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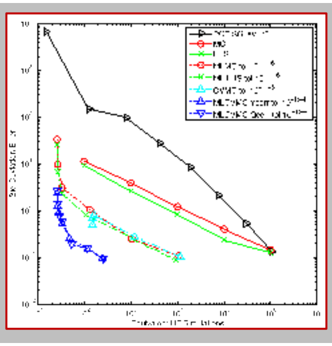
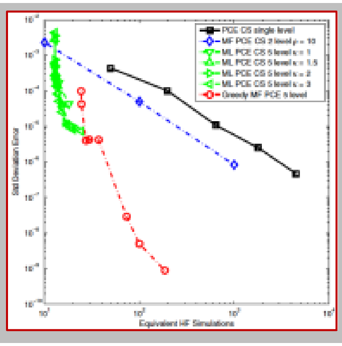
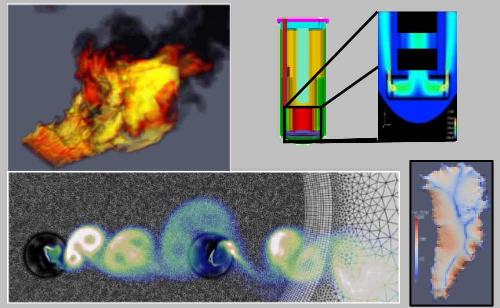




DAKOTA

Explore and predict with confidence



The Dakota Project: Connecting the Pipeline from Uncertainty Quantification R&D to Mission Impact

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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DAKOTA

Explore and predict with confidence.

C++ toolkit that provides a variety of non-intrusive algorithms for performing iterative analysis with simulation codes.

Algorithms: design optimization, model calibration, *uncertainty quantification*, DACE, GSA, parametric studies

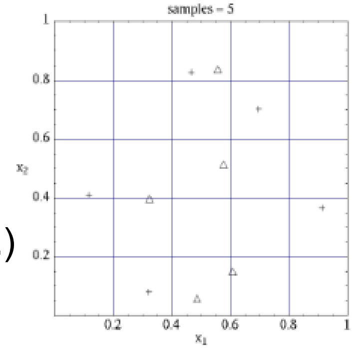
Framework: plug and play method selection, composition of methods/models with nesting, recasting, surrogates

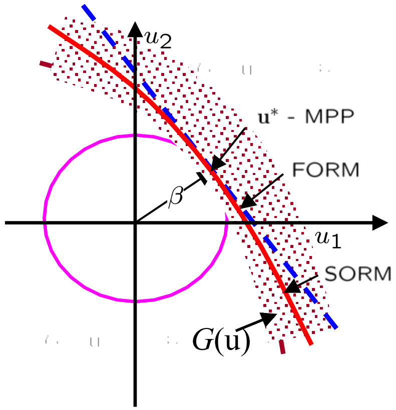
Computing: **supports multiple levels of parallelism for scalability on both capability and capacity HPC resources**

Interfacing: can be used as either a stand-alone application or as a set of library services

Core forward UQ components

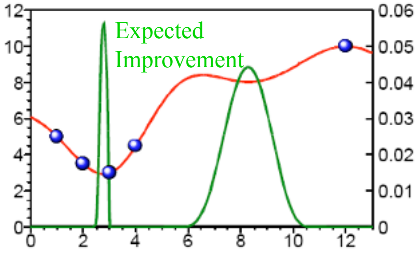
- **Sampling:** Monte Carlo, Latin hypercube; Incremental, Importance
- **Reliability:** Local (FORM, AMV+, TANA/QMEA); Global (EGRA, GPAIS, POF Darts)
- **Stoch. expansion:** PCE (project, regress), SC (nodal, hierarch), FTT (regress, cross appr.)
- **Epistemic:** Interval estimation (local, global); Dempster-Shafer

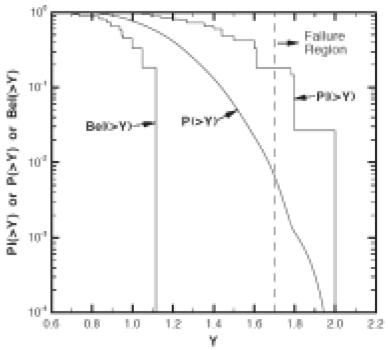




Advanced (multi-component) capabilities

- **Bayesian methods:** QUESO, GPMSA, DREAM, MUQ; Emulator-based MCMC
- **Nested studies:** Mixed aleatory-epistemic UQ; Optimization under uncertainty
- **Multilevel-Multifidelity:** sampling, surrogates, hybrid
- **Dimension reduction:** Active subspaces, adapted basis PCE



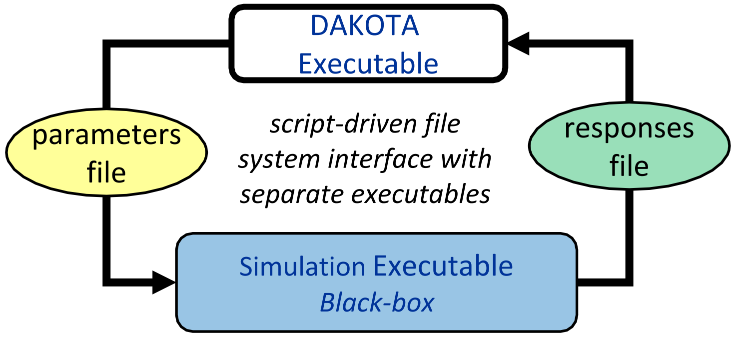


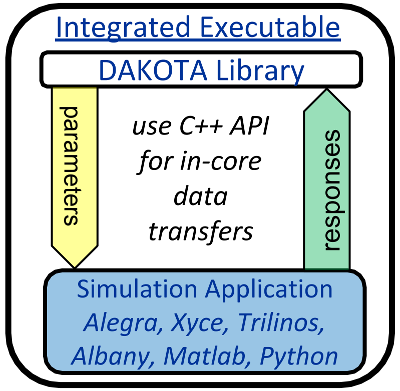
$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

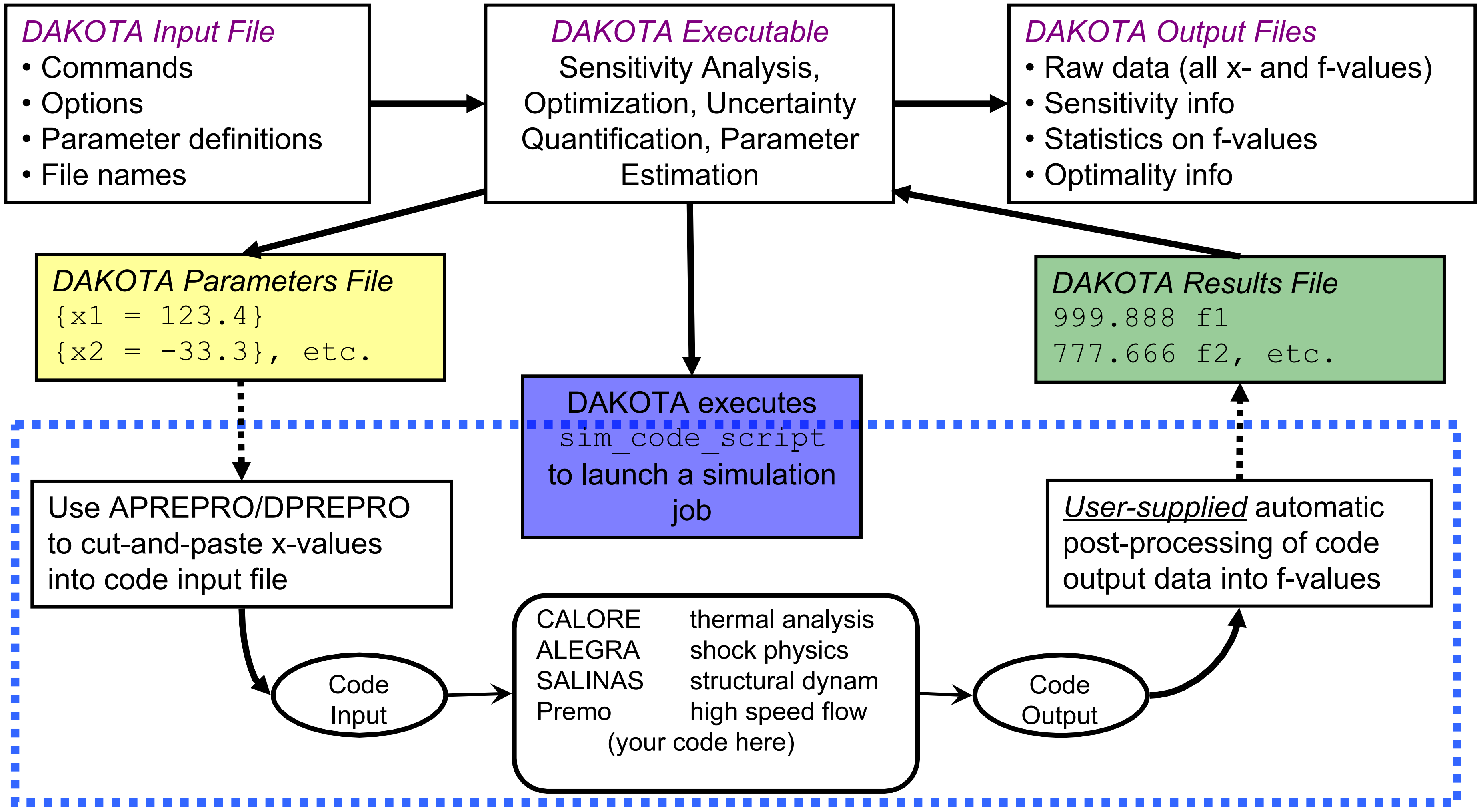
$$R(\boldsymbol{\xi}) \cong \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

Simulation interfacing

- Black box
- Embedded service







Agile Components Vision, ~2012

Non-intrusive (NAND / MDF)

- All residuals eliminated, coupling satisfied
- DAKOTA optimization & UQ

Intrusive to coupling (IDF)

- Indiv. physics residuals eliminated; coupling enforced by opt/UQ
- DAKOTA opt/UQ & ROL opt.

Intrusive to physics (SAND / AAO)

- No residuals eliminated
- ROL opt., Stokhos UQ

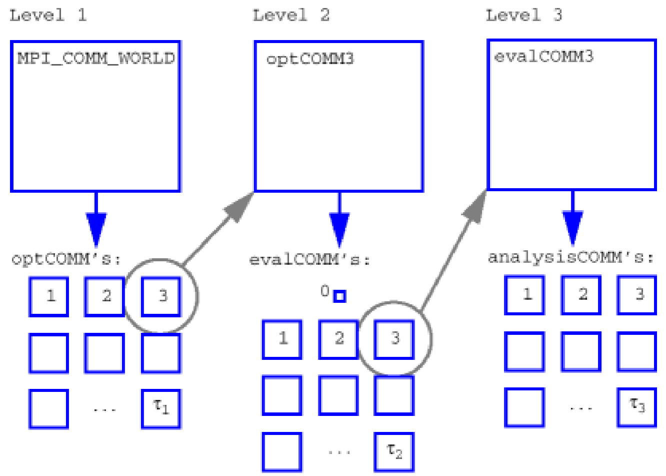
High-Performance Computing for Enabling High-Fidelity Opt/UQ

Exploiting multiple sources of parallelism

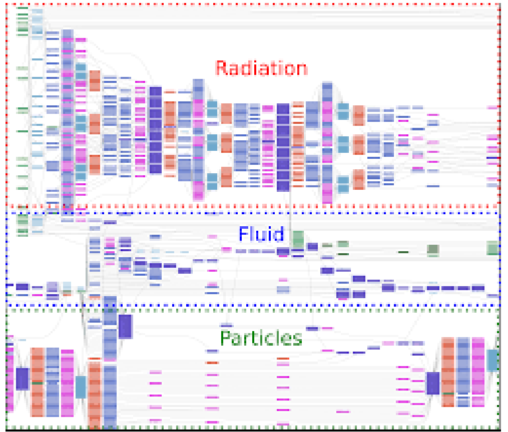
Production (~1998): Multilevel parallelism via MPI + "X" (= asynchronous local system call, fork, thread), effectively separating internal Dakota from external resource scheduling

1. *Algorithmic coarse-grained*: concurrency in data requests:
    - Iterators: Gradient-based, Nongradient-based, Surrogate-based
    - Strategies with concurrent Iterators: Multi-start, Pareto, Hybrid, MINLP
    - Nested Models: OUU/MCUU, Mixed UQ
2. *Algorithmic fine-grained:* computing the internal linear algebra of an opt. algorithm in parallel (e.g., large-scale opt., SAND)
3. *Fn eval coarse-grained:* concurrent execution of separable simulations within a fn. eval. (e.g., multiple loading cases)
4. *Fn eval fine-grained:* parallelization of the solution steps within a single analysis code (e.g., ALEGRA, Xyce, SIERRA)

Recursive partitioning & scheduling with MPI Communicators



Legion task graph for Soleil-X (PSAAP2)



Next-Gen Exploratory (2020): Asynchronous many task (AMT) parallelism

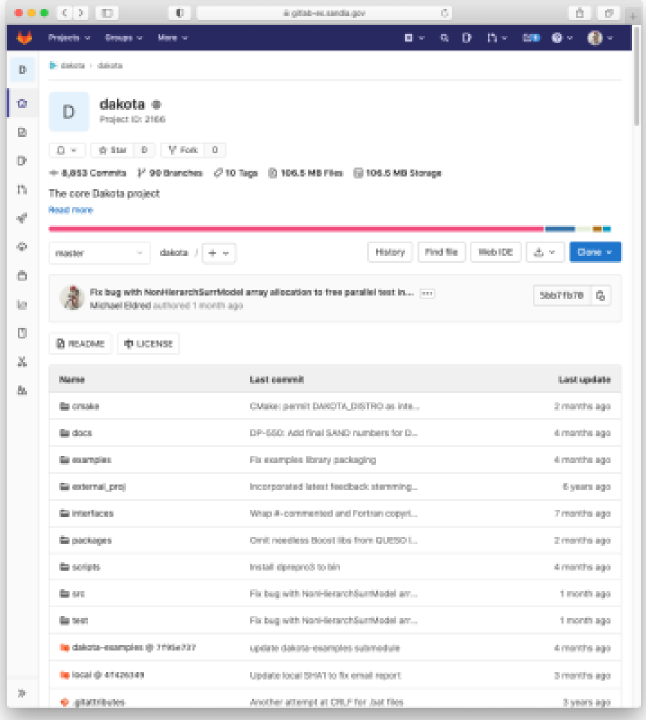
- Ensemble-based UQ workflows amplify the aggregate task graph
    - Heterogeneity in simulation fidelities and computing hardware
    - Fine-grained task optimizations expected to outperform coarse-grained job scheduling
- Collaboration w/ Stanford on Legion + ensembles via PSAAP2, PSAAP3

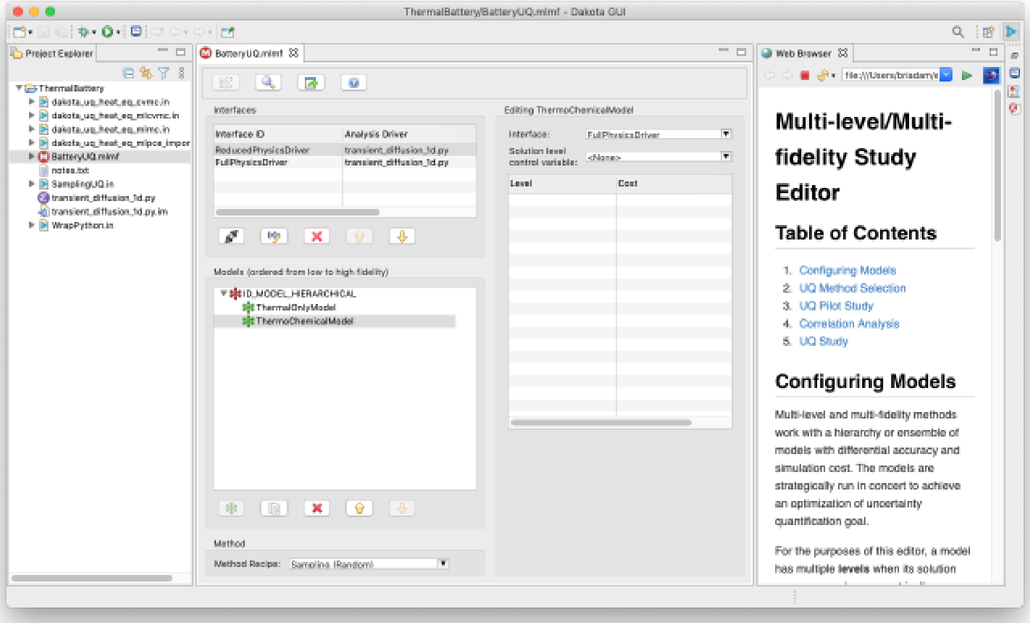
Resources

http://dakota.sandia.gov
Manuals, Publications, Training matls. online

May/November Releases: v6.14 released May 2021
Supported platforms: Linux, Mac, Windows
Modern SQE: Nightly builds/testing, gitlab, cmake
GNU LGPL: free downloads worldwide
Community development: moving to git pull requests
Community support: dakota-users list, [user forums]

Dakota UI: integrate study wizards, docs, pilot analysis for method selection





UQ & Optimization: DOE/DOD Mission Deployment

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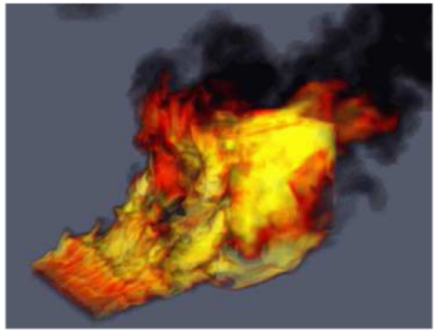
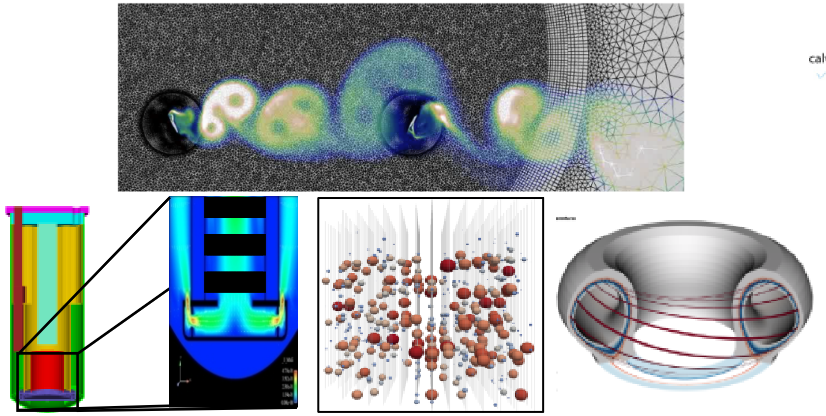
Stewardship (NNSA ASC)

Safety in abnormal environments



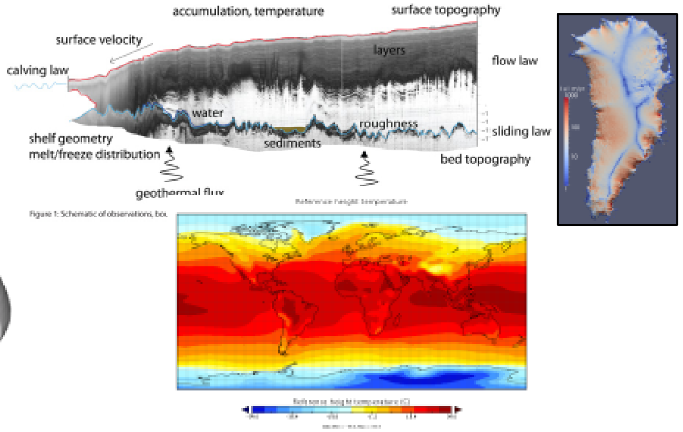
Energy (ASCR, EERE, NE)

Wind turbines, nuclear reactors



Climate (SciDAC, CSSEF, ACME)

Ice sheets, CISM, CESM, ISSM, CSDMS



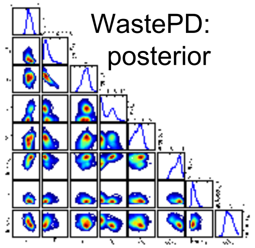
Additional Office of Science:

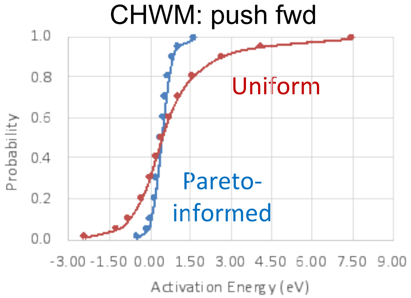
(SciDAC, EFRC, BES)

