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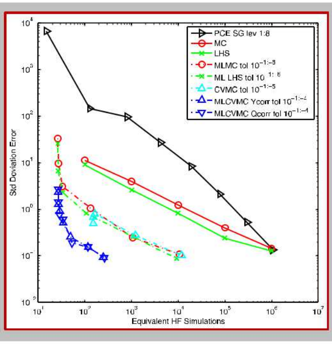
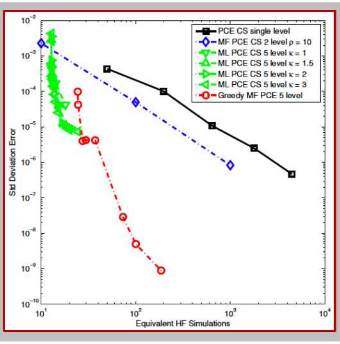
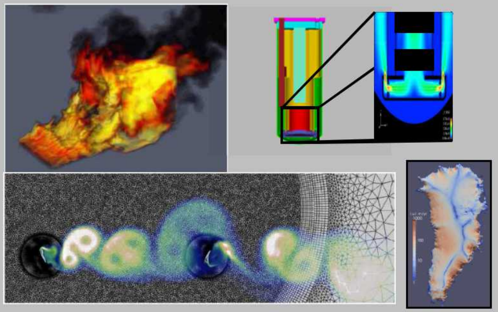




DAKOTA

Explore and predict with confidence



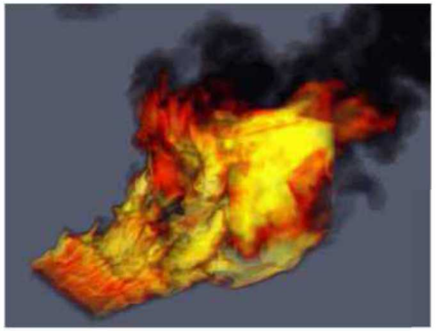
Advanced UQ Methods in Dakota

Michael S. Eldred
Sandia National Laboratories, Albuquerque NM

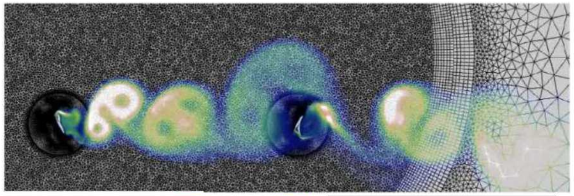
ASC V&V Program Review, May 23, 2019

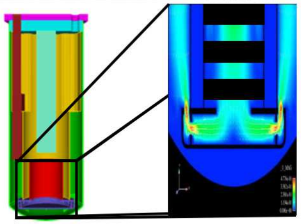
UQ & Optimization: DOE/DOD Mission Deployment

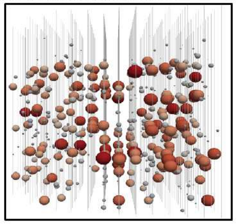
Stewardship (NNSA ASC)
Safety in abnormal environments



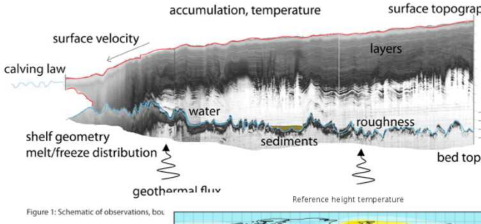
Energy (ASCR, EERE, NE)
Wind turbines, nuclear reactors

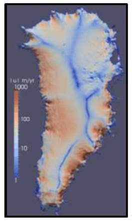


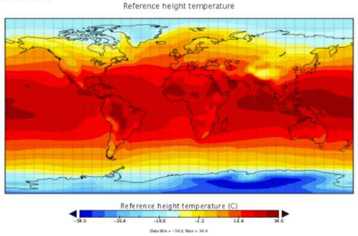




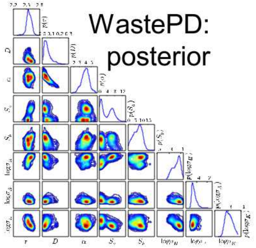
Climate (SciDAC, CSSEF, ACME)
Ice sheets, CISM, CESM, ISSM, CSDMS

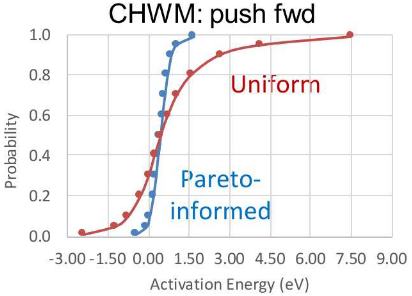


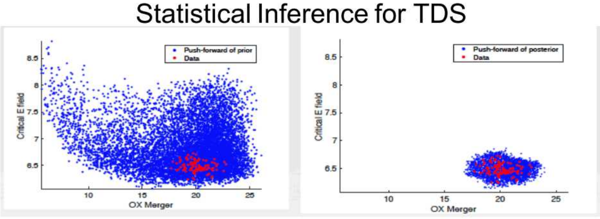




Addtnl. Office of Science:
(SciDAC, EFRC)
Comp. Matls: waste forms / hazardous matls (WastePD, CHWM)
MHD: Tokamak disruption (TDS)







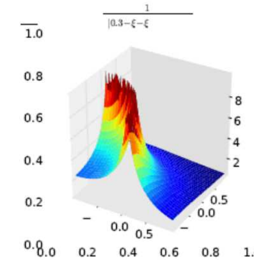
Common theme across these applications:

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

Emphasis on Scalable Methods for High-fidelity UQ on HPC

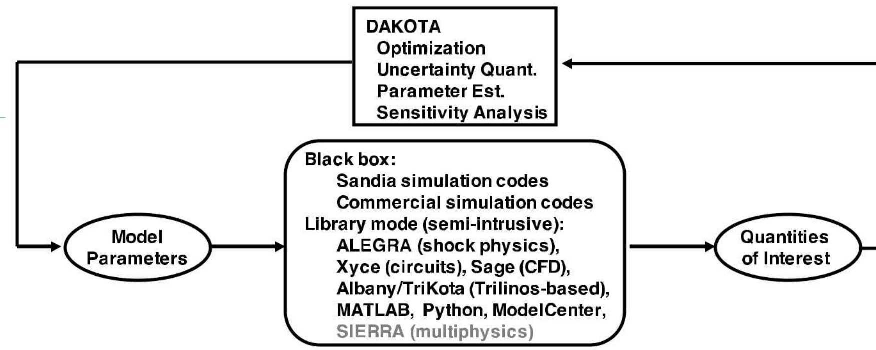
Compounding effects:

