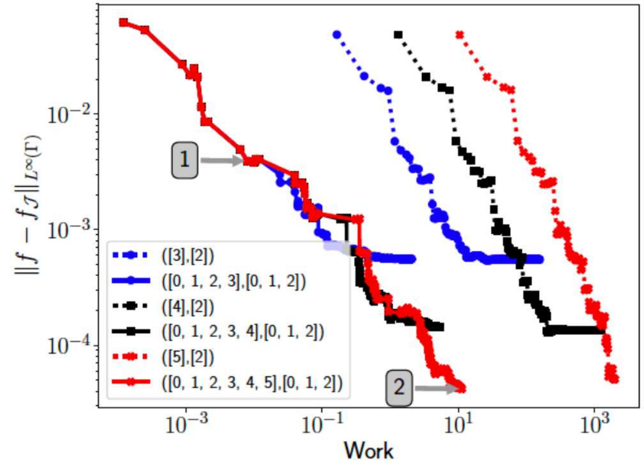
Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-1	198	9	9	9	9
1.e-2	644	198	9	9	9
1.e-3	1802	644	9	9	9
1.e-4	4505	1802	50	9	9

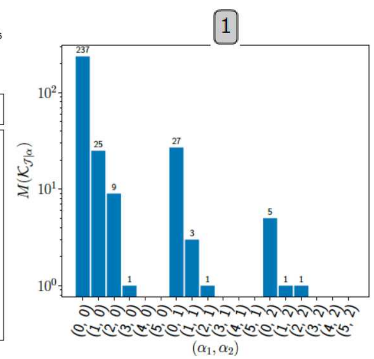
Greedy ML PCE: uniform / generalized SG

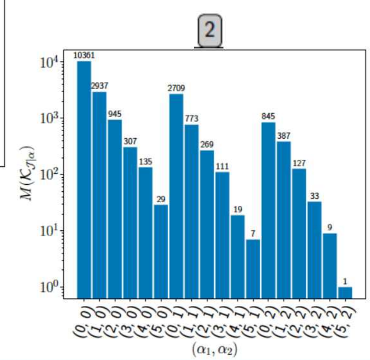


Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-2	43	23	19	19	19
1.e-4	211	83	19	19	19
1.e-6	391	271	156	19	19
1.e-8	1359	743	327	59	19
1.e-10	3535	2311	1039	391	19
1.e-12	10319	5783	2783	1343	43
1.e-14	26655	14991	8063	3703	1535

Greedy multi-index PCE







SWiFT Site Experimental Uncertainty Quantification

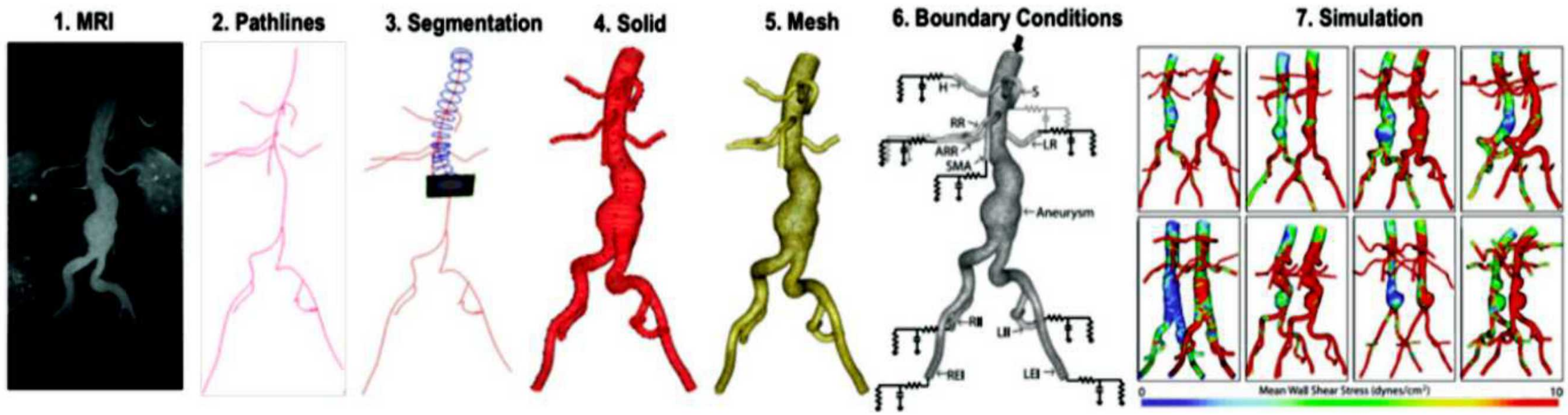
- Inflow Measurements
  - α
  - ρ
  - p
  - RH
  - T
  - TI (sonic)
  - U (sonic)
  - V (sonic)
  - WD (sonic)
- Turbine Measurements
  - Aerodynamic power
  - Rotor speed
  - Aerodynamic torque
  - Rotor thrust
  - Individual blade root loads
  - Yaw heading
  - Yaw misalignment
  - Blade pitch
  - Rotor azimuth
  - Nacelle acceleration
- Wake Measurements
  - DTU Spinner Lidar
  - Wake identification and tracking
  - Turbulence estimators