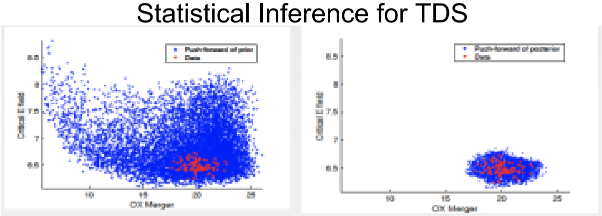
Comp. Matls: waste forms / hazardous matls (WastePD, CHWM)

MHD: Tokamak disruption (TDS)

Quantum Chem: soot modeling







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)

Research Thrusts for UQ

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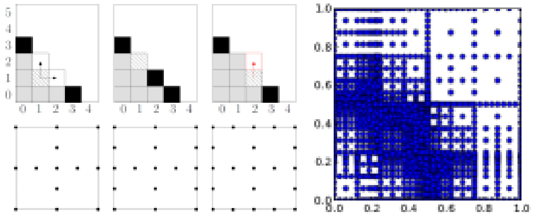
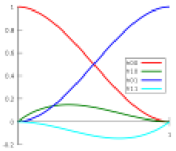
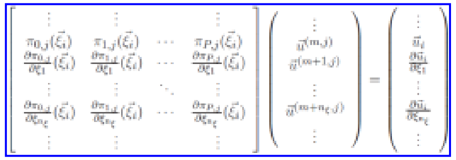
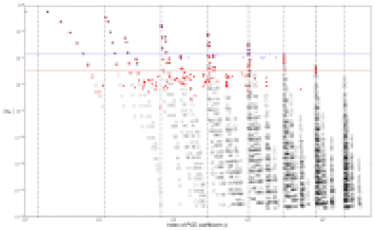
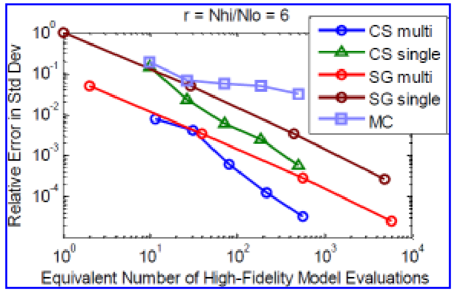
- *Focus:* Compute dominant uncertainty effects despite key challenge of high–{D,Fidelity}
- *Foundational:* Emphasize scalability through exploitation of special structure
  - *Adaptivity:* p- and h- refinement of stochastic expansions
  - *Adjoints:* gradient enhancement for PCE / SC / GP
  - *Sparsity:* compressed sensing
  - *Low rank:* tensor / function train (w/ UMich)
  - *Dimension reduction:* active subspaces (w/ CU Boulder), adapted basis (w/ USC)
- *Building on foundation:* Compound efficiencies
  - Multilevel-Multifidelity with sampling & CS/FT surrogates (new: ROM, NN, GP)
  - Active subspaces/Adapted basis: link dissimilar parameterizations, enhance correlation
- *Building on foundation:* Address complexity w/ component-based approach
  - Emulator-based Bayesian inference, Mixed aleatory-epistemic UQ, Optimization under uncertainty, Optimal experimental design
- Position UQ for next generation architectures
  - *Current (imperative):* multilevel parallelism (MPI comm. partitioning + nested scheduling)
  - *Future (declarative):* collaborations with Legion in Stanford PSAAP{2,3}



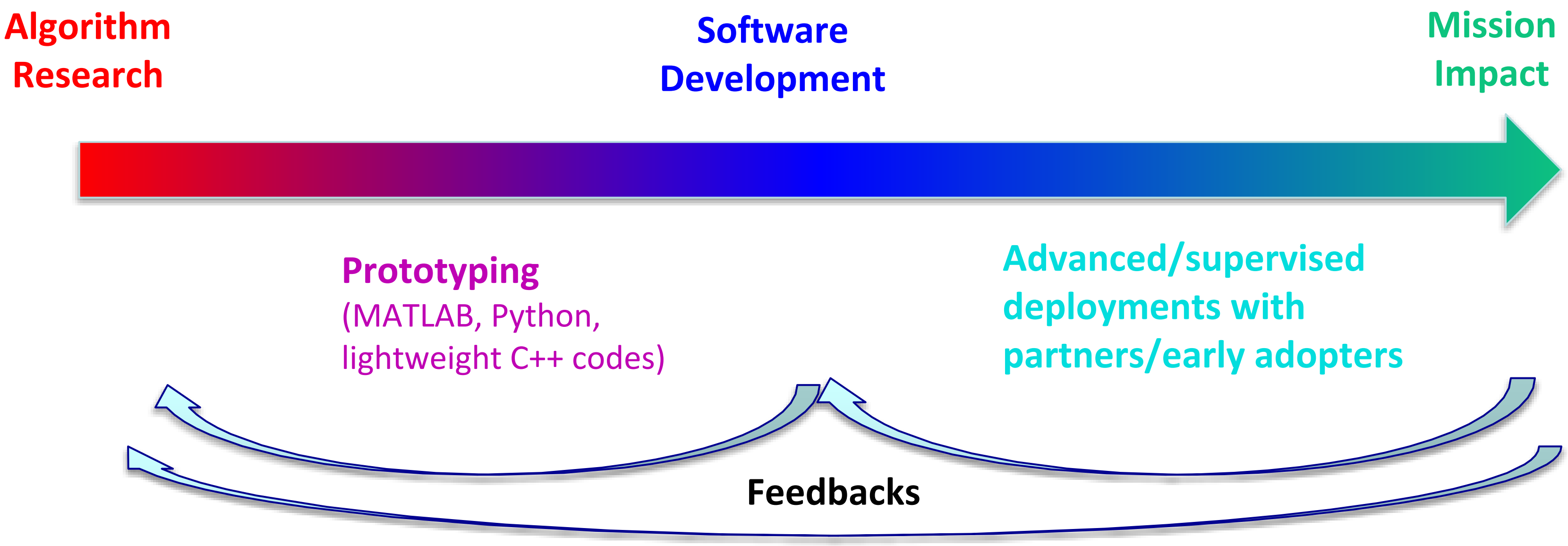








“Science Pipeline” Metaphor



DOD
NASA

Scalable UQ, DUU — DARPA — NASA — Nozzles, Scramjets
Trajectory simulation

DOE/ SC

ASCR — FASTMath UQ — SciDAC Scientific Discovery through Advanced Computing — Tokamaks (OFES) — ENERGY Office of Energy Efficiency & Renewable Energy — EERE, BES

DOE/ NNSA

LDRD — V&V Methods — V&V Software — ASC — Advanced Deployment

"Science Pipeline" Metaphor

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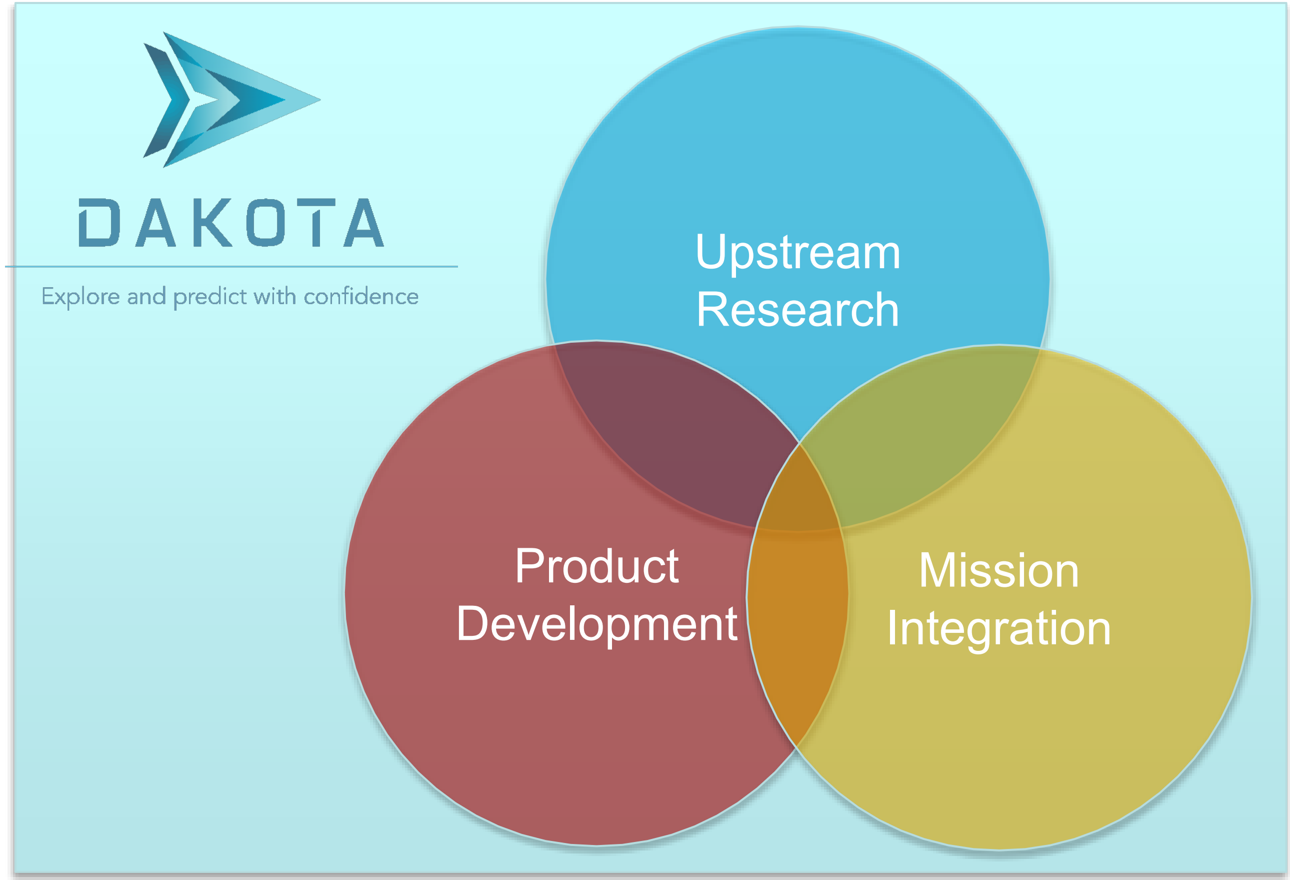
In FY20, we began organizing around the constituent components as project thrusts



- Each thrust has its own team, planning, and set of prioritized goals
- The project defines a set of integrated milestones that emphasize the flow through the R/D/A pipeline

Connecting the pipeline
Selected vignettes in mission-driven R&D

Historical
- UQ modernization for thermal analysis community
- Heavy reliance on 1970s technology in DOE mission work

Current
- Multifidelity methods
- Bayesian inference with MCMC (follow MF UQ)
- Mission connections dominated by HF M&S on HPC
- MCMC = too expensive, posteriors are slow to converge

Looking forward
- Model management with “trustworthy AI/ML”
- Machine learning is the new wild-west!

Connecting the pipeline

Selected vignettes in mission-driven R&D

Historical

- UQ modernization for thermal analysis community

- Heavy reliance on 1970s technology in DOE mission work
  - Mean Value First-Order Second-Moment (MVFOSM)
  - Latin Hypercube Sampling (LHS)

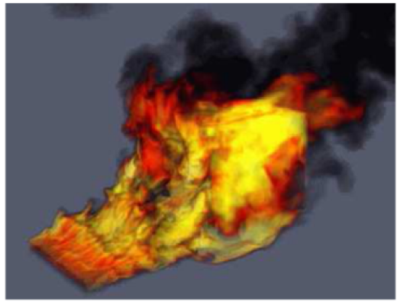
Advanced Deployment: Deploy modern UQ approaches for which barriers to adoption are minimal (~same sample sets):

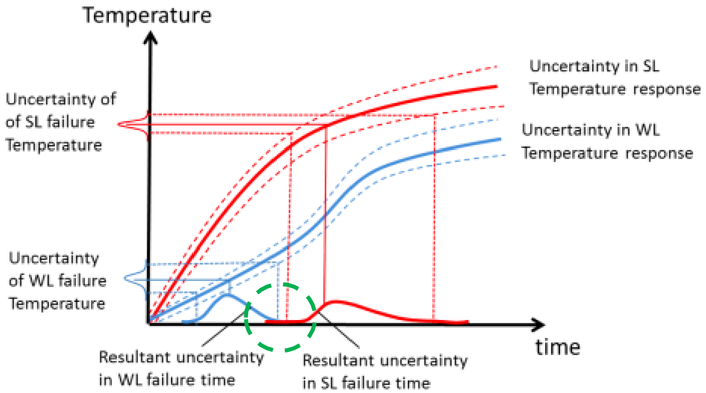
  - L1 sparse grid as alternative to MVFOSM w/ central FD
  - Compressed sensing PCE as post-processor of LHS data

- Can "advanced UQ" demonstrate tangible benefits relative to current MV/LHS approaches?

Leverage these foundations into mixed A-E UQ deployment

- For mixed UQ, are current simplifying assumptions valid, or are we discarding realism for efficiency?





Our starting point here is cultural: gain acceptance for newer UQ approaches from our internal user community. CRITICAL for connecting our R&D to mission impact.

UQ modernization for thermal analysis community (Part 1): PCE methods

Established approach: MVFOSM (linear Taylor series) with central finite differences (2n+1 evaluation stencil)

- Compared to level 1 sparse grid PCE: captures nonlinear main effects and supports nonlinear sensitivity analysis
  - 2n+1 evaluations at Gauss points → quadratic main effects, no interactions
  - First set of active indices within a generalized sparse grid approach
    - Naturally leads to subsequent refinement: Index set(s) with greatest ΔQoI → higher-order main + interaction effects

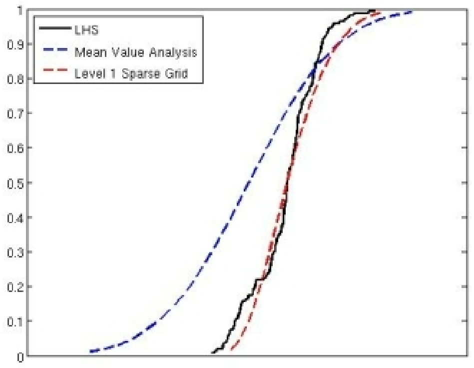
→ Identified cases of mild and severe nonlinearity (MV ok, MV not ok) in thermal response

Established (entrenched?) approach: LHS with coarse sampling (one set of N stratified samples, no replicates)

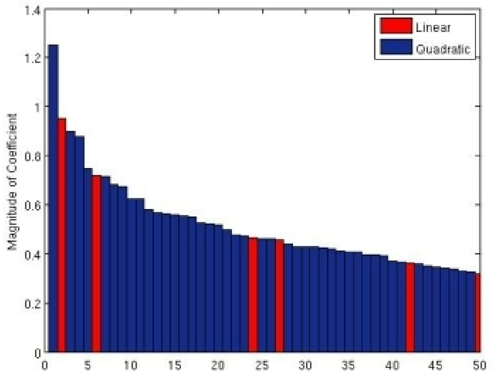
- Post-process this unstructured data using regression PCE
  - *Over-determined:* SVD for low-order expansions
  - *Under-determined:* compressed sensing for higher-order expansion candidates
  - *K-fold cross-validation* → search over {exp. order, noise tol} to mitigate over-fitting of sparse data

→ Identified dominant main + interaction terms within candidate set, efficient GSA via VBD (Sobol' indices)

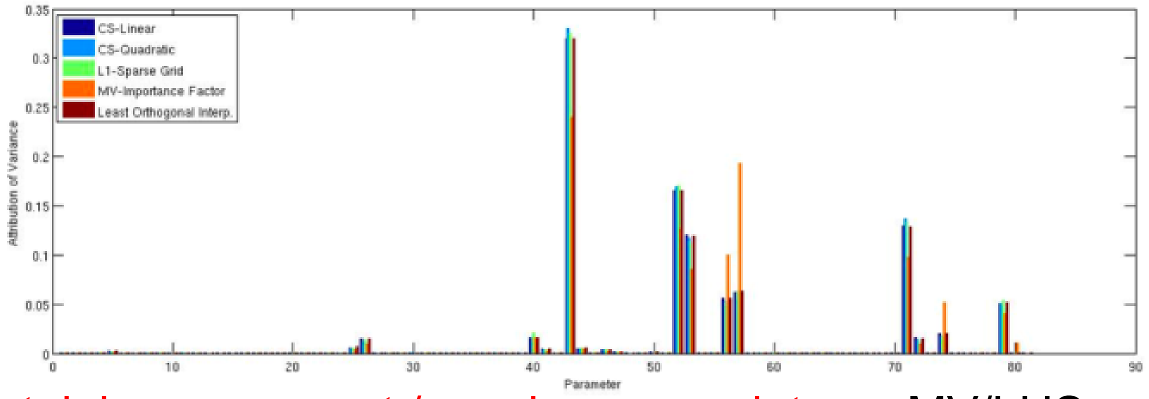
L1 sparse grid



Compressed Sensing

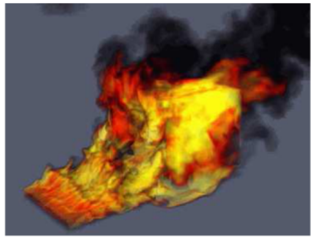


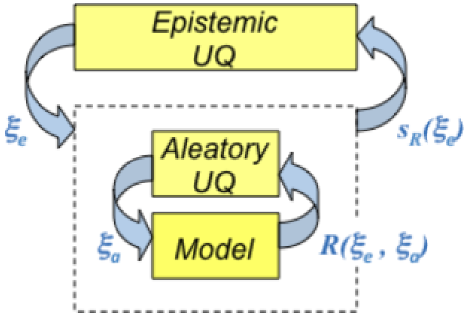
Variance Decomposition



Greater resolution and additional insight while retaining same cost / reusing same data as MV/LHS

UQ modernization (Part 2): Mixed Aleatory-Epistemic Safety Analyses





Context: safety assessments must contend with a mixture of variability + lack of knowledge when computing *probability of loss of assured safety* (PLOAS)

Existing approaches/tools make strong assumptions about the epistemic uncertainty

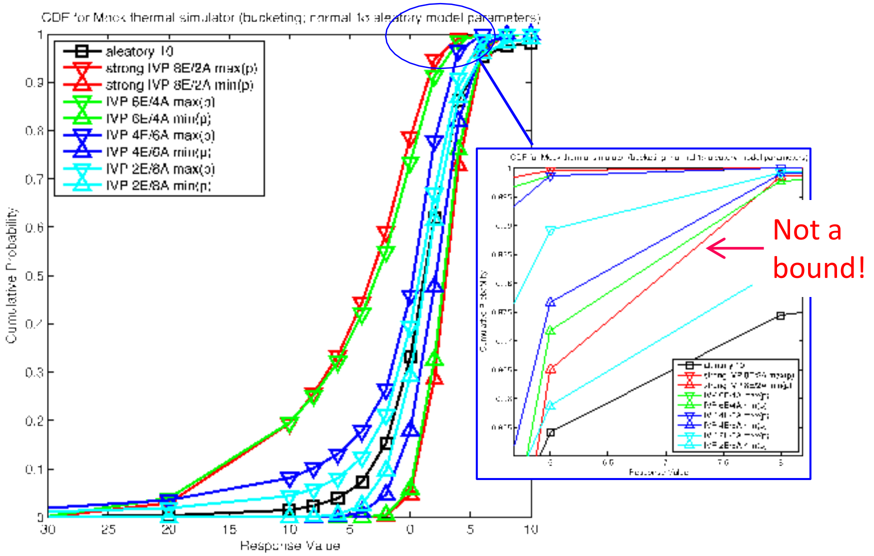
- Rely on nested LHS, which is intractable in general for HF simulations
- Assumption: epistemic UQ is limited to post-processing vars that short circuit nested sampling
    - Arguments can be made that these vars have both reducible and irreducible components and are mis-characterized, and other thermal variables have reducible uncertainty.
    - Investigate impact of these assumptions – are we discarding rigor for tractability?