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



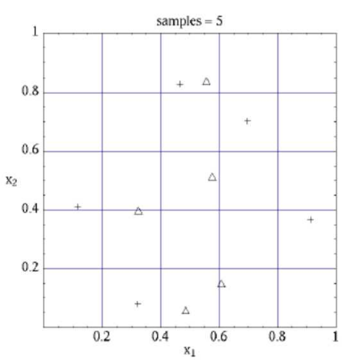
Steward Scalable Algorithms within DAKOTA

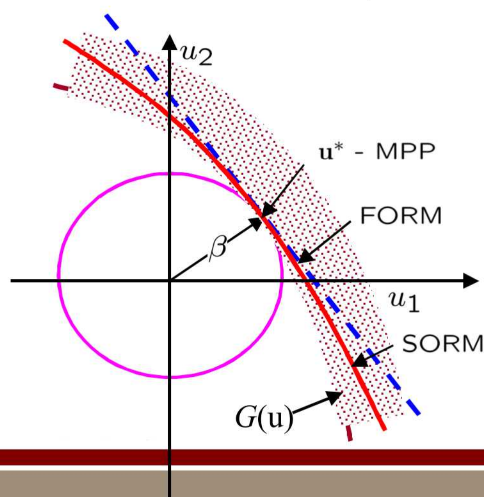
Explore and predict with confidence

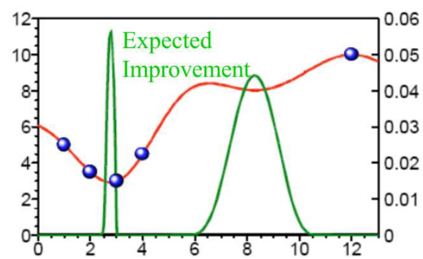


Core (Forward) UQ Capabilities:

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

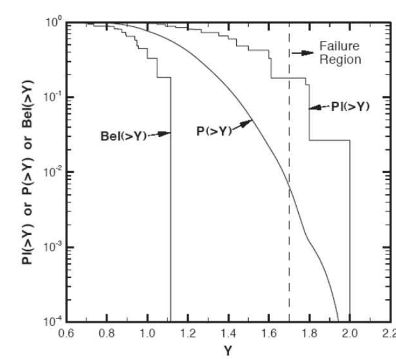






$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

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

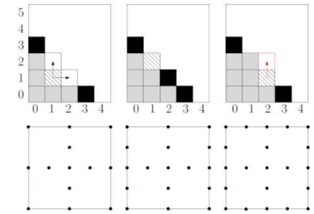


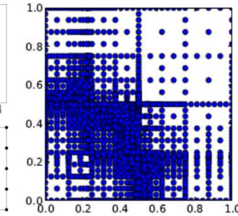
Research Thrusts for UQ

Sandia National Laboratories

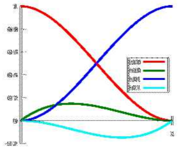
- *Focus:* Compute dominant uncertainty effects despite key challenges

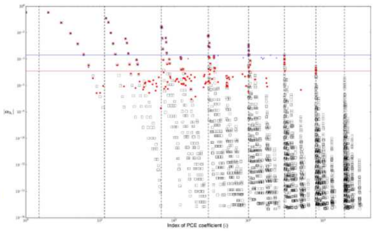
- Emphasize scalability and exploitation of special structure
  - *Adaptivity:* p- and h- refinement of stochastic expansions
  - *Adjoints:* gradient enhancement for PCE / SC / GP
  - *Sparsity:* compressed sensing
  - *Low Rank:* tensor / function train (w/ UMich)
  - *Dimension reduction:* active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





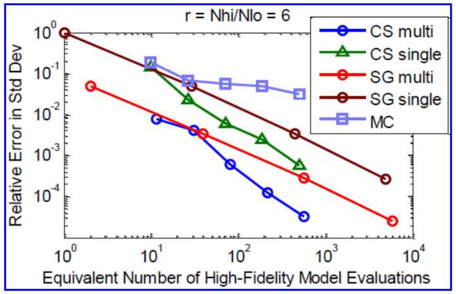
$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ \pi_{0,j}(\vec{\xi}_i) & \pi_{1,j}(\vec{\xi}_i) & \cdots & \pi_{P,j}(\vec{\xi}_i) \\ \frac{\partial \pi_{0,j}}{\partial \xi_1}(\vec{\xi}_i) & \frac{\partial \pi_{1,j}}{\partial \xi_1}(\vec{\xi}_i) & \cdots & \frac{\partial \pi_{P,j}}{\partial \xi_1}(\vec{\xi}_i)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