Ranges for uniform distributions of the three uncertain variables considered in this study.

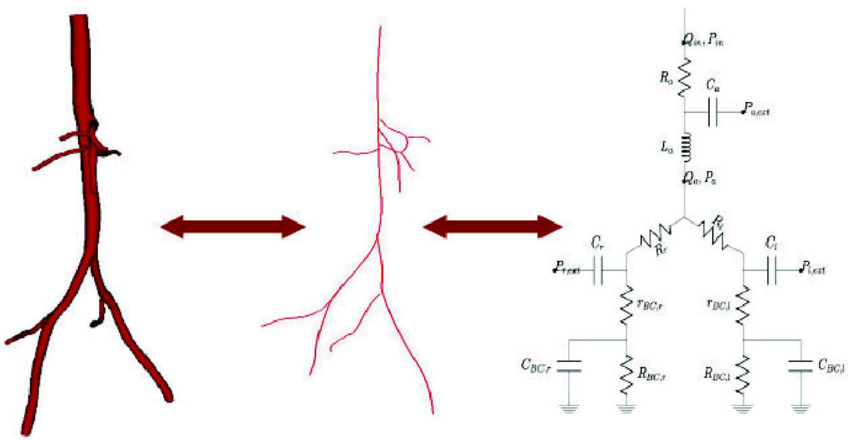
Uncertainty	Minimum	Maxmimum
Speed	6.5 m/s	7.5 m/s
Density	0.97 kg/m^3	1.19 kg/m^3
Yaw	-25^o	25^o