Approach: Dakota enables removal of these strong assumptions and renders mixed A -E studies tractable though use of scalable algorithms that are tailored for each loop

- Epistemic: surrogate-based global optimization (EGO) for interval bounds
- Aleatory: spectral convergence / efficient tail sampling via adaptive PCE

Results: explored spectrum of formulations that provide more realistic A-E separation

- Strong assumptions (red) give conservative probability bounds under specific conditions
- In other cases, bounds on tail probabilities shown to be inaccurate by orders of magnitude, indicating over-prediction of safety / under-prediction of risk
- Accuracy lost where it is most important for PLOAS estimation
  → rigorous aleatory-epistemic modeling is critical for these safety analyses
- Key takeaway (again): socialization of R&D investments → mission impact



Connecting the pipeline
Selected vignettes in mission-driven R&D

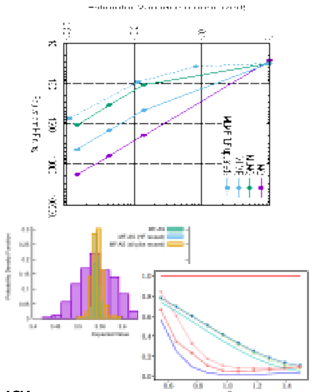
Current

- Multifidelity methods
- Mission connections dominated by HF M&S on HPC

Highly active area with a multifaceted research roadmap

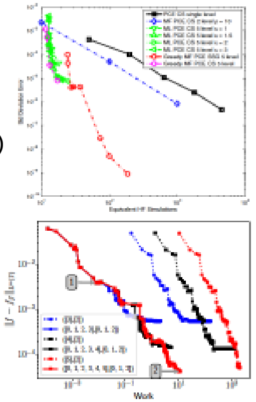
Monte Carlo UQ Methods

- *Production:* optimal resource allocation for multilevel, multifidelity, combined (DARPA EQUiPS, Wind, Cardiovascular)
- *Emerging:* active dimensions (LDRD, SciDAC), generalized fmwk for approx control variates (ASC V&V), goal orientation (rare events), hybrid methods for GSA
- *On the horizon:* control of time avg; model tuning / selection (LDRD)



Surrogate UQ Methods (PCE, SC)

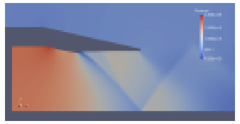
- *Production (v6.10+):* ML PCE w/ projection & regression; ML SC w/ nodal/hierarchical interp; greedy ML adaptation (DARPA SEQUOIA), multilevel fn train (ASC V&V)
- *Emerging:* multi-index stochastic collocation; multiphysics/multiscale integration (ASC V&V); new surrogates (GP, ROM, NN) w/ error mgmt. fmwk (LDRD, SciDAC); learning latent variable relationships (MFNets, LDRD)
- *On the horizon:* unification of surrogate + sampling approaches (LDRD)



Optimization Under Uncertainty

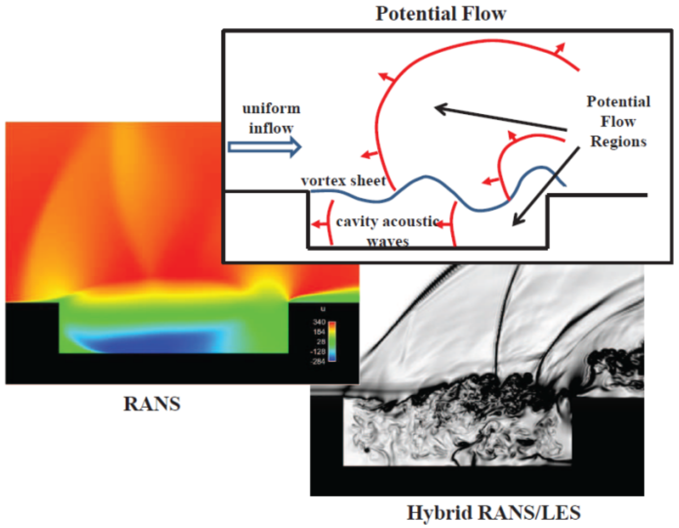
- *Production:* manage simulation and/or stochastic fidelity
- *Emerging:*
  Derivative-based methods (DARPA SEQUOIA)
  - Multigrid optimization (MG/Opt)
  - Recursive trust-region model mgmt.: extend TRMM to deep hierarchies

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



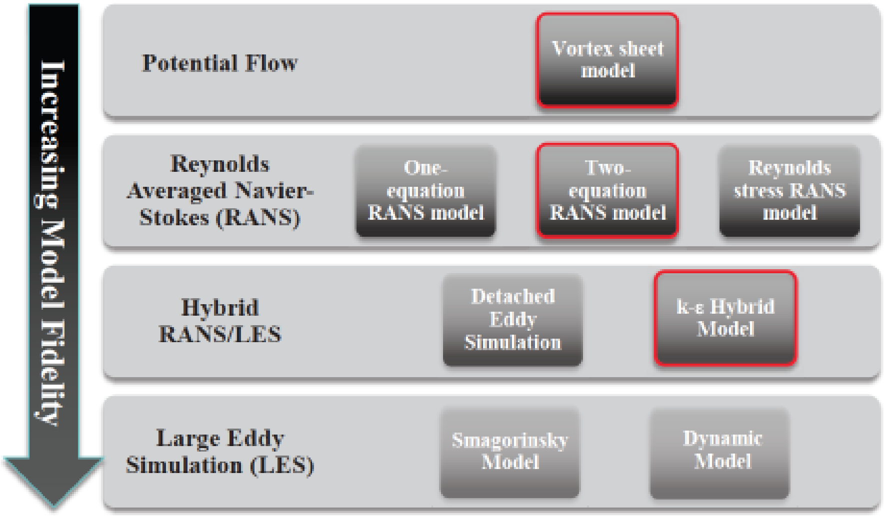
Multiple Model Forms in UQ & Opt

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



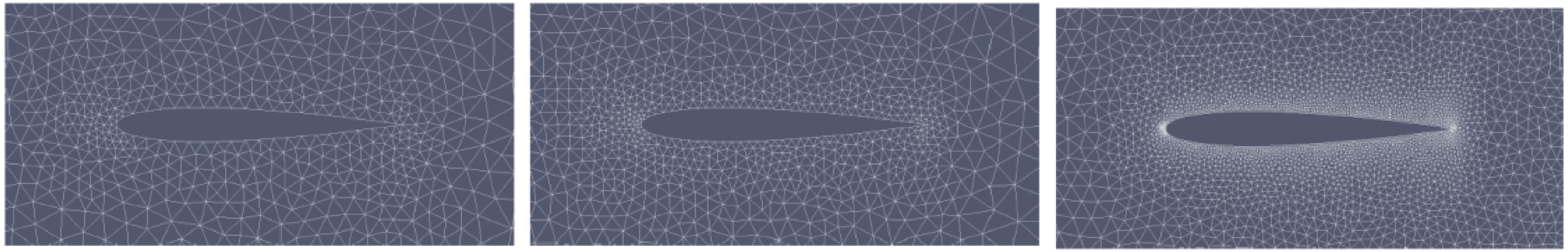
An ensemble of peer models lacking clear preference structure / cost separation: e.g., SGS modeling options

- *With data:* model selection, inadequacy characterization
  - Criteria: predictivity, discrepancy complexity
- *Without (adequate) data:* epistemic model form propagation
  - Intrusive, nonintrusive
- *In MF context:* correlation analysis, model tuning, ensemble selection

Discretization levels / resolution controls

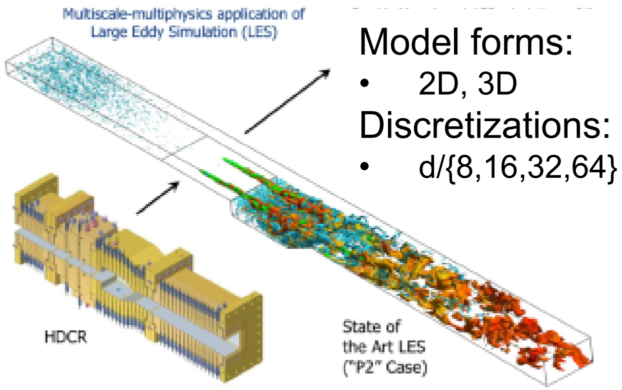
- Exploit special structure: discrepancy → 0 at order of spatial/temporal convergence

Combinations for multiphysics, multiscale



2018/2019 Vignettes: ML, MF, MLMF Monte Carlo

Scramjet



Model forms:
- 2D, 3D

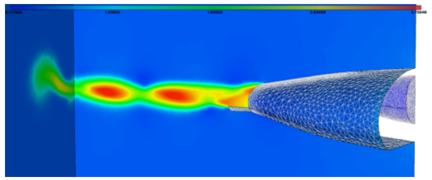
Discretizations:
- d/{8,16,32,64}

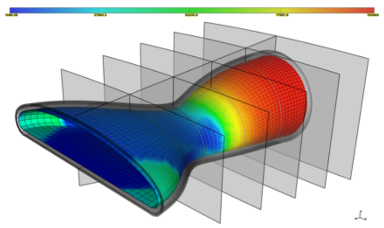
	$P_{0,mean}$	$P_{0,rms,mean}$	M_{mean}	TKE_{mean}	χ_{mean}
P1					
$d/8$	4.02554e-03	1.90524e-06	1.99236e-02	3.34905e-07	4.24520e-03
$d/16$	4.03350e-07	7.77838e-08	6.68974e-05	1.74847e-08	4.40048e-05
P1 updated					
$d/8$	4.05795e-03	1.90612e-06	1.60029e-02	7.53353e-07	9.41403e-04
$d/16$	2.85017e-04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

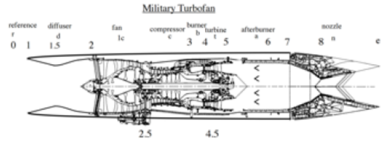
Table 2: Variance for the five QoIs of the P1 unit problem.

No variance decay for higher turbulence levels

UCAV Nozzle





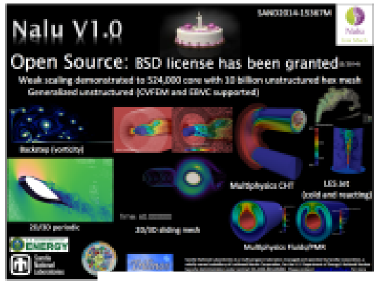


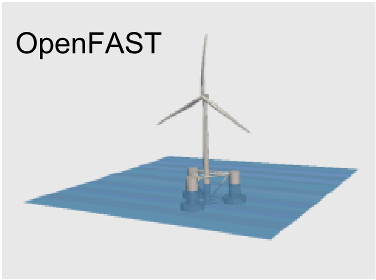
Non-predictive LF stress prior to reformulation

	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 $\varepsilon^2/\varepsilon_0^2 = 0.001$.

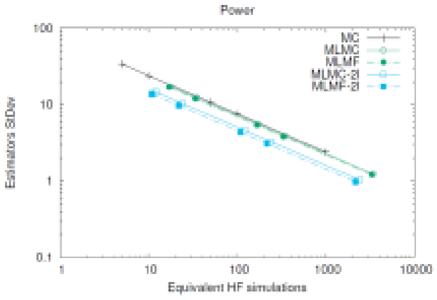
Wind

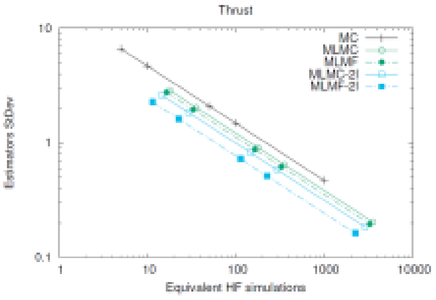




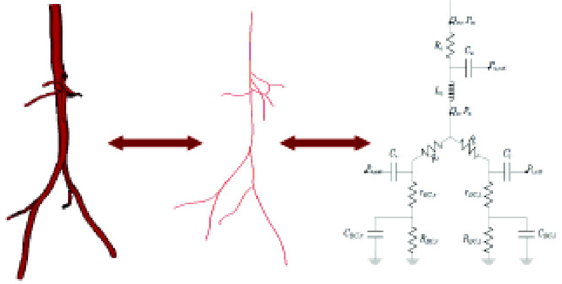
Nalu LES for Q_0 is too coarse with limited predictive value

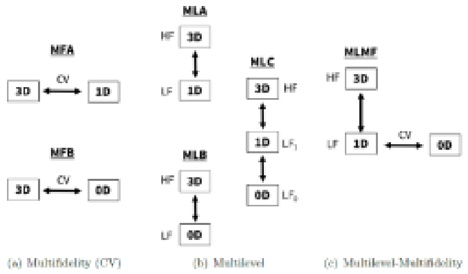
Project basis for ML emulator-based inference to follow





Cardiovascular





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

0D has greater predictive value, for which MF outperforms ML

Recent Deployment Vignettes: ML/MF Monte Carlo/Polynomial Chaos

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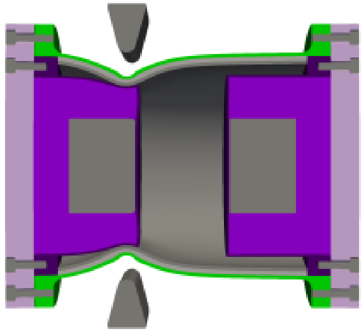
Crash & Burn Multiphysics (ASC L2 Milestone)

Forward UQ w/ explicit (LF) + implicit (HF) SIERRA mechanics

- Multilevel MC across model resolutions for LF model
- Multifidelity MC with HF implicit + selection of most effective LF explicit

Successful demonstration of advanced UQ methods, integrated alongside emerging ASC workflows for multiphysics simulation

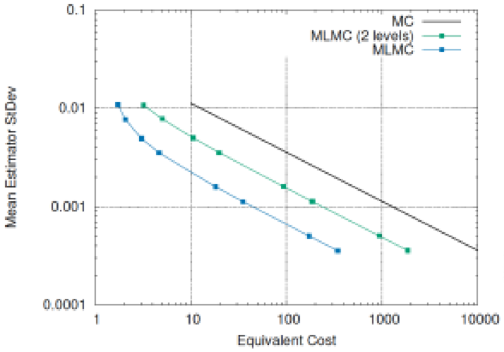


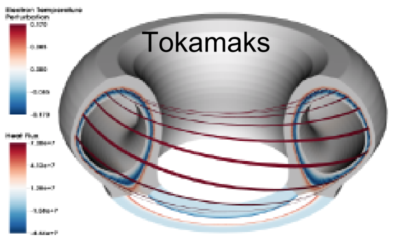
Mechanical loading of mock device

Prediction of Tokamak instability (SciDAC)

Magneto-hydrodynamics (Drekar)

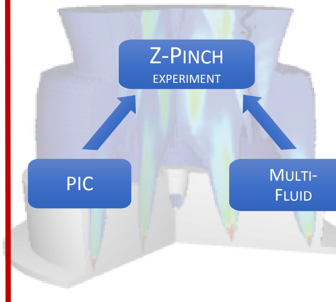
- Model resolutions are well correlated for demo problem
- MLMC is sufficient to obtain 30x reduction in cost for same accuracy



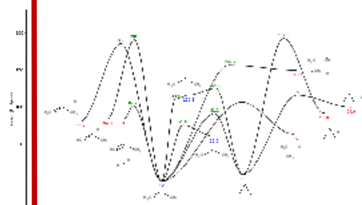


Estimator	N_{400}	N_{200}	N_{100}	Eq. Cost
MC	1273	-	-	1273
MLMC (2 levels)	1	1278	-	236.62
MLMC	1	8	1366	44.36

Emerging



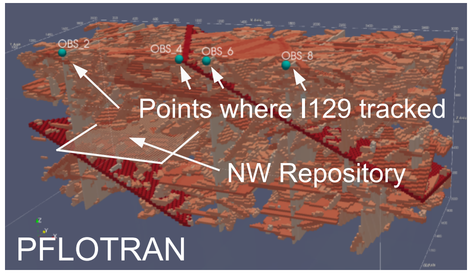
CIS LDRD: non-hierarchical ensemble (models + experiments)

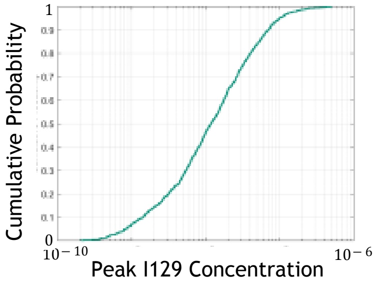


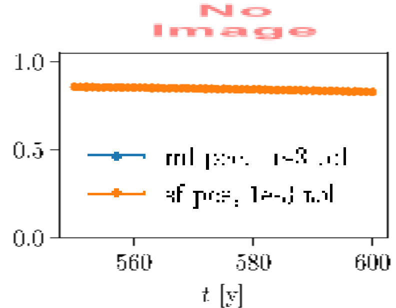
BES QC: exploration of the C_3H_6 PES with KinBot

Geologic Disposal

GDSA example simulation and QOI:



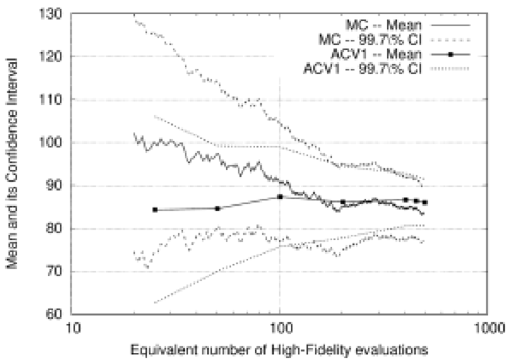




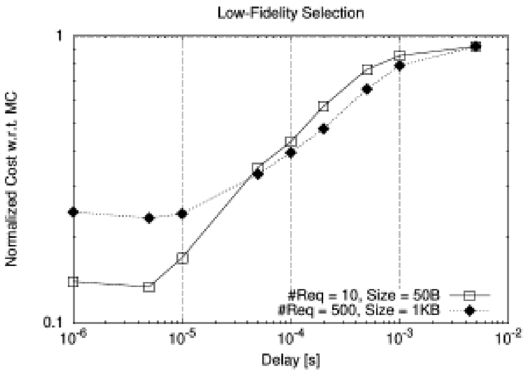
- Deployed MF PCE for GSA to a problem related to geologic disposal safety assessment (GDSA)
- Sobol' indices for model response as fn. of time
- Indices practically identical with ~80 equivalent HF evaluations for MF PCE compared to 713 evaluations for equivalent accuracy SF PCE.

Network Cybersecurity (SECURE GC LDRD)

- Deployed ACV for forward UQ with HF emulation (minimega) and LF discrete event simulation (ns-3)
- Investigated the efficiency of MF UQ by tuning ns-3 models
- Demonstrated increased efficiency for tail est. given a minimega dataset



Forward UQ: ACV1 vs MC



ns-3 tuning effect on ACV performance

Key mission feedbacks

Multilevel performance on elliptic model PDEs is compelling, but does not accurately represent Sandia mission areas

- Extensions for multidimensional hierarchies, including multiphysics / multiscale (multi-index collocation)
- Investments in non-hierarchical MF methods: ACV and MFNets

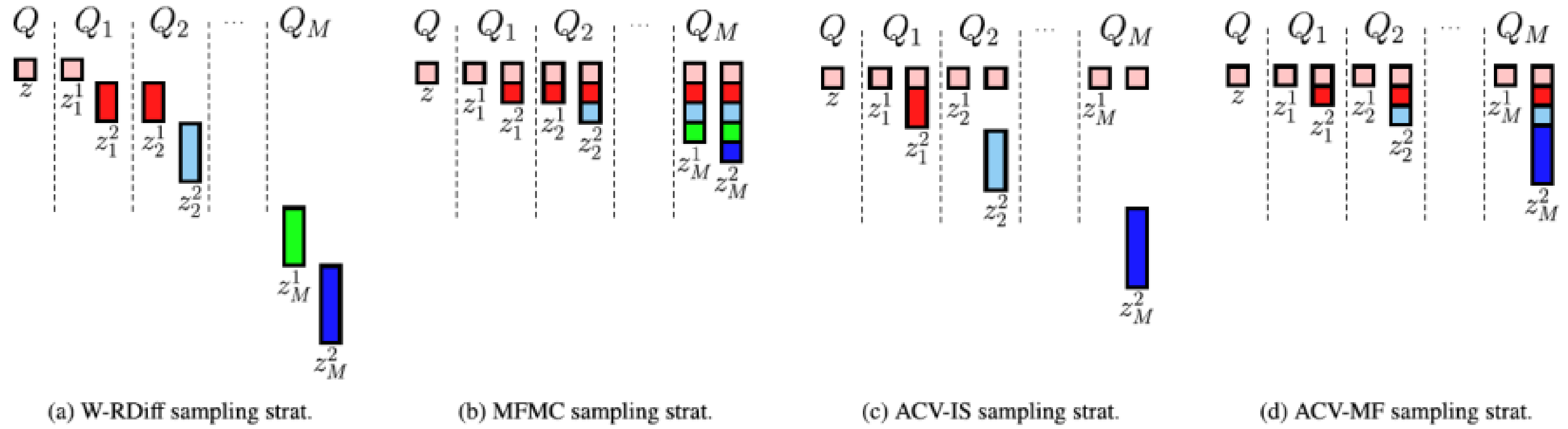
Popular MF approaches neglect important practicalities

- "Oracle" correlations assumed → iterated versions of MFMC, ACV
- Imperfect data → embedded cross validation
- Dissimilar parameterizations → shared subspaces
- Free hyper-parameters → model tuning (currently a joint focus with NASA Langley)
- Stochastic simulation, simulation/surrogate error estimation → extended error management framework