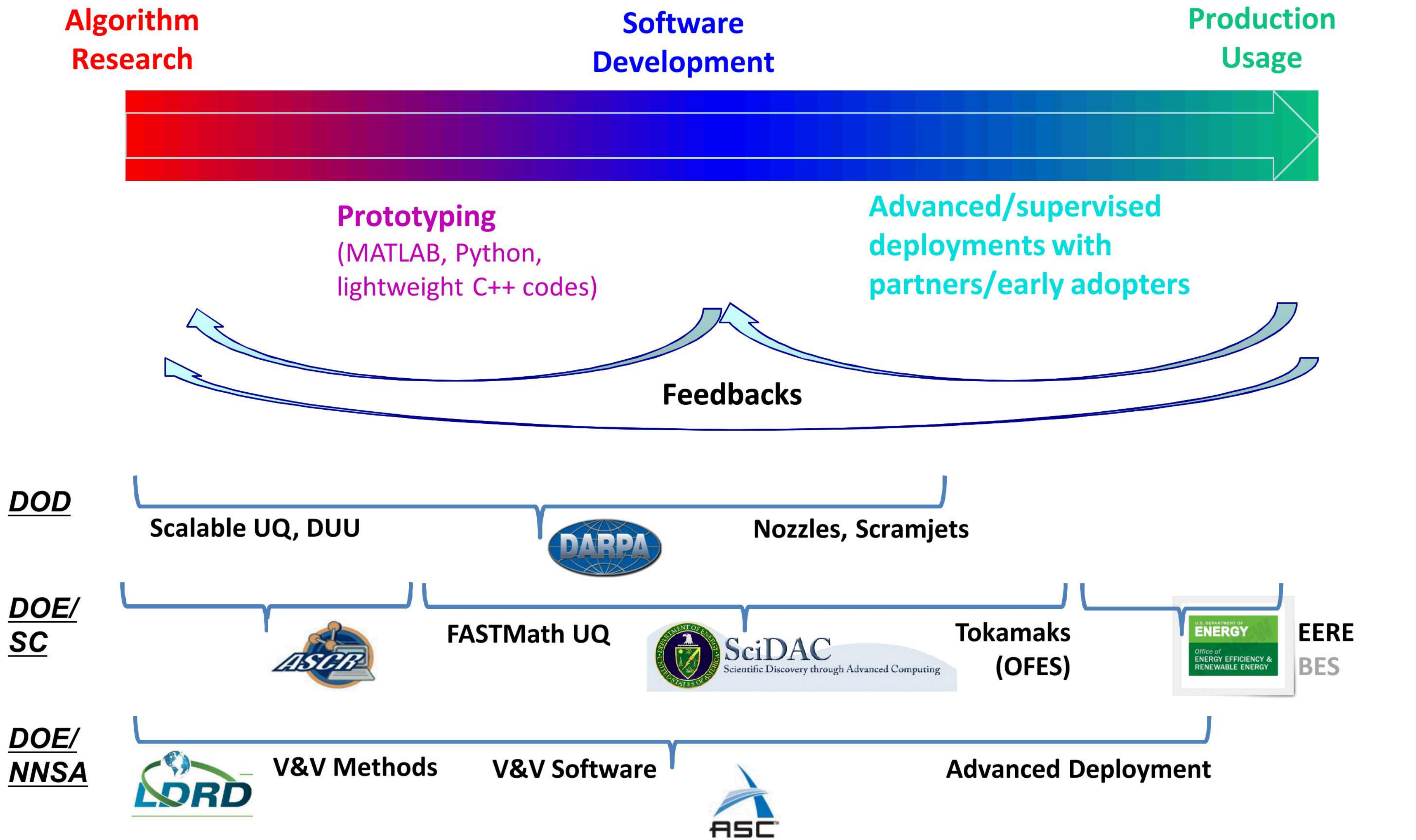
- Compound efficiencies
  - Multilevel-Multifidelity with sampling & CS/FT surrogates (new: ROM, NN)
  - Active subspaces: subspace quadrature, enhance MF control variates

- 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



Multiple Model Forms in UQ & Opt

Discrete model choices for simulation of same physics

A clear hierarchy of fidelity (from low to high)

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

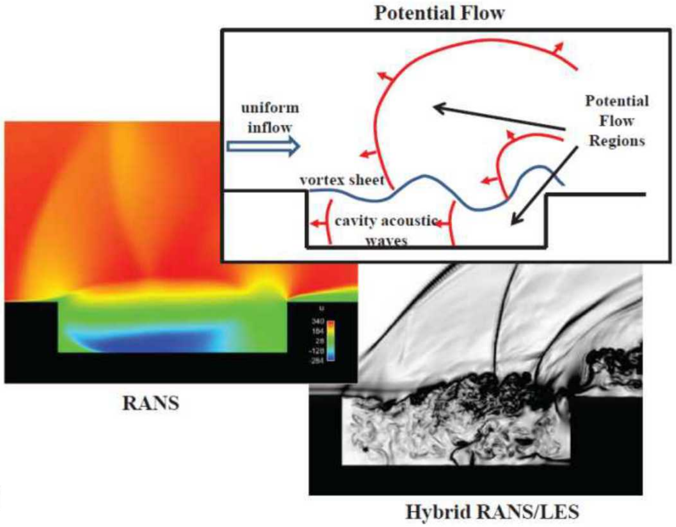
An ensemble of peer models lacking clear preference structure / cost separation: e.g., SGS models

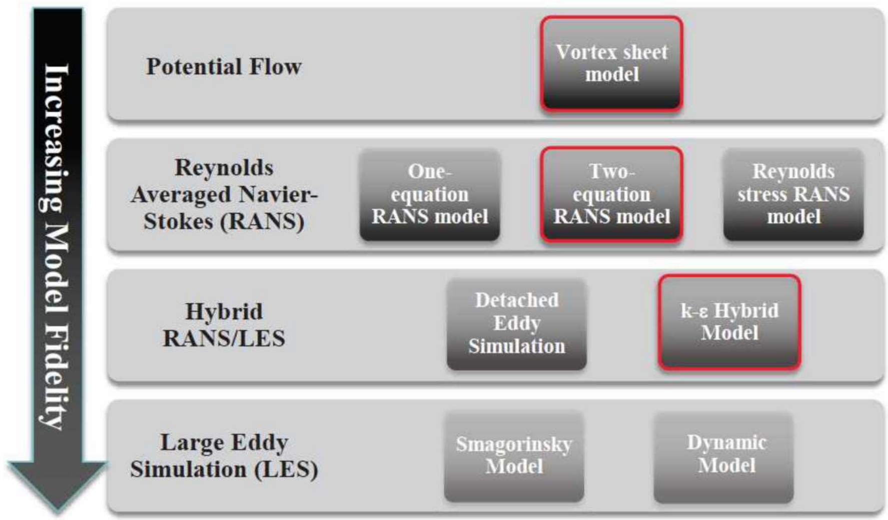
- *With data:* model selection, inadequacy characterization
  - Criteria: predictivity, discrepancy complexity
- *Without (adequate) data:* epistemic model form uncertainty propagation
  - Intrusive, nonintrusive
- *Within MF context:* CV correlation

Discretization levels / resolution controls

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

Combinations for multiphysics, multiscale





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:

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

two sources of error:

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

Looking at the Mean Square Error:

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

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

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:

- $\{M_\ell : \ell = 0, \dots, L\}$ 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

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

- Multilevel Monte Carlo estimator

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

- The Mean Square Error is

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

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

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)

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

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

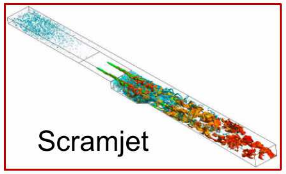
M. Giles, "Multilevel Monte Carlo path simulation," 2008.