Multilevel – Multifidelity Sampling Methods

Cardiovascular flow



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

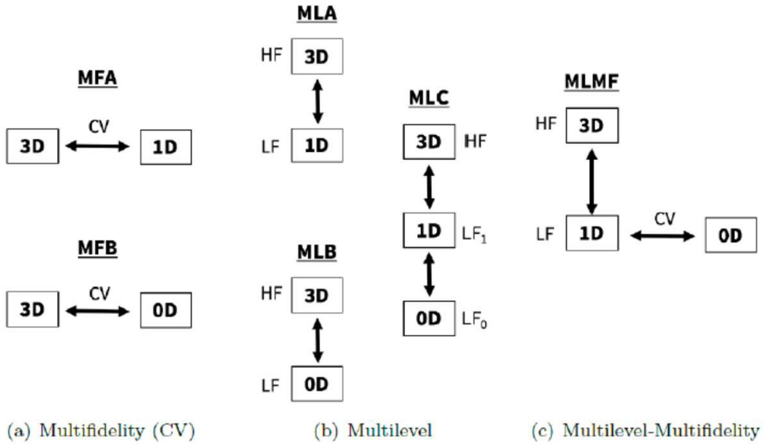


3D Model 1D Model 0D Model

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

Multilevel – Multifidelity Sampling Methods
Cardiovascular flow

Model relationships / graph topologies



Costs to achieve prescribed error tolerance

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

Implies need for not presuming a fixed topology…

Sampling Methods: Classical Control Variate → Multifidelity MC

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

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

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

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

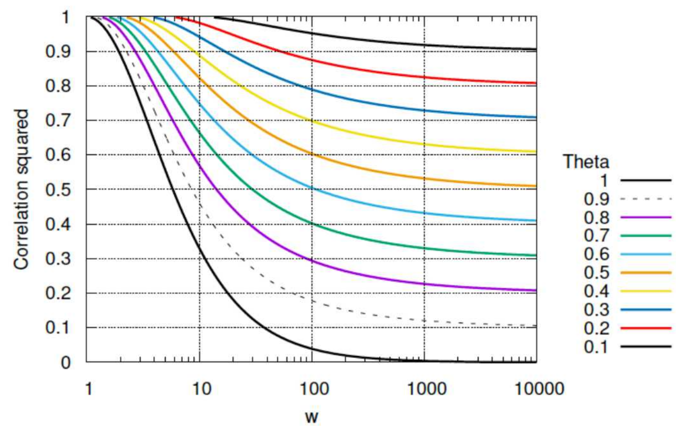
Let's modify the high-fidelity QoI, Q_M^{HF}, to decrease its variance

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

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

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

MFMC cost relative to MC



Minimize CV estimator variance → control param. as before:

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

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

Sampling Methods:
Combining ML and CV for multidimensional model hierarchies

- OUTER SHELL – Multi-level

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

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

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

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

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

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

Optimal sample allocation across discretizations and model forms

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

G. Geraci, E., G. Iaccarino, "A multifidelity control variate approach for the multilevel Monte Carlo technique," CTR Res Briefs 2015.

Multilevel – Multifidelity Sampling Methods

Results on model problem: wave propagation in composites

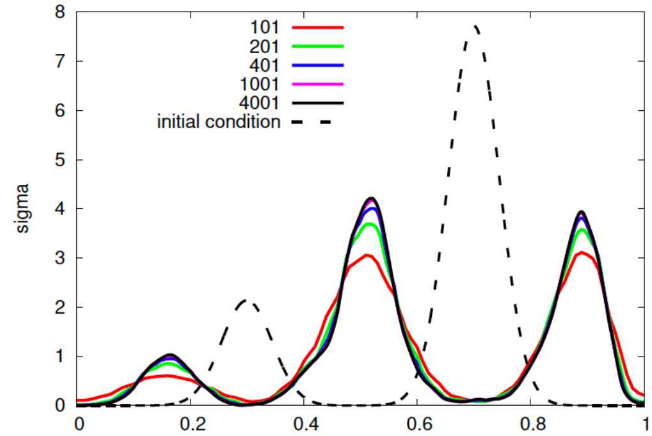
- Rod constituted by 50 layers, two alternated materials (A and B) with constitutive laws

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

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

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

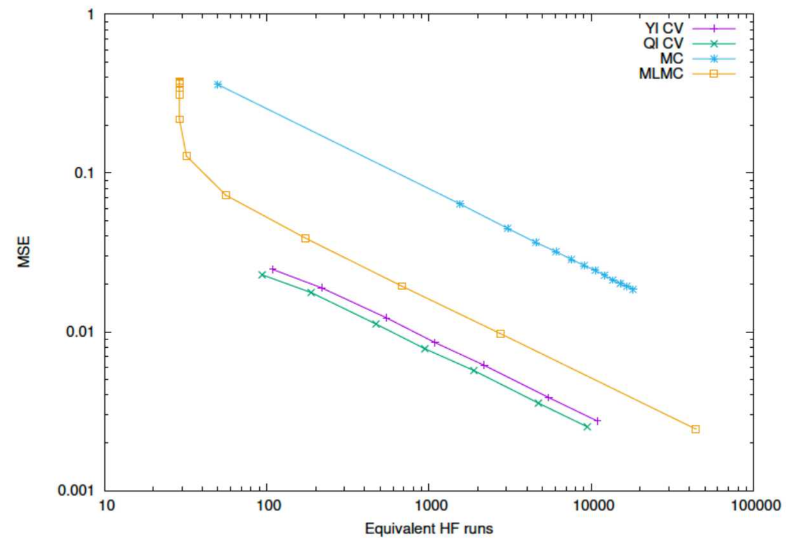
- Spatially varying uncertain density: $\rho(x) = \xi_1 + 0.5 \sin(2\pi x), \xi_1 \sim \mathcal{U}(1.5, 2)$
- Clamped rod as B.C.



28 random variables

Two fidelities, each with 4 discretizations

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



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