Background: multifidelity sampling methods of interest

$$\tilde{Q}(\underline{\alpha}, \underline{z}) = \hat{Q}(\boldsymbol{z}) + \sum_{i=1}^{M} \alpha_i \left(\hat{Q}_i(\boldsymbol{z}_i^1) - \hat{\mu}_i(\boldsymbol{z}_i^2) \right) = \hat{Q}(\boldsymbol{z}) + \sum_{i=1}^{M} \alpha_i \Delta_i(\boldsymbol{z}_i) = \hat{Q} + \underline{\alpha}^T \underline{\Delta}$$

Sample set definitions

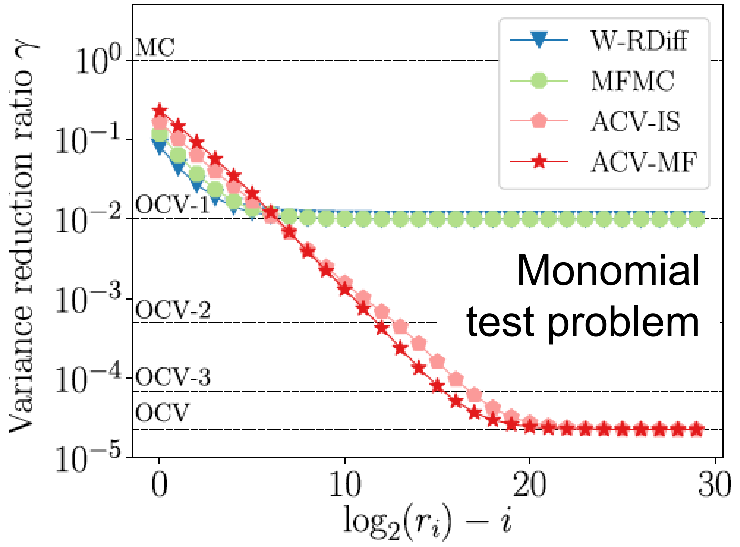


Theoretical perf. bounds for recursive vs. non-recursive

- Recursive limited by variance reduction of perfect μ_1 (OCV-1)
- Non-recursive can exploit potential gap between OCV-1 and OCV

Methods minimize estimator variance over number of truth evals *N* and approximation oversample ratios ***r***

- MFMC has closed form for optimal ***r****,*N** (given ordered/reordered models)
- ACV solves numerically for ***r****,*N** (does not require ordering)



Gorodetsky, Geraci, E., Jakeman, "A generalized approximate control variate framework for multifidelity uncertainty quantification," JCP 408 (2020)

Iterated MFMC

Iterated ACV

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Initialize: select a small shared pilot sample $N^{(0)}$ expected to under-shoot the optimal profile

1) Sample all models

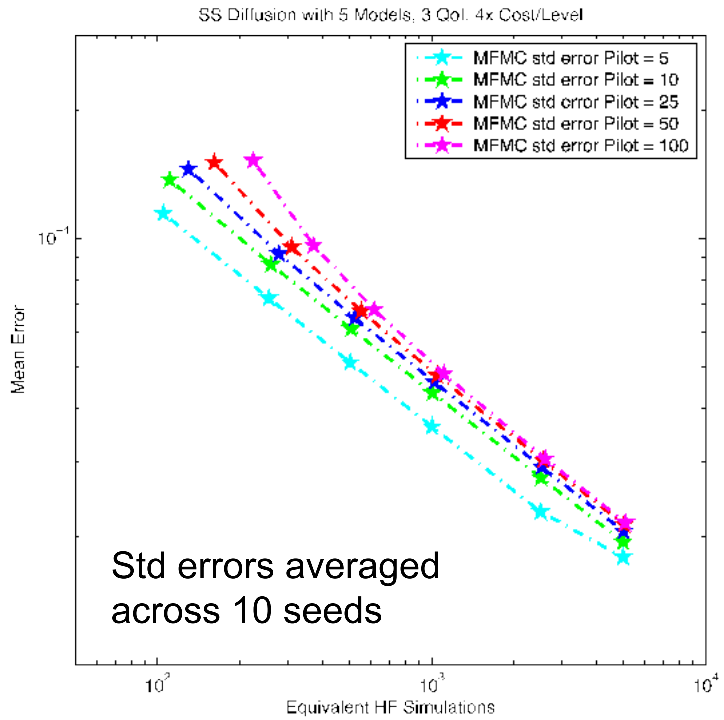
Iterated MFMC:

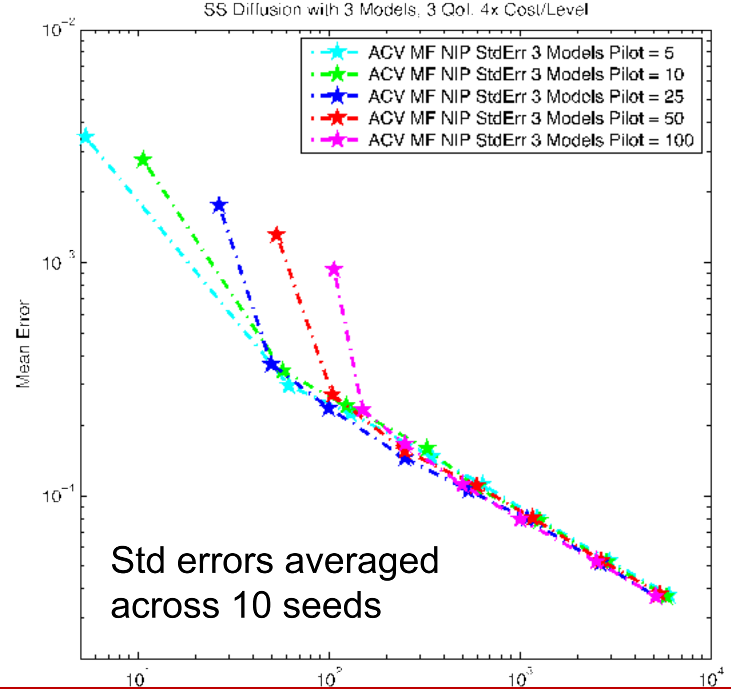
2) $N^{(i)}$ shared samples → Estimate $\rho^2_{LH}{}^{(i)}$ → Estimate $r^{(i)}$
3) Estimate $N^{(i+1)}$ using prescribed { budget C || tolerance ε }
4) Compute one-sided ΔN for shared samples from $N^{(i)}$ to $N^{(i+1)}$
   A. Optional: apply under-relaxation factor γ
   B. If non-zero increment, advance (i) and return to 1)

Iterated ACV:

1) $N^{(i)}$ shared samples → $Cov_{LL}{}^{(i)}$, $Cov_{LH}{}^{(i)}$ ("C", "c") → opt. solver → r^*, N^*
2) Compute one-sided ΔN for shared samples from $N^{(i)}$ to N^*
   A. Optional: apply under-relaxation factor γ
   B. If non-zero increment, advance (i) and return to 1)

Finalize: apply r* for LF eval increments, estimate α → apply controls to compute final expectation(s)





Performance degradation from pilot over-estimation is clearly evident

- Analytic r* reduces numerical burden but also limits flexibility

Performance degradation from pilot over-estimation is *not* significant

- ACV-MF demonstrates greater flexibility / resilience: locates near-optimal solutions that incorporate large pilots
- Starting pts on left are for budget = pilot (moves quickly from MC to ACV)

TO DO: PULL FROM SLIDE COMMENTS?

Surrogates with Greedy MF Refinement: PCE (sparse grids, regression) and FTT (regression):

Integrated MF competition including embedded cross validation

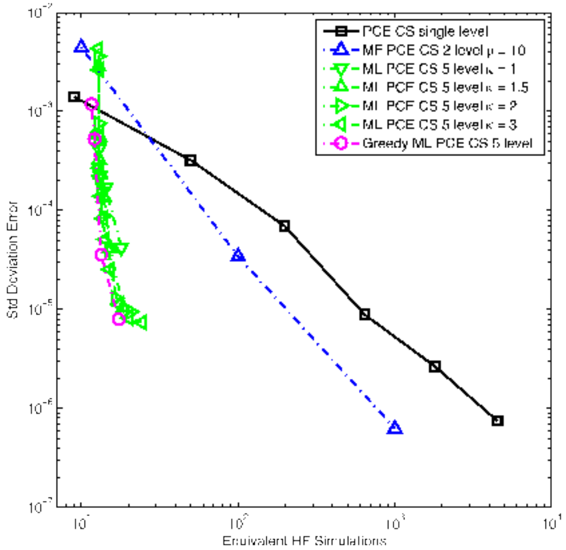
Model problem results

Steady state diffusion

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

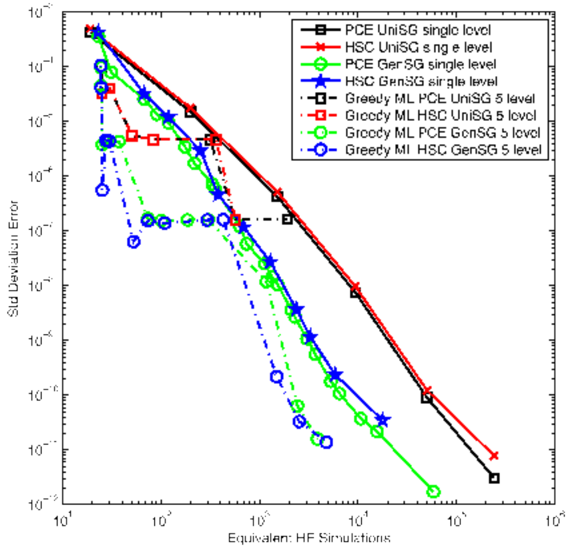
$$u(0,\xi) = 0, \quad u(1,\xi) = 0.$$

Greedy ML PCE: compressed sensing with uniform candidate refinement



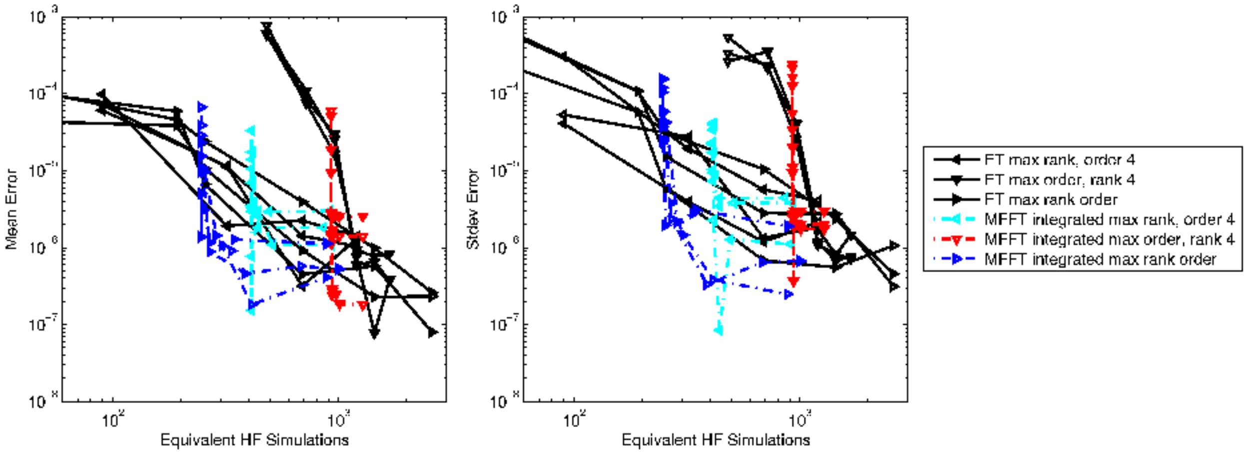
Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-1	198	9	9	9	9
1.e-2	644	198	9	9	9
1.e-3	1802	644	9	9	9
1.e-4	4505	1802	50	9	9

Greedy ML PCE: sparse grids with uniform / generalized refinement

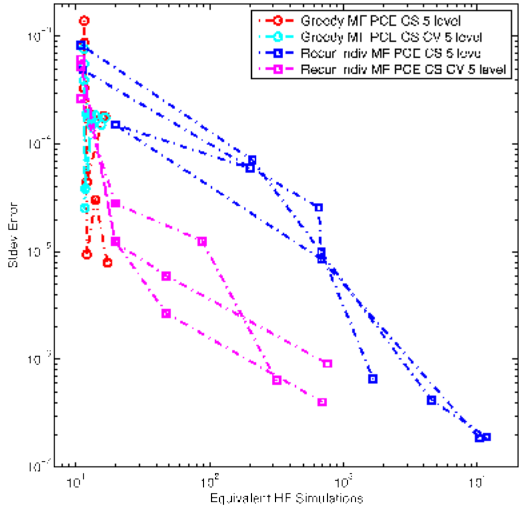


Conv Tol	N_1	N_2	N_3	N_4	N_5
1.e-2	43	23	19	19	19
1.e-4	211	83	19	19	19
1.e-6	391	271	156	19	19
1.e-8	1359	743	327	59	19
1.e-10	3535	2311	1039	391	19
1.e-12	10319	5783	2783	1343	43
1.e-14	26655	14991	8063	3703	1535

Greedy MF FTT regression: *embedded CV over rank, order, both*



Greedy MF PCE regression: *embedded CV over basis order*



Critical for preventing error propagation in recursive emulation schemes

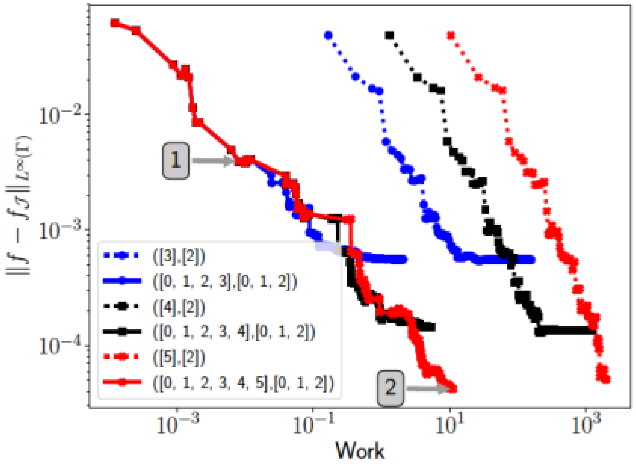
From Multi-Index to (De-)Coupled Multi-Physics

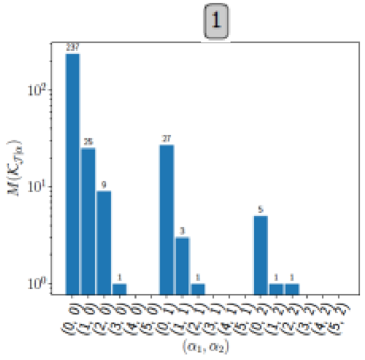
Advection diffusion

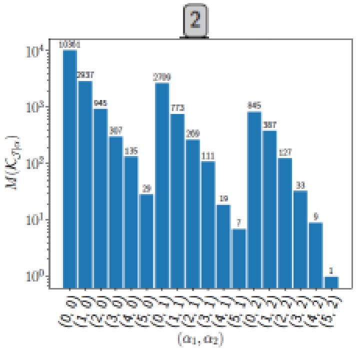
$$\frac{du}{dt}(x_1,t,Z) + a\frac{du}{dx}(x_1,t,Z) - \frac{d}{dx}\left[k(x_1,Z)\frac{du}{dx}(x_1,t,Z)\right] = g(x_1,t,Z) \qquad (x_1,Z)\in(0,1)\times\Gamma$$

$$u(0,t,Z)=0 \quad u(1,t,Z)=0 \quad u(x_1,0,Z)=0,$$

Greedy multi-index PCE: sparse grids with generalized refinement







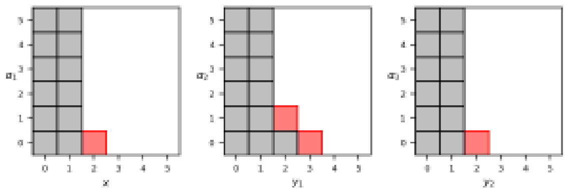
Jakeman, E., Geraci, Gorodetsky, "Adaptive Multi-index Collocation for Uncertainty Quantification and Sensitivity Analysis," in review.

*Multi-level/fidelity/index + **Multiphysics***

- Create multi-index sparse grid (random + model resolution vars) for each physics
- Decouple through surrogates (+ re-representation)
- Compete candidate grid refinements for each physics in terms of impact on system QoI goals per unit cost
- Investigate impact of integrated adaptive refinement
  - Random vars (black box MP, fixed resolution)
  - RV + decoupled MP (fixed resolution)
  - RV + decoupled MP + multilevel resolution

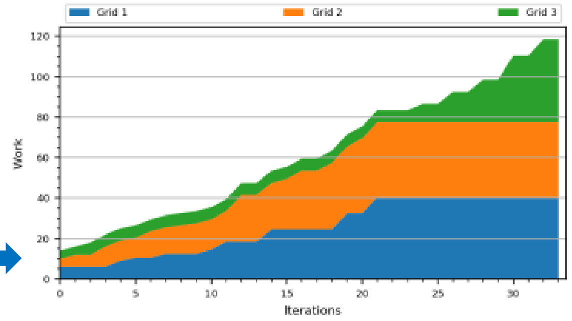
Application test problem:
- System inputs ***x***, model resolutions ***α***, and system QoI ***y₃***
- 3-physics satellite design problem

$$f_1(x, \alpha_1) = y_1$$
$$f_2(y_1, \alpha_2) = y_2$$
$$f_3(y_2, \alpha_3) = y_3$$



Final refinement level for adaptive multiphysics, multilevel manager

Extent of Adaptive Refinement	Equivalent HF Evals
None (Fixed RV, MP, Fid)	6240
RV only (Fixed MP + Fid)	1740
RV + MP (Fixed Fid)	608
RV + MP + MF	119



RV + MF + MP adaptivity reduces expense by 50x

Multilevel – Multifidelity Sampling Methods

Leveraging active directions (ECCOMAS, WCCM)

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- Active subspaces, ridge approximation, adapted basis, …

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

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

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

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

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

  Let's define two sets of variables

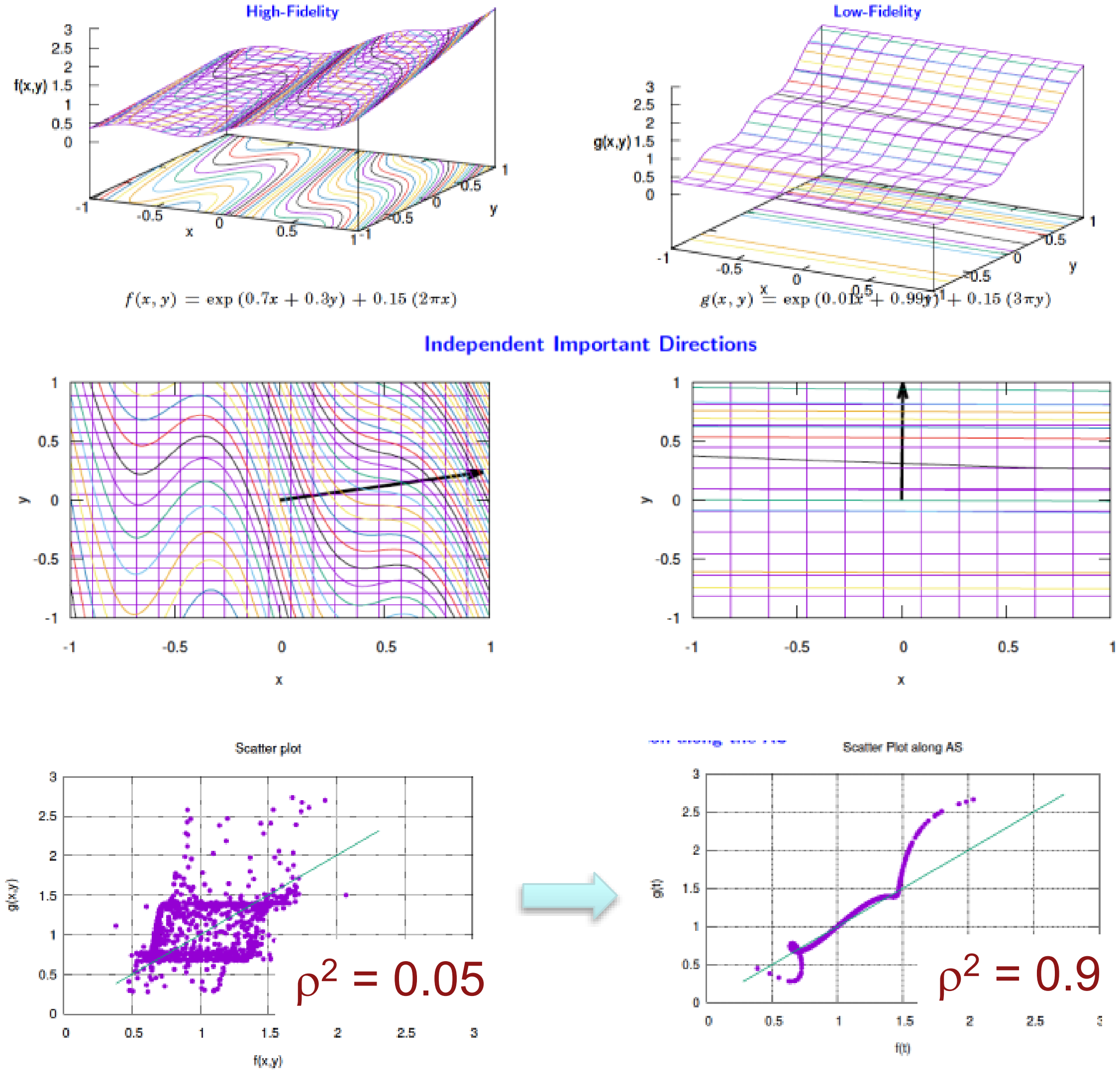
$$\begin{cases} \mathbf{y} = \mathbf{W}_A^{\mathrm{T}} \mathbf{x} \in \mathbb{R}^n & \text{(Active)} \\ \mathbf{z} = \mathbf{W}_I^{\mathrm{T}} \mathbf{x} \in \mathbb{R}^{(m-n)} & \text{(Inactive)} \end{cases} \implies \mathbf{x} = \mathbf{W}_A \mathbf{y} + \mathbf{W}_I \mathbf{z} \approx \mathbf{W}_A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