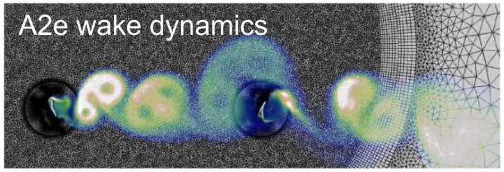
Research & Development in Multifidelity Methods

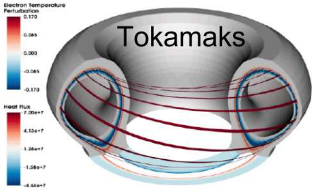
Sandia National Laboratories

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





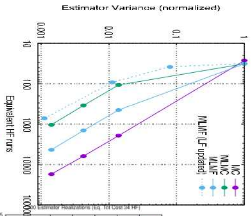


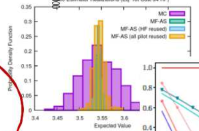
SECURE GC

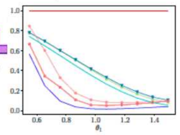
Emerging mission areas: abnormal thermal, Z-pinch MagLIF, quantum chemistry

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)

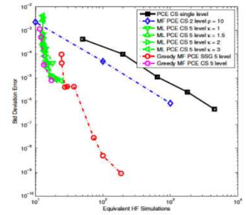


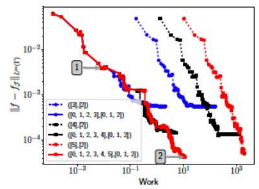




Surrogate UQ Methods (PCE, SC)

- *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

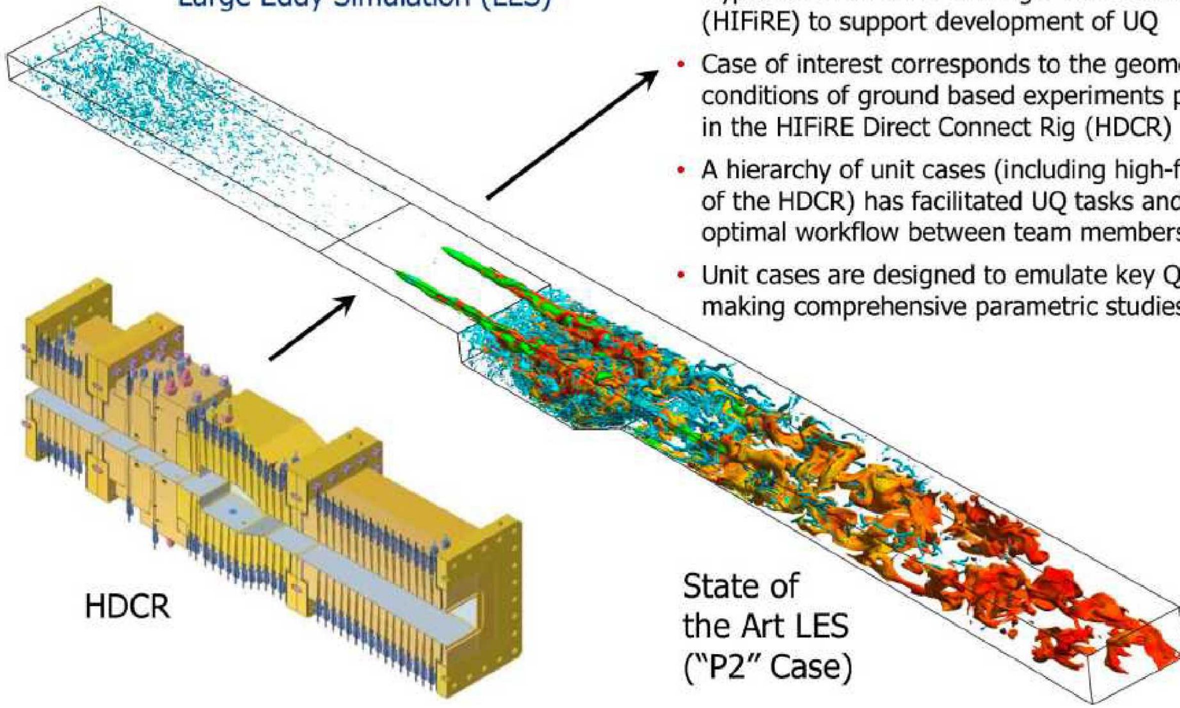
- *Emerging:*
  Derivative-based methods (DARPA SEQUOIA)
  - Multigrid optimization (MG/Opt)
  - Recursive trust-region model mgmt.: extend TRMM to deep hierarchies

  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)

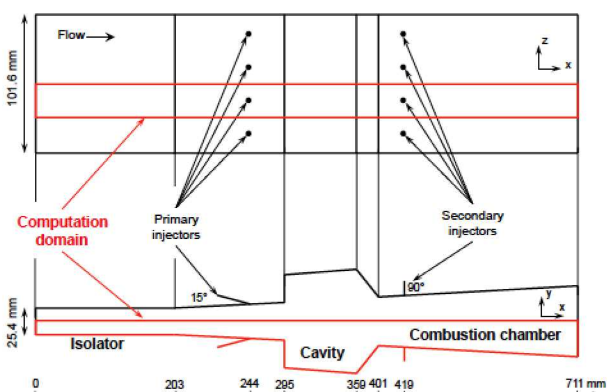
Key Challenge: existing ML/MF/MI performance is compelling on (elliptic) model problems, but significant generalization required for engineering applications with non-trivial model relationships

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

Multiscale-multiphysics application of Large Eddy Simulation (LES)

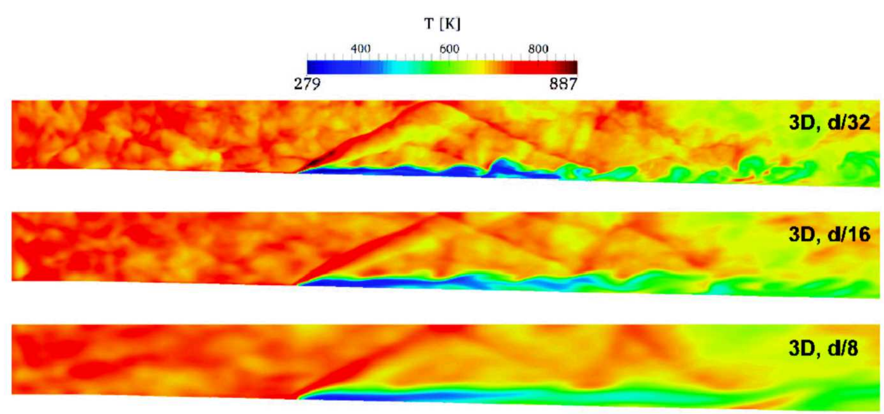


- Provided benchmark LES calculations of the Hypersonic International Flight Research Experiment (HIFiRE) to support development of UQ
- Case of interest corresponds to the geometry and conditions of ground based experiments performed in the HIFiRE Direct Connect Rig (HDCR)
- A hierarchy of unit cases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