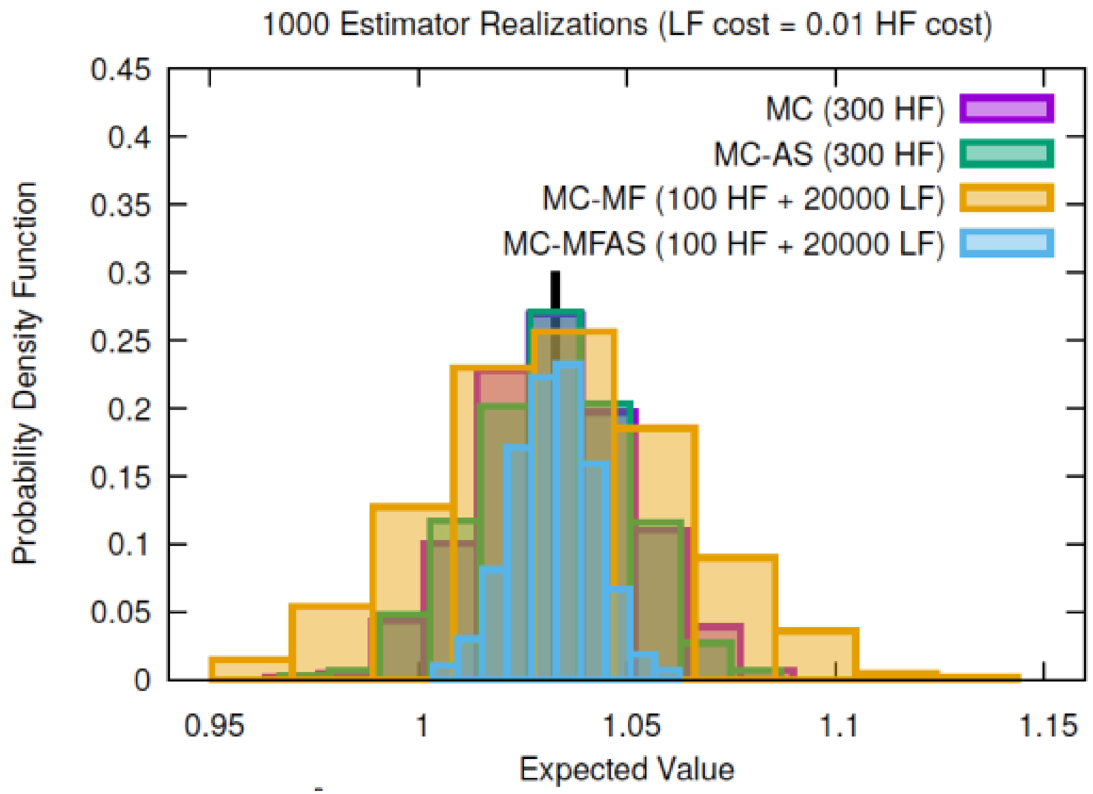
- Main ideas:
  - For each model independently one can compute active directions
  - Sample along these shared active directions and map back to original model coords.
  - Principal directions for a shared QoI can bridge dissimilar parameterizations and demonstrate underlying shared processes

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

Multilevel – Multifidelity Sampling Methods

Research Direction: leveraging active directions (example 1)





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

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

Exploration of hyper-parameter model tuning

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Tunable model problem (from JCP paper on ACV*)

- 1 parameter is tunable: θ_1
- 2 parameters are fixed: $\theta = \pi/2$, $\theta_2 = \pi/6$

Model Definitions

$$Q = \sqrt{11} y^5$$
$$Q_1 = \sqrt{7}\left(\cos\theta_1 x^3 + \sin\theta_1 y^3\right)$$
$$Q_2 = \sqrt{3}\left(\frac{\sqrt{3}}{2}x + \frac{1}{2}y\right), \quad \text{where} \quad x, y \sim \mathcal{U}(-1,1)$$

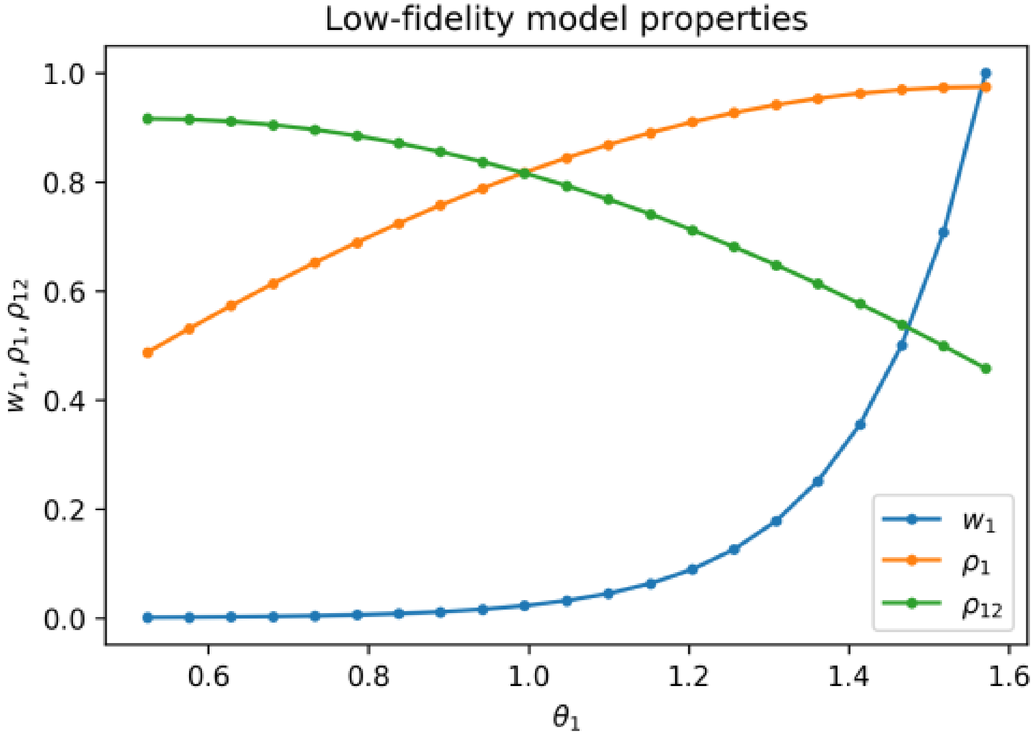
Correlations (variances are scaled to 1)

	Q	Q_1	Q_2
Q	1	$\frac{\sqrt{77}}{9}\sin\theta_1$	$\frac{\sqrt{33}}{14}$
Q_1	*sym*	1	$\frac{\sqrt{21}}{10}\left(\sin\theta_1 + \sqrt{3}\cos\theta_1\right)$
Q_2	*sym*	*sym*	1

θ_1 controls:

- Correlations among models ρ_1 and ρ_{12};
- Cost of evaluating Q_1 according to the cost law

$$\log w_1 = \log w_2 + \frac{\log w_2 - \log w}{\theta_2 - \theta}(\theta_1 - \theta_2)$$
$$\text{with} \quad w = 1 \quad \text{and} \quad w_2 = 10^{-3}$$



* Gorodetsky, Geraci, E., Jakeman, "A generalized approximate control variate framework for multifidelity uncertainty quantification," JCP 408 (2020)

Exploration of hyper-parameter model tuning

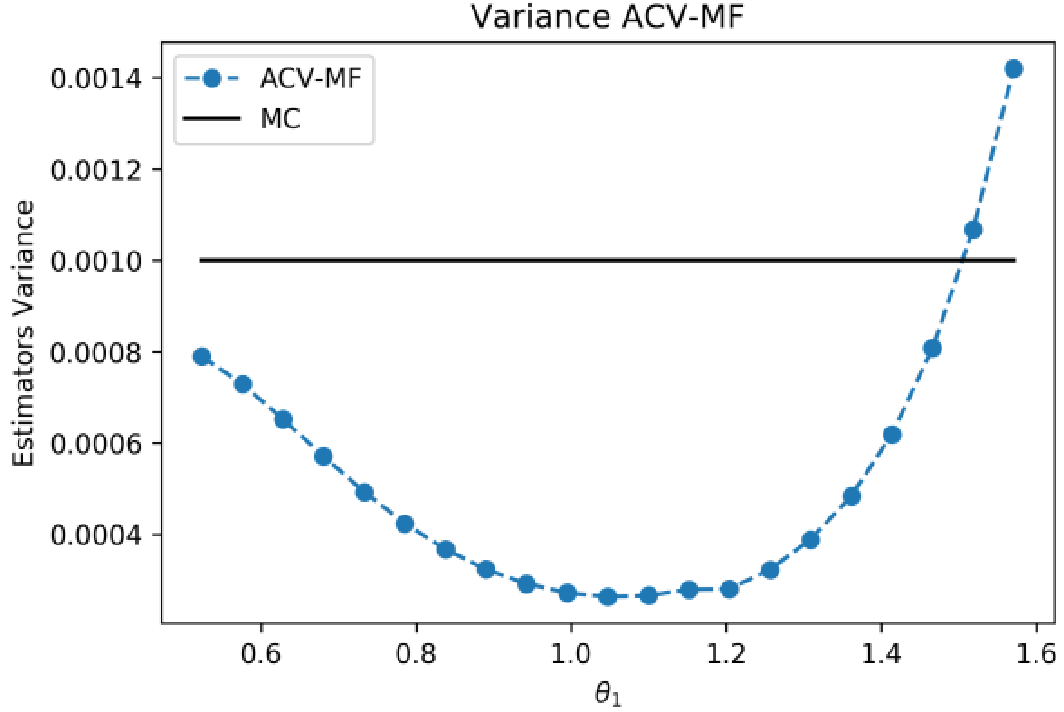
Model tuning performed within the context of a particular estimator (here, ACV-MF)

$$\underset{\theta_1, N, r_1, r_2}{\text{argmin}} \frac{1}{N}\left(1 - R^2_{ACV-MF}(\theta_1, r_1, r_2)\right) \quad \text{s.t.} \quad \mathcal{C}^{tot} = N\left(w + \sum_{i=1}^{2} w_i r_i\right) \leq \mathcal{C}_{target} = 1000$$

Nested or AAO optimization:

- For ACV, hyper-parameters integrate as additional decision vars for minimizing estimator variance
- For analytic allocation cases (e.g., MFMC), there is no need for AAO opt. and we simplify to argmin_θ since $\rho(\theta), w(\theta) \rightarrow r^*, N^* \rightarrow R^{2*}$

Mid-fidelity model (Q_1) is tuned for ACV at ~ midpoint $\theta_1^* = \pi/3$



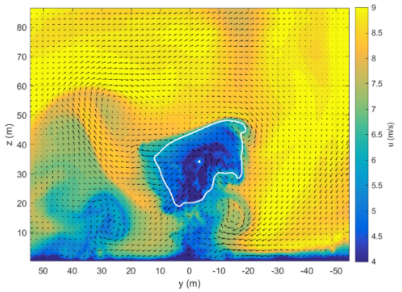
Connecting the pipeline

Selected vignettes in mission-driven R&D

Current

- Bayesian inference with MCMC (follow MF UQ)
- MCMC = too expensive, slow to converge, poor reliability

Inverse UQ:
Characterization of input uncertainties through data assimilation

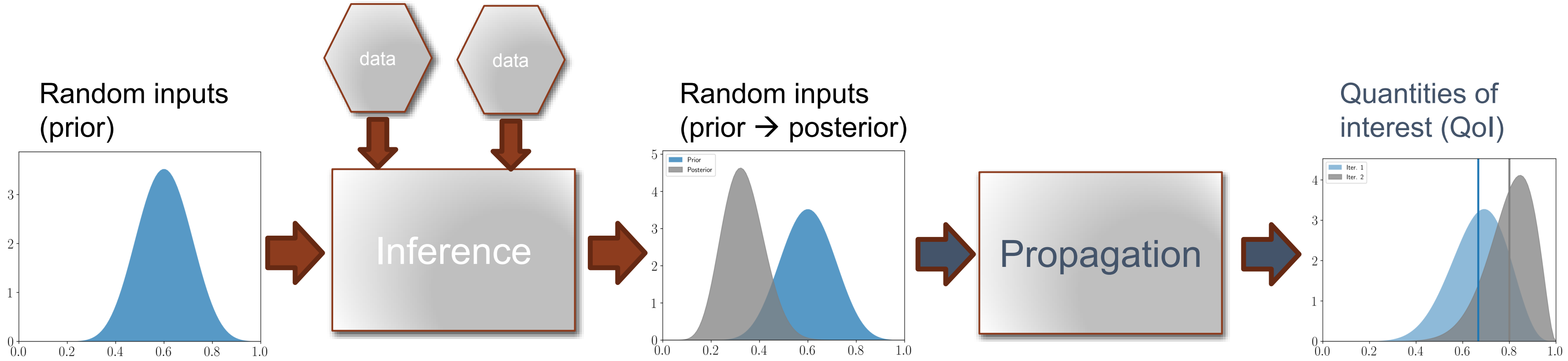


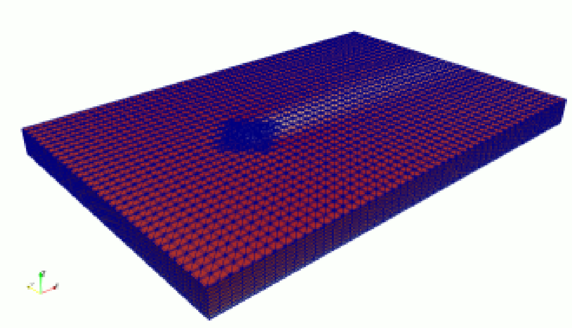
Nalu-Wind simulated wake data 5D downwind (inference target is averaged)

Atmosphere to electrons (A2e)

- **Forward UQ:** WindSE resolutions (RANS) within Greedy MF PCE
- **Data assimilation:** integrate wake data from experiments / HF LES
- **Opt. Under Uncertainty:** wind plant design using SNOWPAC + MLMC

FY19 EERE: Emulator-based Bayesian inference leveraging multifidelity PCE





(ML-MF) Emulator-based Bayesian inference

MCMC sampling performed on emulator, leveraging differentiable emulator structure

- Pre-solve for MAP (maximum a posteriori probability) point: full Newton min of –log(posterior)
- Accurate MCMC proposal: emulator derivatives → Hessian of misfit → MVN proposal covariance
  - mitigates sample rejection in high D: for 10D Rosenbrock test, 98% rejection rate reduced to 30%

$$p(\mathbf{d}|\xi) = \exp\left[-\frac{1}{2}(f(\xi)-\mathbf{d})^T \Gamma_{\mathbf{d}}^{-1}(f(\xi)-\mathbf{d})\right]$$

Gaussian Likelihood

$$-\log\left[p(\mathbf{d}|\xi)\right] = \frac{1}{2}(f(\xi)-\mathbf{d})^T \Gamma_{\mathbf{d}}^{-1}(f(\xi)-\mathbf{d}) = M(\xi)$$

Negative Log Likelihood = Misfit

$$\nabla_\xi^2 M(\xi) = \nabla_\xi f(\xi)^T \Gamma_{\mathbf{d}}^{-1} \nabla_\xi f(\xi) + \nabla_\xi^2 f(\xi) \cdot \left[\Gamma_{\mathbf{d}}^{-1}(f(\xi)-\mathbf{d})\right]$$

Hessian of Misfit

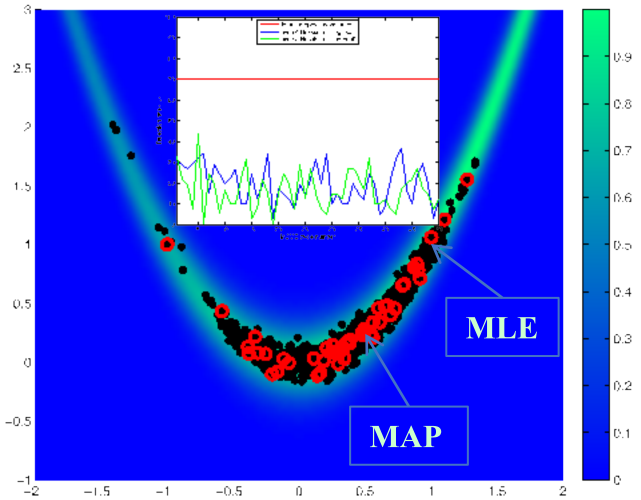
Gauss-Newton approx. Hessian
(if only emulator grads)

Laplace approx.: MVN proposal covariance defined by inverse Hessian of negative log posterior

$$-\log \pi_d(\xi) = M(\xi) - \log \pi_0(\xi)$$

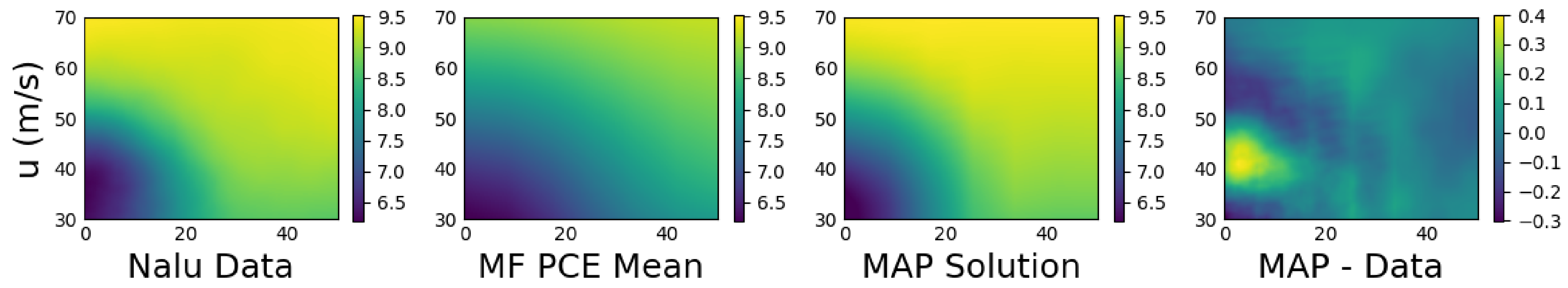
- augmenting misfit: Hessian of negative log prior provides regularization for priors w/ curvature (normal, beta, gamma)
- Posterior Hessian-based proposal balances likelihood and prior, performing better than either alone

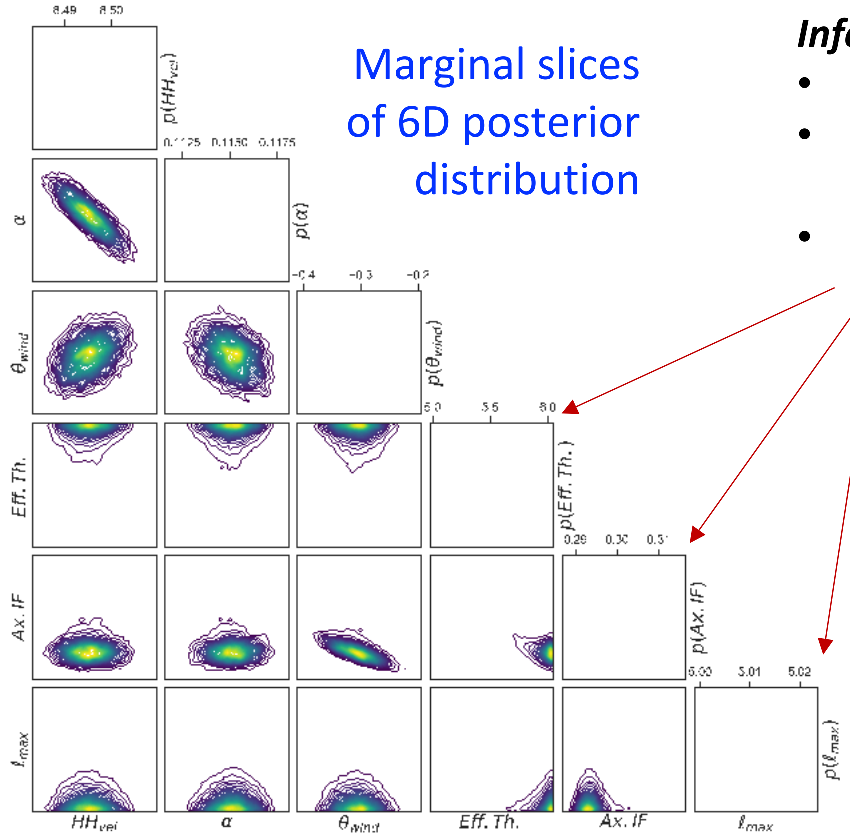
Rosenbrock Problem; Prior ~ N(0,1)



WindSE (RANS) Inference Results for MF PCE

Inference results for u compared to Nalu Data:





Marginal slices of 6D posterior distribution

Inference Details

- MCMC chain of 250k samples → effective sample sizes of $10^3 - 10^4$
- MAP solution has *Eff. Th.*, l_{max} at bounds
  - significant improvement in wake capturing relative to mean soln
- Data is informative, especially for *Eff. Th.*, l_{max}, *Ax. IF*
  - significant info gain w.r.t. uniform priors

Impacts

- 5x speedup for forward emulation using MF PCE
- Inverse problem comes for free (post-processing of MF PCE using Hessian-preconditioned MCMC)
  - Added expense: iteratively refine MF PCE in regions of high posterior probability
- Reduction of epistemic RANS uncertainty through assimilation of LES data
- Demonstration of Robust / Reliable Inference at affordable cost: effective alternative to simulation-based MCMC (and ML MCMC)

Connecting the pipeline

Selected vignettes in mission-driven R&D

Looking forward

- Model management with ”trustworthy AI/ML”
- Machine learning is the new wild-west!

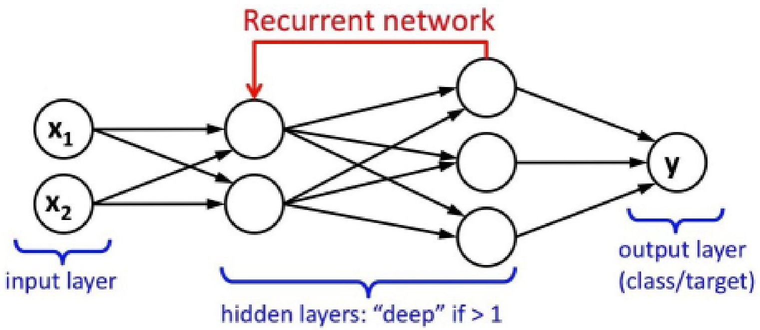
Within DOE, much effort is currently being invested in “UQ for Machine Learning”

- General recognition that AI/ML models must be used with care
- Goal: estimates of prediction variance due to uncertainty in quality of network training

Challenge: “Machine Learning for UQ” leveraging these estimates

- Given emerging capabilities for NN prediction variance + our experience in MF surrogates, extend our model management / data fusion approach to incorporate AI/ML models

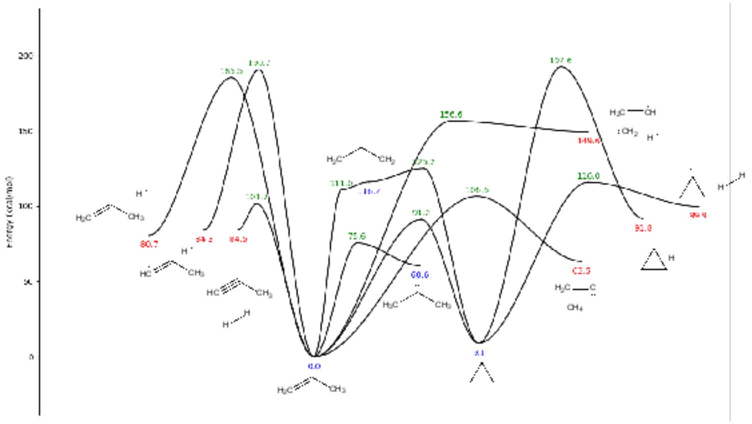
Opportunity to demonstrate a rigorous approach



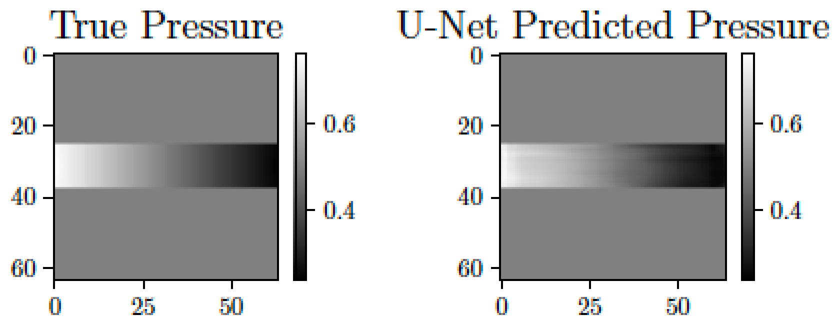
From “Implementation of RNN, LSTM, and GRU,” C.C. Chatterjee

Model Management for UQ with Machine Learning

Quantum Chemistry



Fluid Dynamics



Discrepancy-based, Sequence-based, Hybrid architectures

- Motivated by existing MF approaches (Monte Carlo, PCE)

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

- Mapping from *x* to HF QoI is composed of multiple (traditional) feed-fwd NNs, one per model in hierarchy
  - Following first NN mapping x → Q_0, can map x → Δ_l or Q_{l-1} → Q_l or combine x,Q_{l-1} → Q_l *or* x,Δ_{l-1} → Δ_l
- Differential training: tailor to predictive value vs. cost, targeting decay in mapping complexity

Greedy MF refinement / Active learning

- Compete candidate grid refinements across parameter and model investments for MF prediction of PES for heavy carbon clustering (soot)

Convolutional encoder/decoder assembly networks

- inspired by the recent success in image classification and segmentation shown by deep convolutional encoder-decoder networks (DCNN)
- We investigate encoding-decoding DCNN where fidelities are learned all-at-once during training.

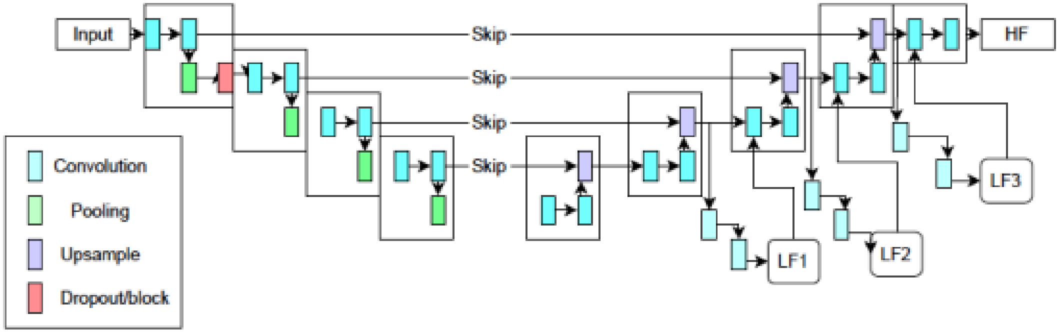


Fig. 3 Schematic representation of the proposed multifidelity network with explicit feedback.

Model Management for UQ Aggregating Additional Error Models

- Beyond MC estimator variance + residual bias
- Must be estimable and controllable
  - Prediction variance in surrogates
  - Underlying simulation stochasticity →
  - …
- Intent is AAO optimization over all relevant parameters (generalized "model management" for aggregate MSE)
  - Special cases (as below) may collapse to smaller optimizations, given explicit theory for portions

E.g., within SNL:

- Turbulent flows/Combustion: finite time-window used for flow stats
- Radiation transport: finite number of particle histories
- Subsurface transport (repositories): finite number of transport domains

- ξ is the vector of **UQ parameters**
- η is a vector of inaccessible RV that notionally represents the **variability in the solver**
- Every time we run the solver, we get an **elementary realization** $f = f(\xi, \eta)$
- **Running for a fixed** $\xi^{(i)}$ multiple times (*replicas*) generates $\left\{ f(\xi^{(i)}, \eta^{(j)}) \right\}_{j=1}^{N_\eta}$
- The QoI for UQ is obtained by **averaging** f (for a fixed ξ):

$$Q(\xi) = \mathbb{E}_\eta[f] \approx \frac{1}{N_\eta} \sum_{j=1}^{N_\eta} f(\xi^{(i)}, \eta^{(j)}) = \tilde{Q}(\xi)$$

Sampling UQ, *e.g.* mean estimator, is accomplished with **two nested sampling estimators**

$$\mathbb{E}[Q] \approx \frac{1}{N_\xi} \sum_{i=1}^{N_\xi} \tilde{Q}^{(i)} = \frac{1}{N_\xi} \sum_{i=1}^{N_\xi} \left[\frac{1}{N_\eta} \sum_{j=1}^{N_\eta} f(\xi^{(i)}, \eta^{(j)}) \right]$$

$$\mathbb{V}ar\left[\hat{Q}^{MC}\right] = \frac{\mathbb{V}\mathbf{ar}\left[\mathbf{Q}(\xi)\right] + \mathbb{E}\left[\frac{\sigma_\eta^2(\xi)}{\mathbf{N}_\eta}\right]}{N_\xi}$$

$$\tilde{\rho}^2 = \frac{\left(\mathrm{Cov}\left[\tilde{Q}^{HF}, \tilde{Q}^{LF}\right]\right)^2}{\mathbb{V}ar\left[\tilde{Q}^{HF}\right] \mathbb{V}ar\left[\tilde{Q}^{LF}\right]} \longrightarrow \boxed{\tilde{\rho}^2 = \frac{\rho^2}{1 + \rho^2 \tilde{\tau}}}$$

$$\text{where} \quad \tilde{\tau} = \frac{\mathbb{V}ar\left[Q^{LF}\right] \frac{\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{N_\eta^{\mathrm{HF}}} + \mathbb{V}ar\left[Q^{HF}\right] \frac{\mathbb{E}\left[\sigma^2_{\eta,\mathrm{LF}}\right]}{N_\eta^{\mathrm{LF}}} + \frac{\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]\mathbb{E}\left[\sigma^2_{\eta,\mathrm{LF}}\right]}{N_\eta^{\mathrm{HF}} N_\eta^{\mathrm{LF}}}}{\left(\mathrm{Cov}\left[\tilde{Q}^{HF}, \tilde{Q}^{LF}\right]\right)^2}$$

$$\tilde{r}^\star = \sqrt{\frac{1-\rho^2}{1-\rho^2+\rho^2\tilde{\tau}} \frac{N_\eta^{\mathrm{HF}}}{N_\eta^{\mathrm{LF}}}} \sqrt{\frac{\rho^2}{1-\rho^2} \frac{\mathcal{C}^{\mathrm{HF}}}{\mathcal{C}^{\mathrm{LF}}}} = \tilde{R}r^\star \quad \leftarrow \textbf{LF oversampling}$$

$$\tilde{\Lambda} = 1 - \frac{\tilde{R}r^\star - 1}{\tilde{R}r^\star} \frac{\rho^2}{1+\rho^2\tilde{\tau}} \quad \leftarrow \textbf{variance reduction}$$

$$N_\xi^\star = \frac{\mathbb{V}ar\left[Q^{HF}\right] + \frac{1}{N_\eta^{\mathrm{HF}}}\mathbb{E}\left[\sigma^2_{\eta,\mathrm{HF}}\right]}{\varepsilon^2} \tilde{\Lambda} \quad \leftarrow \textbf{HF samples}$$

$$\mathcal{C}_{tot} = N_\xi \tilde{\mathcal{C}}_{\mathrm{HF}} + \tilde{r} N_\xi \tilde{\mathcal{C}}_{\mathrm{LF}} = N_\xi \mathcal{C}^{\mathrm{HF}} \left(N_\eta^{\mathrm{HF}} + Rr \frac{\mathcal{C}^{\mathrm{LF}}}{\mathcal{C}^{\mathrm{HF}}} N_\eta^{\mathrm{LF}} \right) \quad \leftarrow \textbf{Total cost}$$

Summary Remarks

Dakota: a flexible, extensible software tool for UQ

- Algorithms: design optimization, model calibration, UQ, DACE, GSA, parametric studies
- Framework: plug and play method selection, composition of methods/models with nesting, recasting, surrogates
- Computing: multiple levels of parallelism for scalability on both capability / capacity HPC
- Interfacing: either a stand-alone application or a set of library services

The Pipeline from Upstream Research → Product Development → Mission Integration

- Vignettes:
  - *UQ Modernization efforts*
  - *Multifidelity methods*
  - *Robust / affordable Bayesian inference*
  - *"ML for UQ" leveraging "UQ for ML"*

Lessons Learned:

- Milestones and other "advanced deployment" opportunities: critical for demonstration and socialization of emerging methodologies
- Organizing around these principles has helped us formalize the different roles and ensure their health
- Feedbacks from these mission integration efforts are identifying the most critical directions for R&D investment
- …

Extra

MF deep Neural Networks for Quantum Chemistry

Discrepancy-based Multifidelity NN modeling

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

- Motivated by MF approaches for Monte Carlo and stochastic emulation
- Decomposition-based approach: mapping from *x* to HF QoI is composed of multiple feed-forward NNs, one per model in hierarchy
- Differential training: tailor to predictive value vs. cost, targeting decay in mapping complexity
- Following first NN mapping x → Q_0, can map either x → Δ_l or Q_{l-1} → Q_l

Recurrent architecture for MF NN

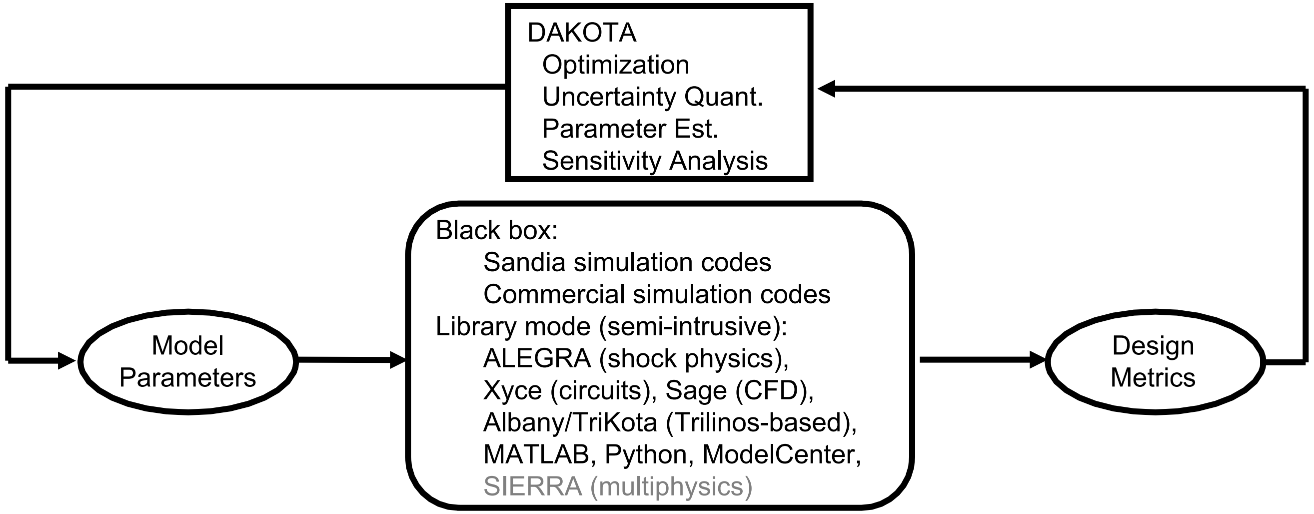
- Used for modeling a sequence, typically for time-dependence
- Our sequence is the model dependence mapping Q_{l-1} → Q_l
- As for co-kriging / GPs, correlation → benefits in integrated modeling
- Approach can be applied to any DAG → generalized model dependency
- Explore LSTM, independent RNN, hierarchical RNN

Greedy MF refinement / Active learning

- Compete candidate grid refinements across parameter and model investments for MF prediction of PES for heavy carbon clustering (soot)

DAKOTA

Explore and predict with confidence



Iterative systems analysis

Multilevel parallel computing

Simulation management

http://dakota.sandia.gov

Manuals, Publications, Training matls. online

Releases: v6.14 released in May

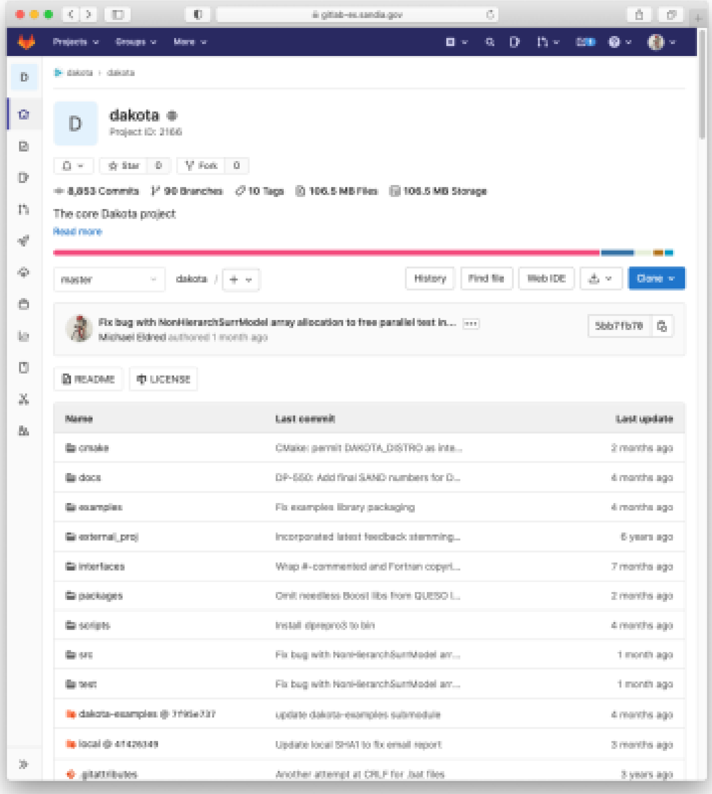
Supported platforms: Linux, Mac, Windows

Modern SQE:; Nightly builds/testing, gitlab, Cmake

GNU LGPL: free downloads worldwide

Community development: moving to pull request model

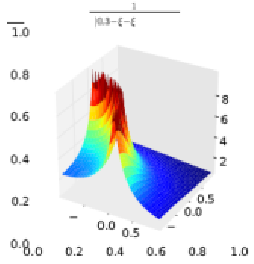
Community support: dakota-users list, [user forums]



Emphasis on Scalable Methods for High-fidelity UQ on HPC

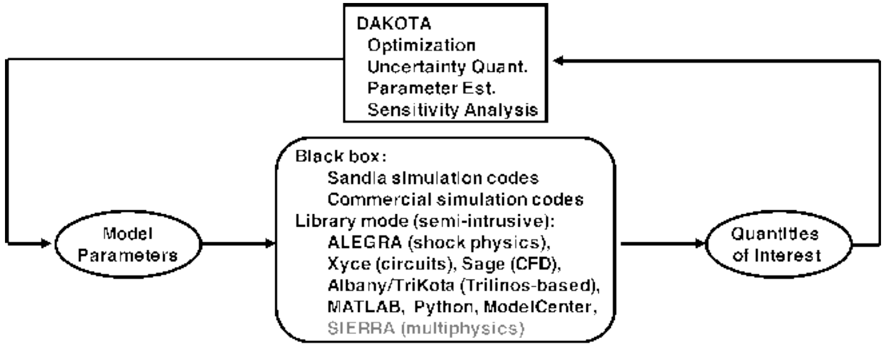
Compounding effects:

- 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)



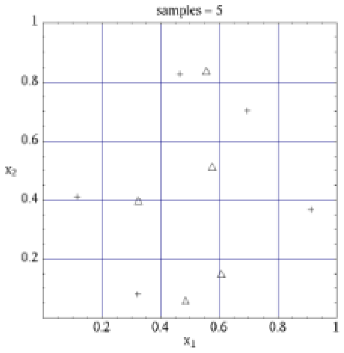
Steward Scalable Algorithms within DAKOTA