Model forms:
- 2D, 3D

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

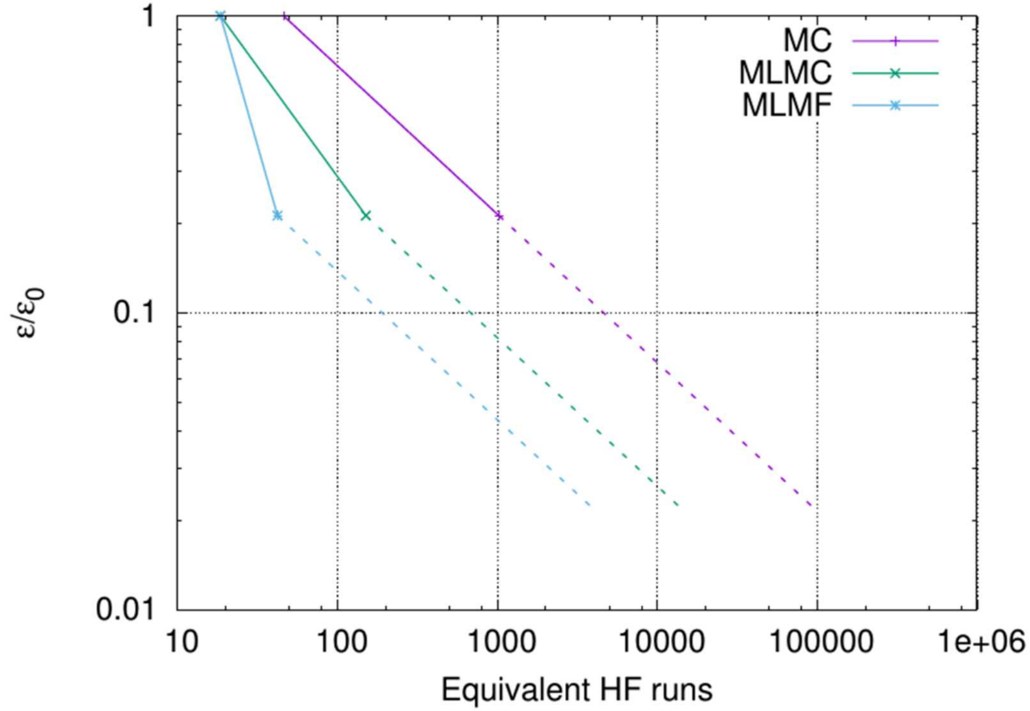


Initial Deployment of MLCV MC for Scramjet UQ

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

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

UQ Approach: MLCV algorithm described previously.



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

TABLE: Computational cost.

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

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

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

Updated Deployment of MLCV MC for Scramjet UQ

Sandia National Laboratories

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

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

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

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

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

Multilevel – Multifidelity Sampling Methods

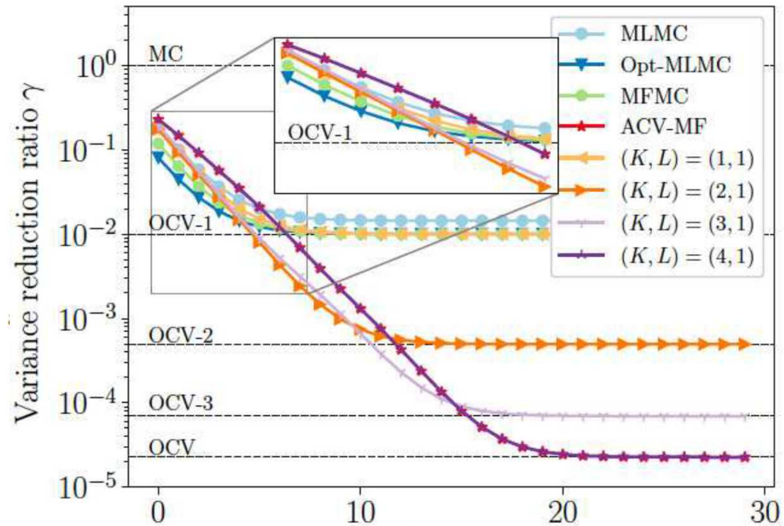
Sandia National Laboratories

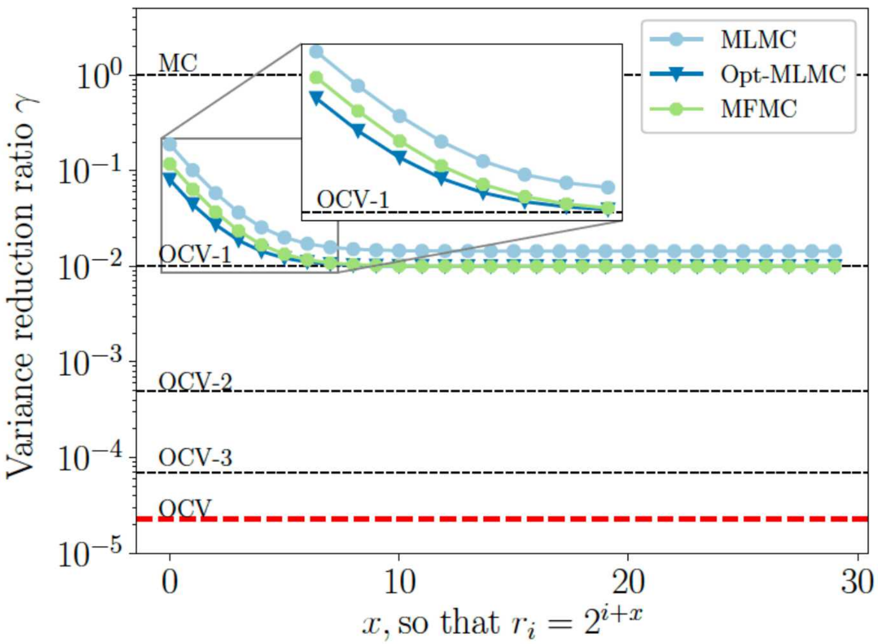
Research Direction: Generalized framework for approx. control variates