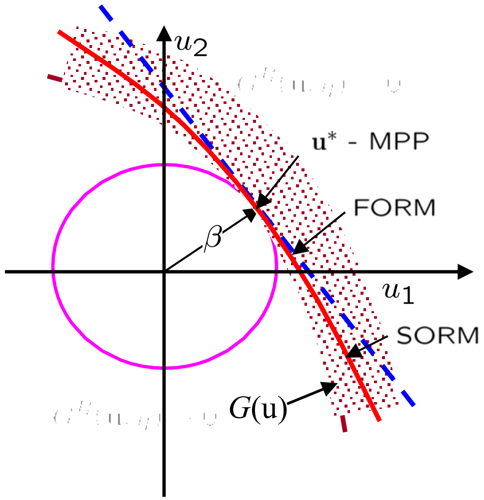
Explore and predict with confidence

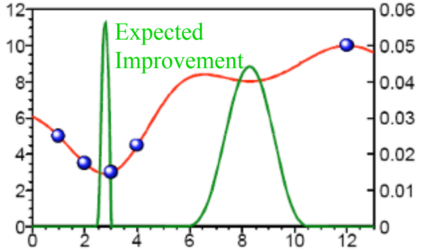


Core (Forward) UQ Capabilities:

- 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

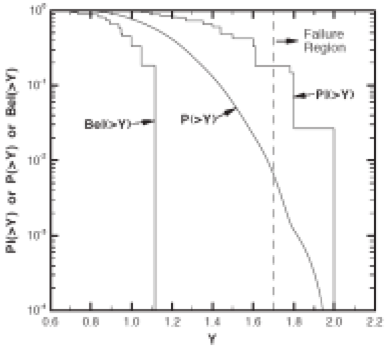




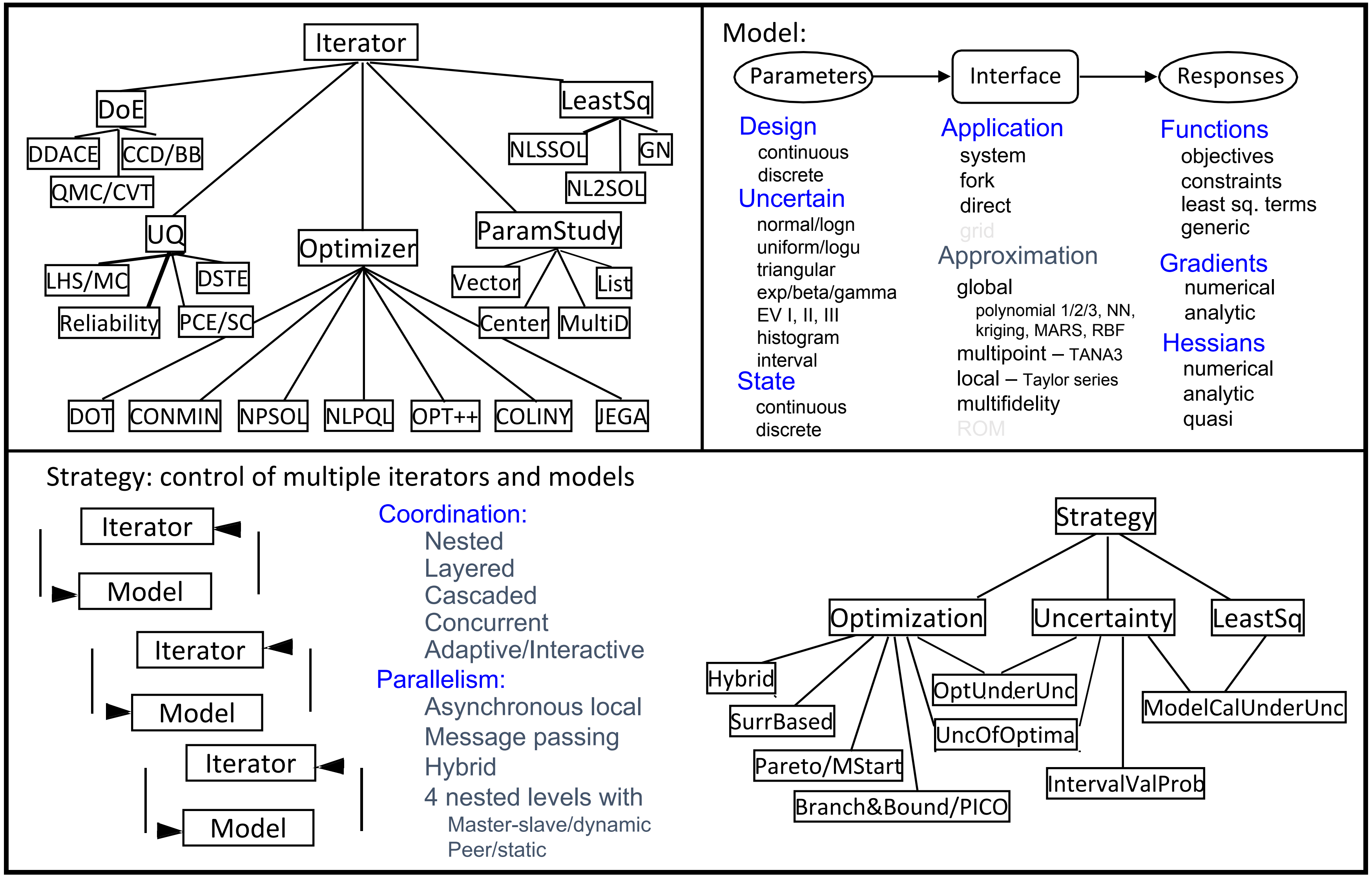


$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

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



DAKOTA Framework

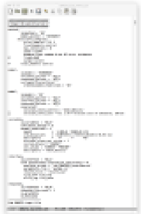


High-Level Vision for Next Generation Architecture

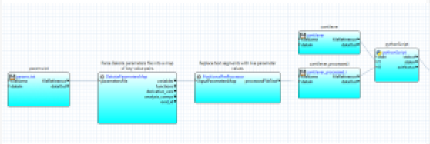
Dakota-MPI, Dakota-X, Py-Dakota, …

Front ends
(Research to Production)

Input file editors



Stand-alone GUI



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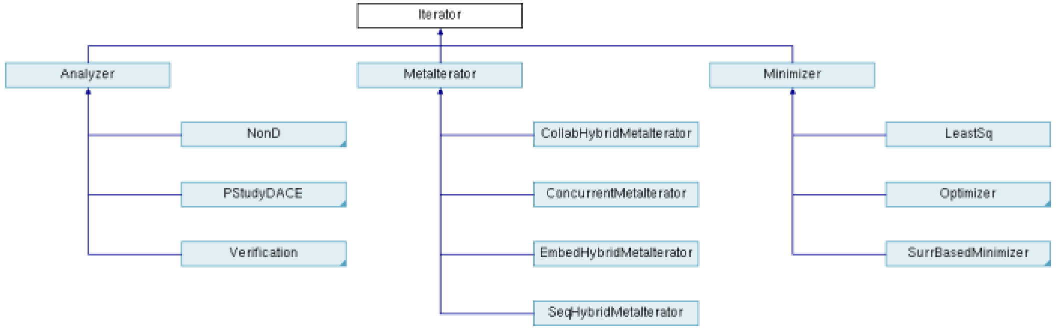
Algorithm Core
(Iterators, Models, …)



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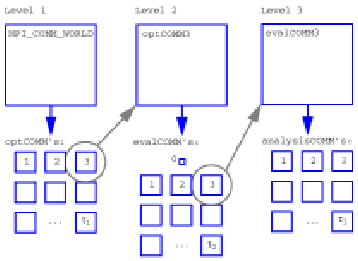
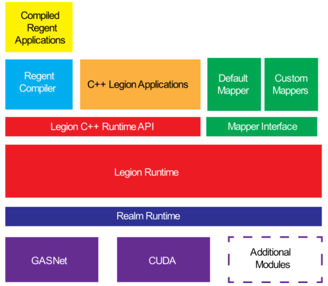
Back ends
(Black box to Embedded plug-ins)

MPI + "X"



AMT



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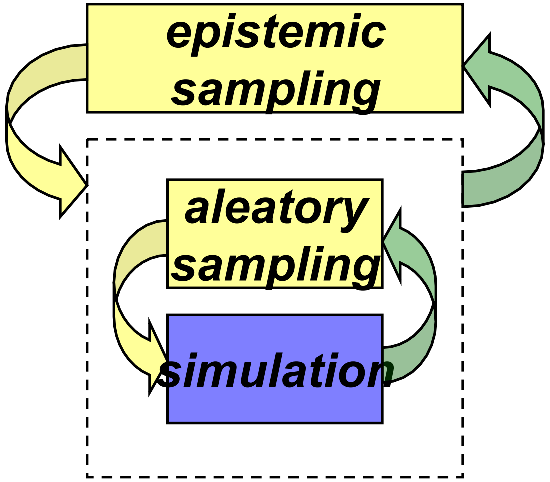
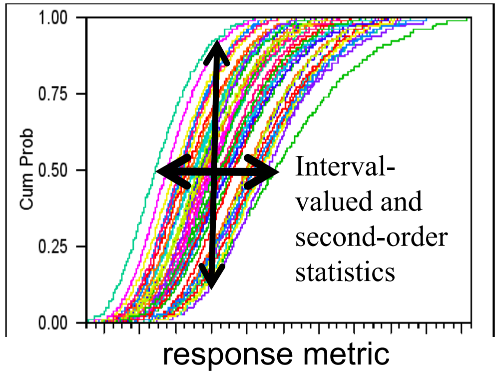
Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

Epistemic uncertainty (aka: subjective, reducible, lack of knowledge uncertainty): insufficient info to specify objective probability distributions



Traditional approach: nested sampling

- Expensive sims → under-resolved sampling (especially @ outer loop)
- Under-prediction of credible outcomes



Algorithmic approaches

- Interval-valued probability (IVP), *aka* probability bounds analysis (PBA)
- Dempster-Shafer theory of evidence (DSTE)
- Second-order probability (SOP), *aka* probability of frequency

Increasing epistemic structure (stronger assumptions)

Address accuracy and efficiency

- Inner loop: stochastic exp. that are epistemic-aware (aleatory, combined)
- Outer loop:
  - IVP, DSTE: opt-based interval estimation, global (EGO) or local (NLP) ⇨
  - SOP: nested stochastic exp. (nested expectation is only post-processing in special cases)

$$\begin{array}{ll} \text{minimize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \end{array}$$

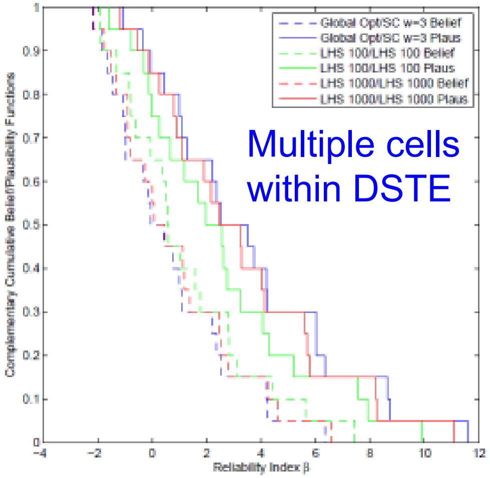
$$\begin{array}{ll} \text{maximize} & M(s) \\ \text{subject to} & s_L \leq s \leq s_U \end{array}$$

Mixed Aleatory-Epistemic UQ:
IVP, SOP, and DSTE based on Stochastic Expansions

Sandia National Laboratories

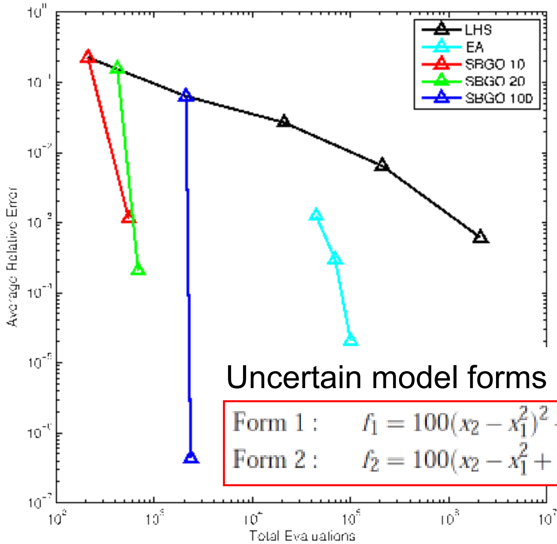
Interv Est Approach	UQ Approach	Expansion Variables	Evaluations (Fn, Grad)	Area	β
IVP SC SSG Aleatory: β interval converged to 5-6 digits by 300-400 evals					
EGO	SC SSG w = 1	Aleatory	(84/91, 0/0)	[75.0002, 374.999]	[-2.26264, 11.8623]
EGO	SC SSG w = 2	Aleatory	(372/403, 0/0)	[75.0002, 374.999]	[-2.18735, 11.5900]
EGO	SC SSG w = 3	Aleatory	(1260/1365, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
EGO	SC SSG w = 4	Aleatory	(3564/3861, 0/0)	[75.0002, 374.999]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 1	Aleatory	(21/77, 21/77)	[75.0000, 375.000]	[-2.26264, 11.8623]
NPSOL	SC SSG w = 2	Aleatory	(93/341, 93/341)	[75.0000, 375.000]	[-2.18735, 11.5901]
NPSOL	SC SSG w = 3	Aleatory	(315/1155, 315/1155)	[75.0000, 375.000]	[-2.18732, 11.5900]
NPSOL	SC SSG w = 4	Aleatory	(891/3267, 891/3267)	[75.0000, 375.000]	[-2.18732, 11.5900]
IVP nested LHS sampling: converged to 2-3 digits by 10^8 evals					
LHS 100	LHS 100	N/A	($10^4/10^4$, 0/0)	[80.5075, 338.607]	[-2.14505, 8.64891]
LHS 1000	LHS 1000	N/A	($10^6/10^6$, 0/0)	[76.5939, 368.225]	[-2.19883, 11.2353]
LHS 10^4	LHS 10^4	N/A	($10^8/10^8$, 0/0)	[76.4755, 373.935]	[-2.16323, 11.5593]

Fully converged area interval = [75., 375.], β interval = [−2.18732, 11.5900]



Multiple cells within DSTE

Interval est w/ mixed-integer global opt



Uncertain model forms (Rosenbrock)

Form 1 : $f_1 = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$

Form 2 : $f_2 = 100(x_2 - x_1^2 + .2)^2 + (0.8 - x_1)^2$

Drekar RANS turbulence: Spalart-Allmaras, k-ε with Neumann BC, k-ε with Dirichlet BC

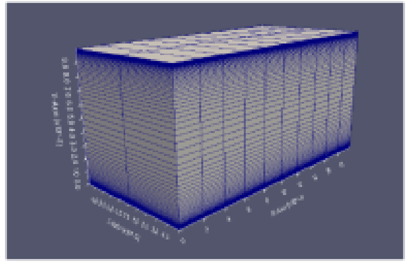


Figure 4. The steady-state x-velocity for typical realization computed using a RANS model in Drekar.

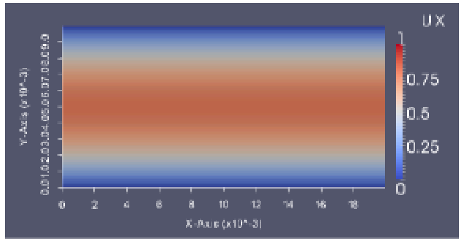
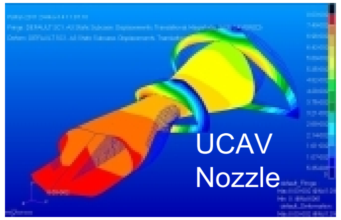


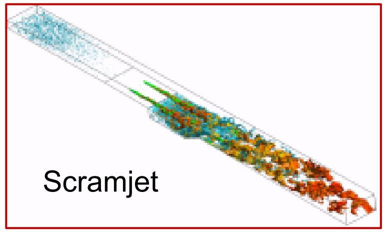
Figure 5. The steady-state x-velocity for typical realization computed using a RANS model in Drekar.

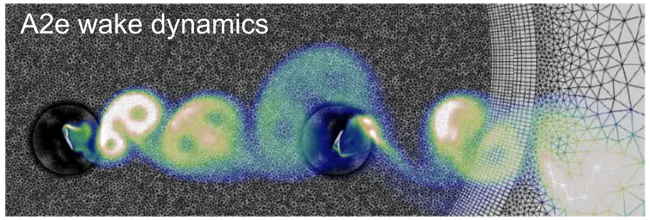
Method	Outer Evals	Total Evals	μ_{ux}	$\mu_{pressure}$
LHS	10	250	[0.727604, 2.78150]	[32.6109, 282.237]
SBGO	17	425	[0.622869, 4.44624]	[21.7321, 297.957]

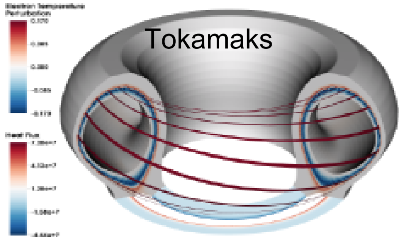
Multifidelity Methods: Sampling UQ, Surrogate UQ, OUU

2018/2019:

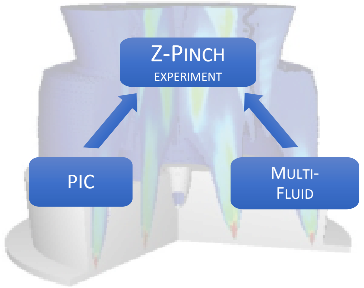


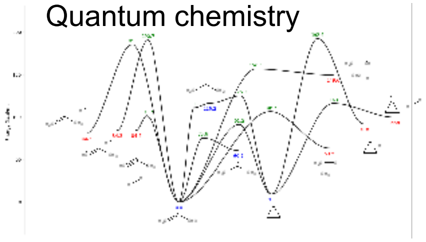


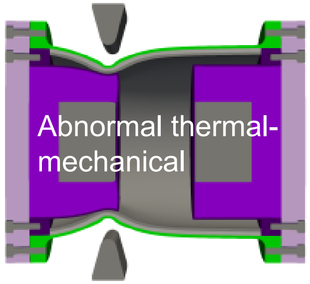


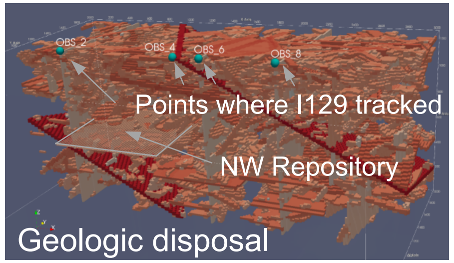


2020/2021:



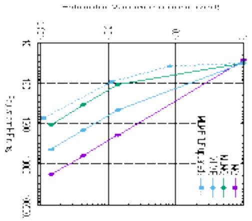


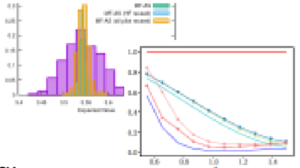




Monte Carlo UQ Methods

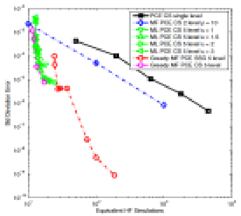
- *Production:* optimal resource allocation for multilevel, multifidelity, combined (DARPA EQUiPS, Wind, Cardiovascular)
- *Emerging:* active dimensions (LDRD, SciDAC), generalized fmwk for approx control variates (ASC V&V), goal orientation (rare events), hybrid methods for GSA
- *On the horizon:* control of time avg; model tuning / selection (LDRD)

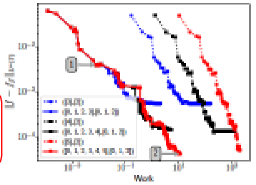




Surrogate UQ Methods (PCE, SC)

- *Production (v6.10+):* ML PCE w/ projection & regression; ML SC w/ nodal/hierarchical interp; greedy ML adaptation (DARPA SEQUOIA), multilevel fn train (ASC V&V)
- *Emerging:* multi-index stochastic collocation; multiphysics/multiscale integration (ASC V&V); new surrogates (GP, ROM, NN) w/ error mgmt. fmwk (LDRD, SciDAC); learning latent variable relationships (MFNets, LDRD)
- *On the horizon:* unification of surrogate + sampling approaches (LDRD)

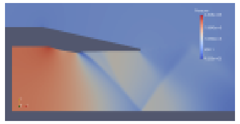




Optimization Under Uncertainty

- *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 Scramjet)
  - SNOWPAC (w/ MIT, TUM) with goal-oriented MLMC error estimates
- *On the horizon:* Gaussian process-based approaches: multifidelity EGO; Optimal experimental design (OED)



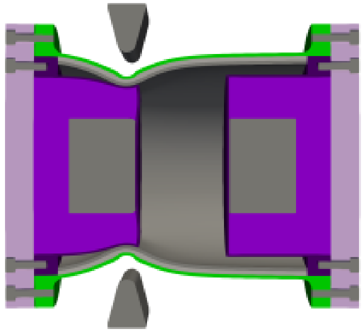
Recent Deployment Vignettes: ML/MF Monte Carlo/Polynomial Chaos

Crash & Burn Multiphysics (ASC L2 Milestone)