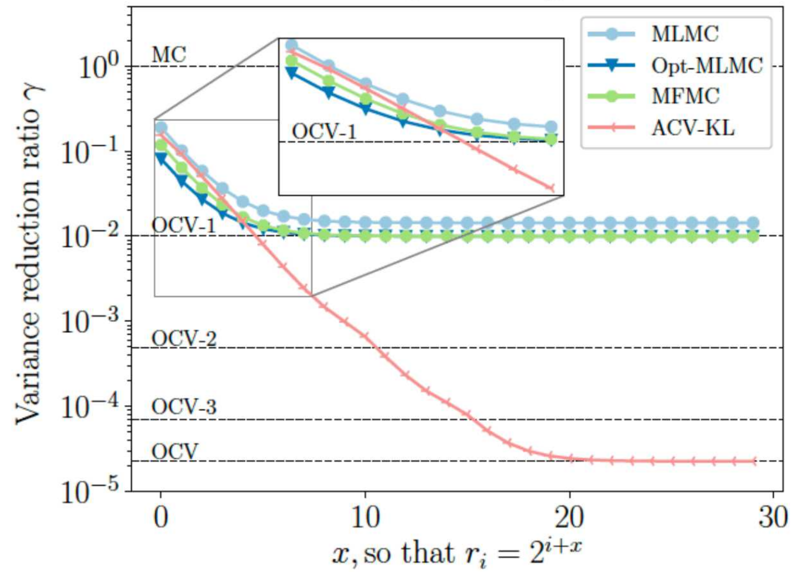
- Unification of ML and CV approaches
- Look beyond (recursive) model pairings

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

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







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

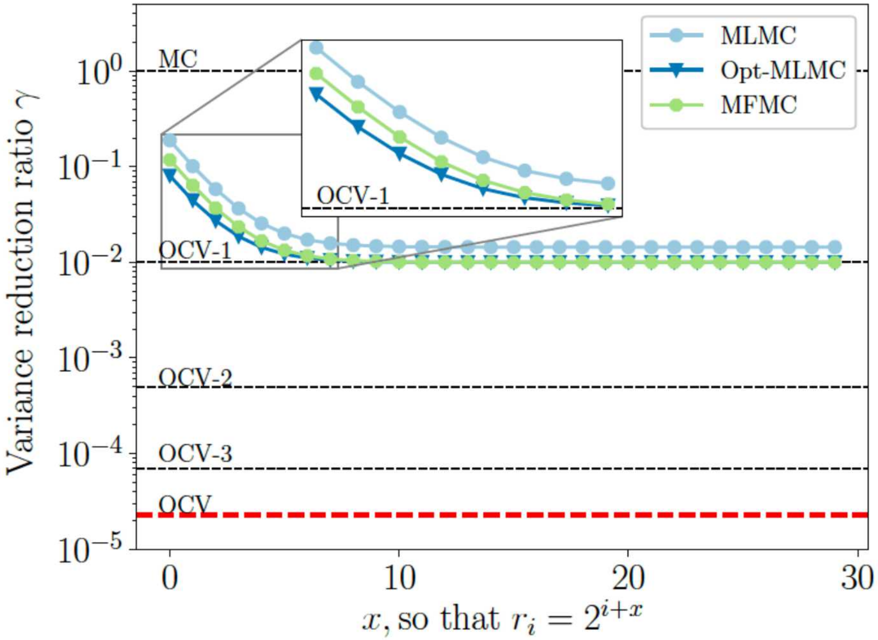
Multilevel – Multifidelity Sampling Methods

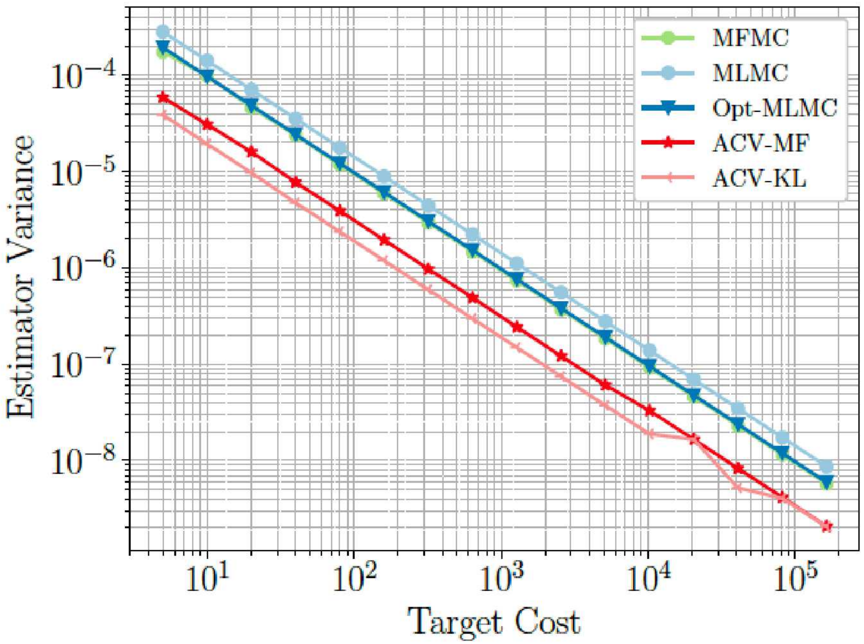
Research Direction: Generalized framework for approx. control variates

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

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

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





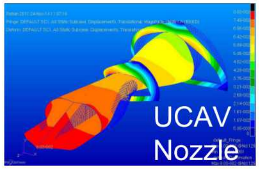
A. Gorodetsky, G. Geraci, E., J. Jakeman "A Generalized Framework for Approximate Control Variates," arxiv.org/abs/1811.04988

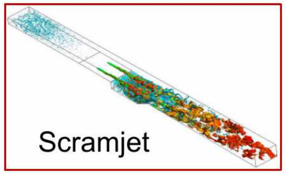
Research & Development in Multifidelity Methods

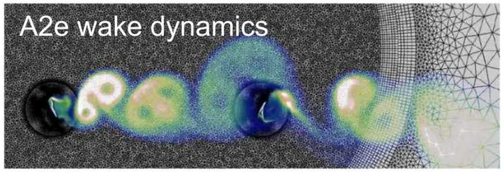
Sandia National Laboratories

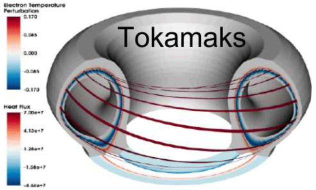
Recurring R&D theme: couple scalable algorithms with exploiting a (multi-dimensional) model hierarchy

- ➢ 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





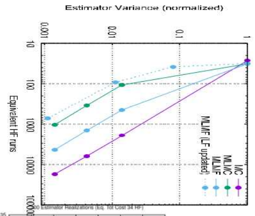


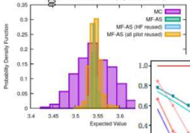


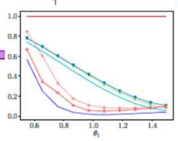
Emerging mission areas: abnormal thermal, Z-pinch MagLIF, quantum chemistry

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)

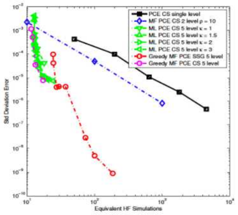


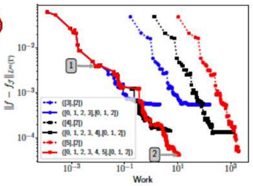




Surrogate UQ Methods (PCE, SC)

- *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

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

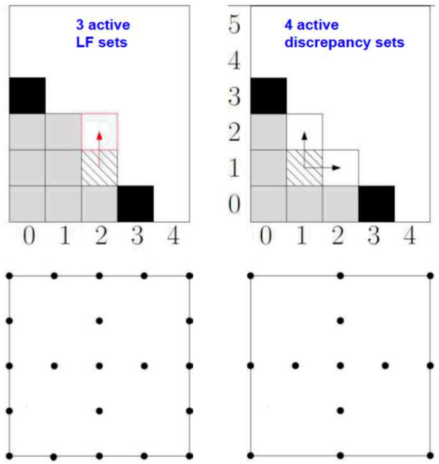
Compete refinement candidates across model levels: max induced change / cost

- 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

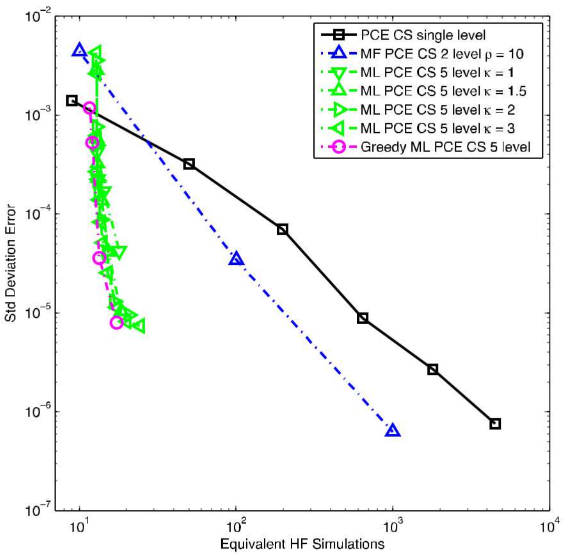
Level candidate generators:

- *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.)



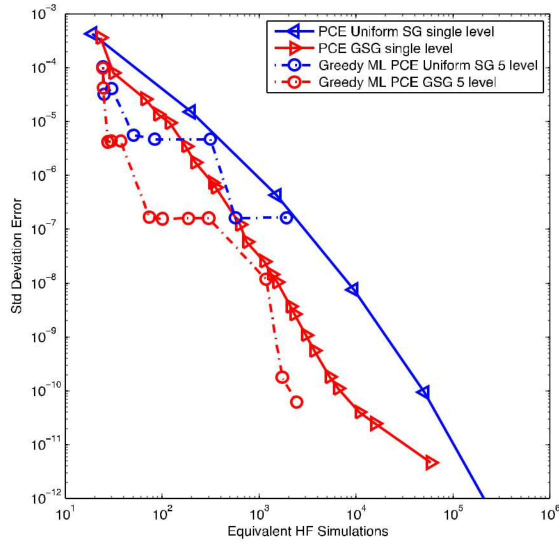
Multilevel / Multi-index PCE: greedy competition across models

Greedy ML PCE: uniform CS



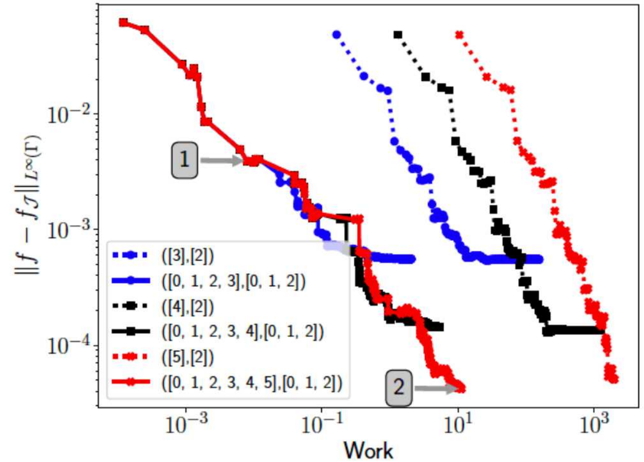
Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-1	198	9	9	9	9
1.e-2	644	198	9	9	9
1.e-3	1802	644	9	9	9
1.e-4	4505	1802	50	9	9

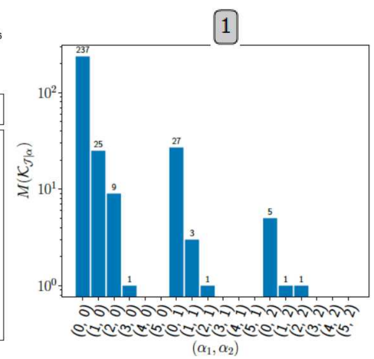
Greedy ML PCE: uniform / generalized SG

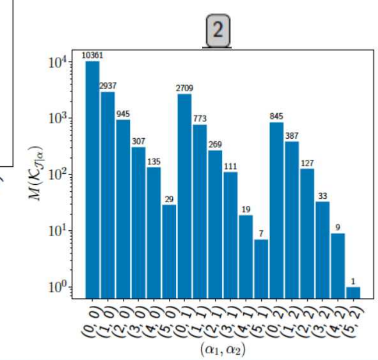


Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-2	43	23	19	19	19
1.e-4	211	83	19	19	19
1.e-6	391	271	156	19	19
1.e-8	1359	743	327	59	19
1.e-10	3535	2311	1039	391	19
1.e-12	10319	5783	2783	1343	43
1.e-14	26655	14991	8063	3703	1535