Forward UQ w/ explicit (LF) + implicit (HF) SIERRA mechanics

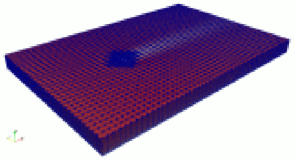
- Multilevel MC across model resolutions for LF model
- Multifidelity MC with HF implicit + selection of most effective LF explicit

Successful demonstration of advanced UQ methods, integrated alongside emerging ASC workflows for multiphysics simulation



Mechanical loading of mock device

A2e Wind (EERE Milestone)

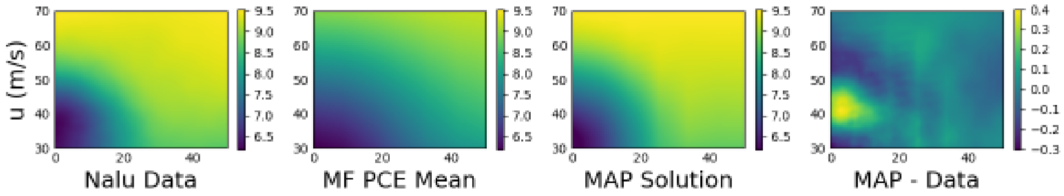


- **Forward UQ:** LES + potential flow in MLMF MC
- **Data assimilation:** integrate experimental wake data from SWiFT facility
- **Opt. Under Uncertainty:** wind plant design using SNOWPAC + MLMC

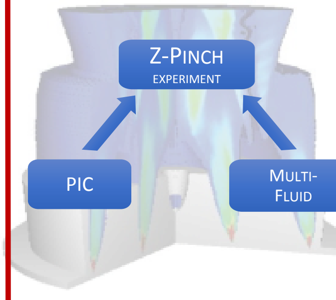
FY19 EERE program milestone:

Emulator-based Bayesian inference leveraging multifidelity PCE

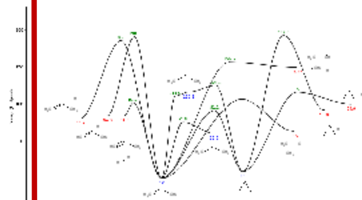
- 5x speedup for forward emulation; inverse problem via post-processing using Hessian-preconditioned Markov chain Monte Carlo



Emerging



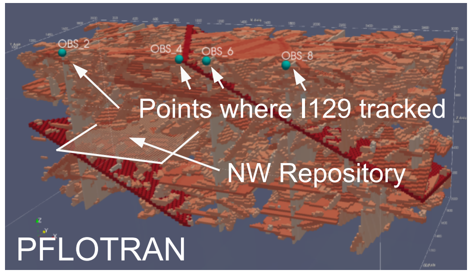
CIS LDRD: non-hierarchical ensemble (models + experiments)

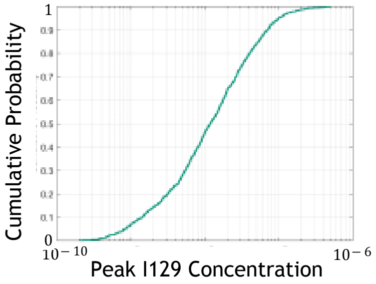


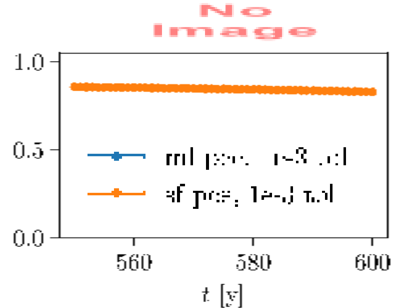
BES QC: exploration of the C_3H_6 PES with KinBot

Geologic Disposal

GDSA example simulation and QOI:



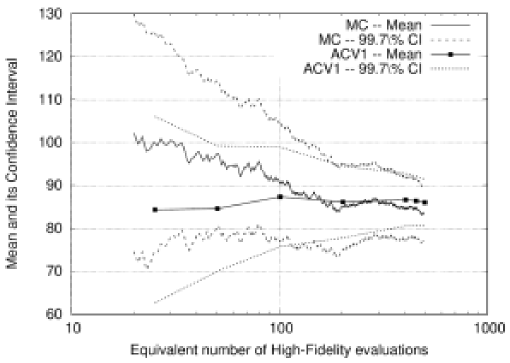




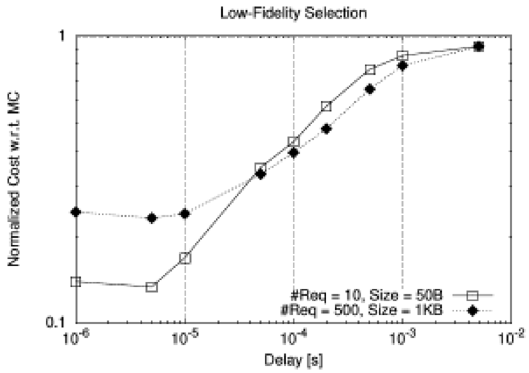
- Deployed MF PCE for GSA to a problem related to geologic disposal safety assessment (GDSA)
- Sobol' indices for model response as fn. of time
- Indices practically identical with ~80 equivalent HF evaluations for MF PCE compared to 713 evaluations for equivalent accuracy SF PCE.

Network Cybersecurity (SECURE GC LDRD)

- Deployed ACV for forward UQ with HF emulation (minimega) and LF discrete event simulation (ns-3)
- Investigated the efficiency of MF UQ by tuning ns-3 models
- Demonstrated increased efficiency for tail est. given a minimega dataset



Forward UQ: ACV1 vs MC



ns-3 tuning effect on ACV performance

SciDAC Partnership: FASTMath/UQ + TDS

Prediction of a basic Tokamak instability using Drekar:

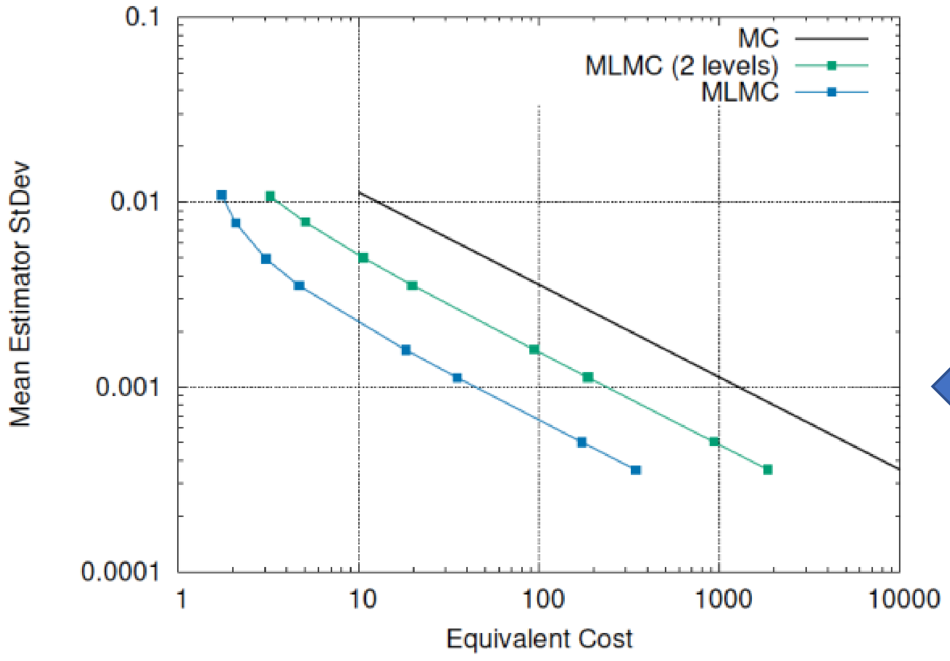
- Multilevel hierarchy: 3 discretizations (constant CFL)

Level	#cores	Run Time [s]	Normalized cost
100×100	72	2.567e+02	0.0307
200×200	108	1.029e+03	0.1844
400×400	144	4.186e+03	1.0000

Pilot sample: 20 samples per level

400	200	100
1.000000000000000	0.999999000457186	0.999967798992103
0.999999000457186	1.000000000000000	0.999969313474247
0.999967798992103	0.999969313474247	1.000000000000000

TABLE: Correlation matrix



Estimator	N_{400}	N_{200}	N_{100}	Eq. Cost
MC	1273	-	-	1273
MLMC (2 levels)	1	1278	-	236.62
MLMC	1	8	1366	44.36

TABLE: Samples allocation per model and total equivalent cost corresponding to an estimator standard deviation equal to $1E-3$

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 $M_0 < M_1 < \dots < M_L \stackrel{\text{def}}{=} M$
- Estimation of $\mathbb{E}[Q_M]$ by means of correction w.r.t. the next lower level

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

- Multilevel Monte Carlo estimator

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

- The Mean Square Error is

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

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

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)

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

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

Background: multifidelity Monte Carlo (MFMC)

Sandia National Laboratories

Correlations
Costs → Optimal LF over-sample $r_i^* = \sqrt{\frac{w_1(\rho_{1,i}^2 - \rho_{1,i+1}^2)}{w_i(1-\rho_{1,2}^2)}}$ → HF samples from budget $m_1^* = \frac{p}{\boldsymbol{w}^T \boldsymbol{r}^*}$

Following ρ estimation, budget p exhausted
→ No iteration

$$\alpha_i^* = \frac{\rho_{1,i}\sigma_1}{\sigma_i}$$ → Expectations from shared, refined

Background: approximate control variate (ACV)

C = covariance matrix among Q_i
c = covariance vector among Q_i and Q

$$\underline{\alpha}^{\text{ACV-IS}} = -\left[\mathbf{C} \circ \mathbf{F}^{(IS)}\right]^{-1}\left[\operatorname{diag}\left(\mathbf{F}^{(IS)}\right) \circ \mathbf{c}\right]$$

$$\mathbb{V}\text{ar}\left[\hat{Q}^{\text{ACV-IS}}(\underline{\alpha}^{\text{ACV-IS}})\right] = \frac{\mathbb{V}\text{ar}[Q]}{N}\left(1 - R^2_{\text{ACV-IS}}\right), \text{ where } R^2_{\text{ACV-IS}} = \boldsymbol{a}^T\left[\mathbf{C} \circ \mathbf{F}^{(IS)}\right]^{-1}\boldsymbol{a}$$

$$\underline{\alpha}^{\text{ACV-MF}} = -\left[\mathbf{C} \circ \mathbf{F}^{(MF)}\right]^{-1}\left[\operatorname{diag}\left(\mathbf{F}^{(MF)}\right) \circ \mathbf{c}\right],$$

$$\mathbb{V}\text{ar}\left[\hat{Q}^{\text{ACV-MF}}(\underline{\alpha}^{\text{ACV-MF}})\right] = \frac{\mathbb{V}\text{ar}[Q]}{N}\left(1 - R^2_{\text{ACV-MF}}\right), \text{ where } R^2_{\text{ACV-MF}} = \boldsymbol{a}^T\left[\mathbf{C} \circ \mathbf{F}^{(MF)}\right]^{-1}\boldsymbol{a}$$

$\boldsymbol{a} = [\operatorname{diag}(\mathbf{F}^{(IS)}) \circ \bar{\mathbf{c}}]$ *and* $\mathbf{F}^{(IS)} \in \mathbb{R}^{M\times M}$ *has elements*

$$\mathbf{F}^{(IS)}{}_{ij} = \begin{cases} \frac{r_i-1}{r_i}\frac{r_j-1}{r_j} & \text{if } i \neq j \\ \frac{r_i-1}{r_i} & \text{otherwise} \end{cases}.$$

$\boldsymbol{a} = [\operatorname{diag}(\mathbf{F}^{(MF)}) \circ \bar{\mathbf{c}}]$ *and* $\mathbf{F}^{(MF)} \in \mathbb{R}^{M\times M}$ *has elements*

$$\mathbf{F}^{(MF)}{}_{ij} = \begin{cases} \frac{\min(r_i,r_j)-1}{\min(r_i,r_j)} & \text{if } i \neq j \\ \frac{r_i-1}{r_i} & \text{otherwise} \end{cases}.$$

← Differs only in off-diagonal terms + sample sets

$$\min_{N,\underline{r},K,L} \log(J_{ACV}(N,\underline{r},K,L)) \quad \text{subject to } N\left(w + \sum_{i=1}^{M} w_i r_i\right) \leq C, \quad N \geq 1, \quad r_1 \geq 1$$

Optimal r*,N* w/i budget from ***C*,*c*** estimates → No iteration

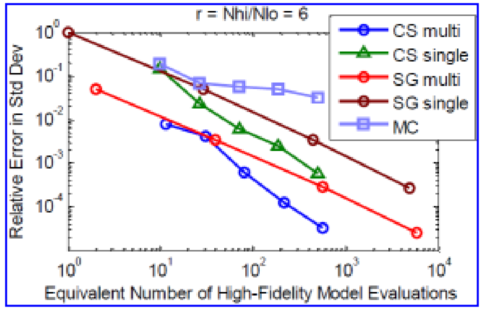
Peherstorfer, Willcox, Gunzburger, “Optimal Model Management For Multifidelity Monte Carlo Estimation”, SISC, Vol. 38, No. 5.
Gorodetsky, Geraci, E., Jakeman, “A generalized approximate control variate framework for multifidelity uncertainty quantification,” JCP 408 (2020)

Formulations for Multilevel PCE / SC

Starting point (2012): prescribed ML/MF resolutions w/ adaptivity

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

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



Rate estimation

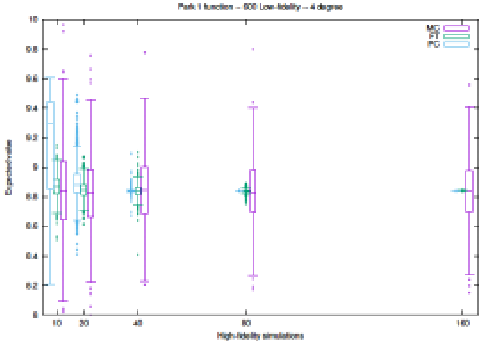
1. Optimal resource allocation: parameterize estimator variance → optimal N_l

Global κ and $\gamma > 0$

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

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

Main challenge: abrupt transitions in sparse / low rank recovery



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

Recovery theory

2. Restricted Isometry Property (RIP) for sparse recovery (BLUE for OLS, FTT N_l scaling w/ rank)

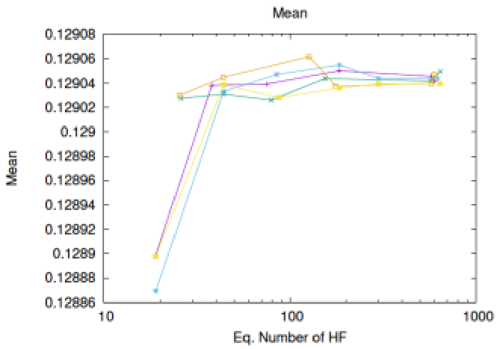
$$N_l \geq s_l \, log^3(s_l) \; L_l \, log(C_l)$$

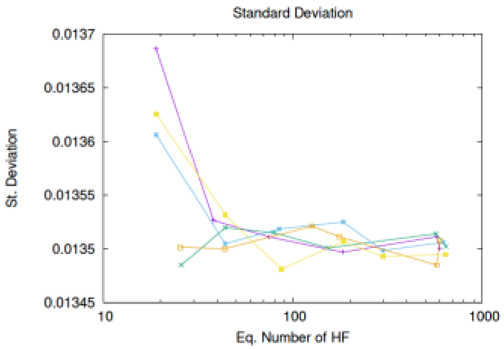
Jakeman, Narayan, and Zhou, 2016

Main challenge: compressible fns

→ increasing s

→ feedback not well controlled for CS (better for FTT?)





Greedy

3. Greedy Multilevel refinement

ML competition with multiple level candidate generators

Main challenges: scalable refinement schemes, loss of precision

Surrogate approaches: Greedy multilevel refinement

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

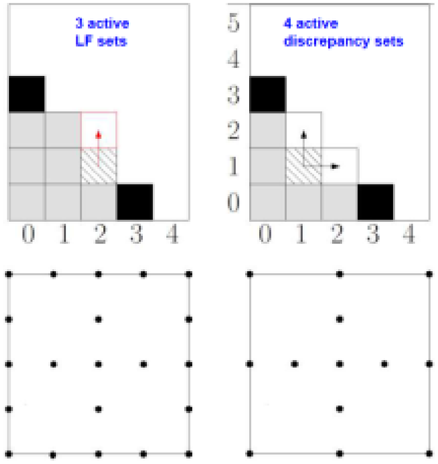
<u>Compete refinement candidates across model levels:</u> max induced change / cost

- 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

<u>Level candidate generators:</u>

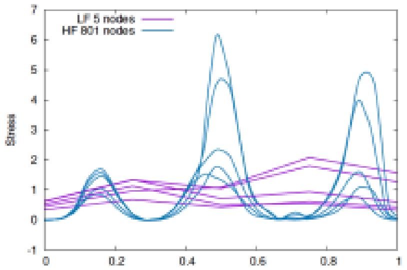
- *Uniform refinement:* 1 exp order / grid level candidate per model level
  - Tensor / sparse grids: projection PCE, nodal/hierarchical SC
  - Regression PCE: least squares / compressed sensing
- *Anisotropic refinement:* 1 exp order / grid level candidate per model level
  - Tensor / sparse grids
- *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.)



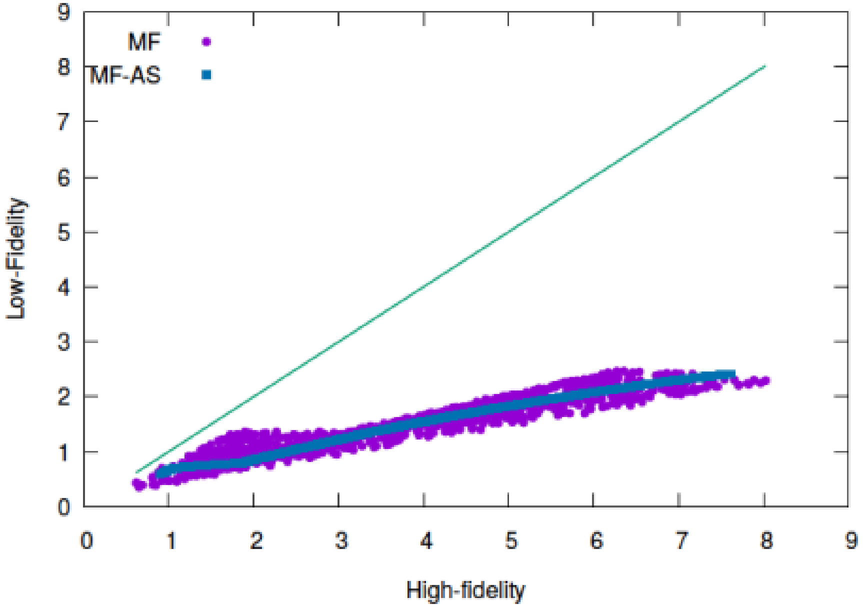
Multilevel – Multifidelity Sampling Methods

Research Direction: leveraging active directions (example 2)

Wave propagation test problem

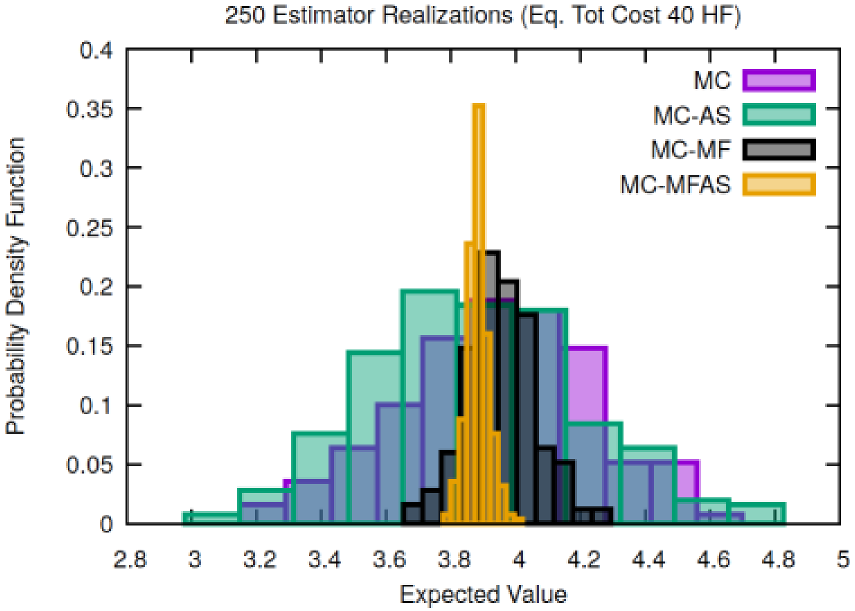


	N_x	N_t	Δ_t
Low-fidelity	5	50	36×10^{-4}
High-fidelity	801	600	30×10^{-5}



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

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



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

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