Greedy multi-index PCE







Advanced UQ Methods in Dakota (ASC V&V Methods) – Mike Eldred

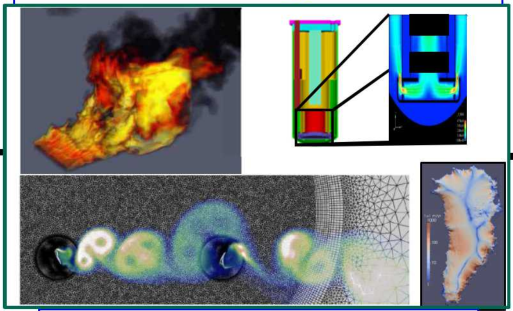
Background

- Emphasis on UQ with high-fidelity simulation models: SOA in computational M&S w/ HPC
  → Severe simulation budget constraints (e.g., handful of HF runs)
  → Significant dimensionality, driven by model complexity
  → Can make fwd propagation / inference / OUU / OED untenable
- Multiple model fidelities / discretizations are often available that trade accuracy for cost
  - In CFD for example, common model fidelities include potential flow, inviscid Euler, RANS, and LES / DNS, each potentially supporting multiple spatio-temporal resolutions

Approach, Metrics, and Outcomes

- Exploit special problem structure when available
- Leverage all available information sources
- Scalable architecture for ensemble computing
- Coordination/Communication
  - Dakota team in 1463, 8754, 1424, 1544, et al.
  - Many academic collaborations: Stanford, MIT, UMich, USC, UT Austin, CU Boulder, Duke, et al.
  - Lab collaborations: LANL-ESA, LLNL A (UQ Pipeline), ORNL
- Assumptions & limitations:
  - Avoid simplifying assumptions → generalized frameworks, UQ risk mitigations
    - Sampling: robust, noise-tolerant
    - Surrogate: exploit special structure

Defense / Energy / Climate

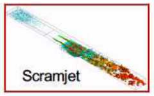


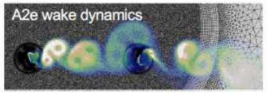
DOE/NNSA, DOE/SC, DOD

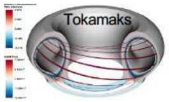
Impact

- Healthy research to production pipeline
- Mission applications across DOE/NNSA, DOE/SC, DOD

Recent / current MLMF deployments:

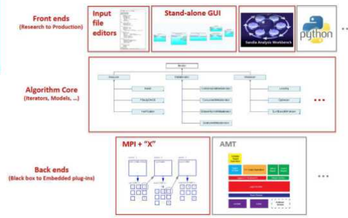


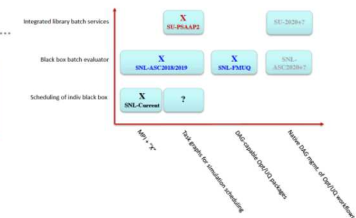




Emerging mission areas: abnormal thermal, Z-pinch MagLIF, quantum chemistry

Strategic Vision





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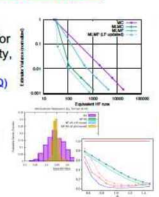

Informs

Polynomial Chaos UQ Methods

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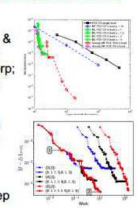

Informs

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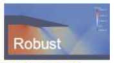


Extra

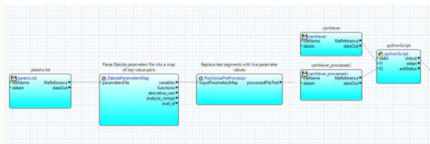
High-Level Vision for Next Generation Architecture

Dakota-MPI, Dakota-X, Py-Dakota, …

Front ends
(Research to Production)

Input file editors

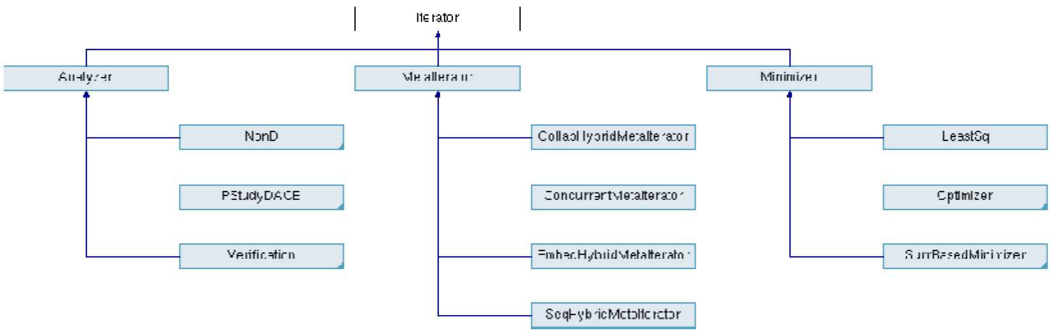
Stand-alone GUI



python

…

Algorithm Core
(Iterators, Models, …)



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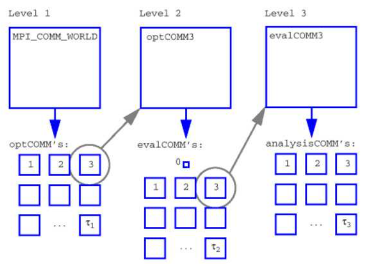
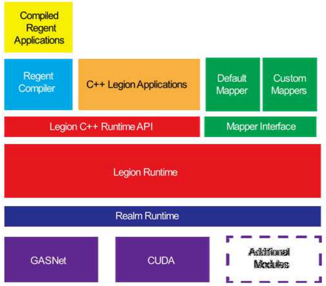
Back ends
(Black box to Embedded plug-ins)

MPI + "X"



AMT



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An Initial Capability Roadmap

At least two dimensions of evolving capability / complexity