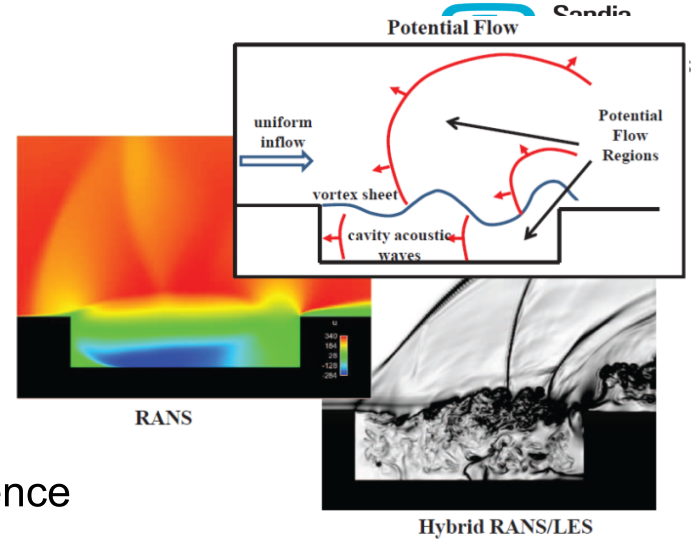
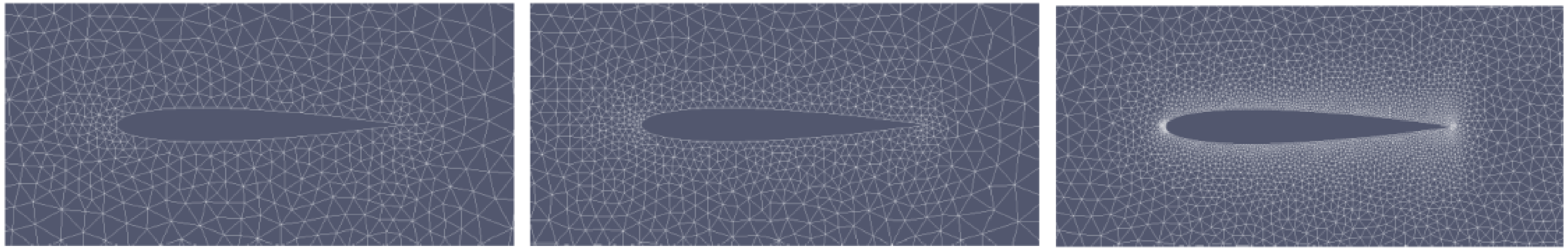
What is Multifidelity UQ?



Simulation alternatives

- Distinct model forms from solving different equation sets
  - Significant cost separation but discrepancy is more complex
- Discretization levels / resolution controls
  - Exploit special structure: discrepancy → 0 at order of spatial/temporal convergence
- Combinatorial ensemble for multiphysics, multiscale



Single-fidelity approaches are widespread and typical model development practices lead to an error imbalance

- A single high-fidelity model, with spatial/temporal resolution appropriately addressed through solution verification
- Effective resolution of deterministic bias, but often leading to large stochastic errors (e.g. from restricted sampling)

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

Mean Square Error:

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

- Multifidelity UQ optimizes the allocation of simulation resources subject to achieving an error target…

Multifidelity UQ Example: optimal resource allocation in Multilevel MC

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Expectations are distributed across levels to decompose variance:

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

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

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

Design variable to optimize

$$\begin{aligned} \text{minimize} \quad & \mathcal{C}(\hat{Q}_M^{ML}) = \sum_{\ell=0}^{L} N_\ell \mathcal{C}_\ell \\ \text{s.t.} \quad & \sum_{\ell=0}^{L} N_\ell^{-1} \mathbb{V}ar(Y_\ell) = \varepsilon^2/2 \end{aligned}$$

Minimize aggregate cost

Balance deterministic and stochastic errors

KKT Optimality →

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

Level independent | Level dependent

Optimal sample profile

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

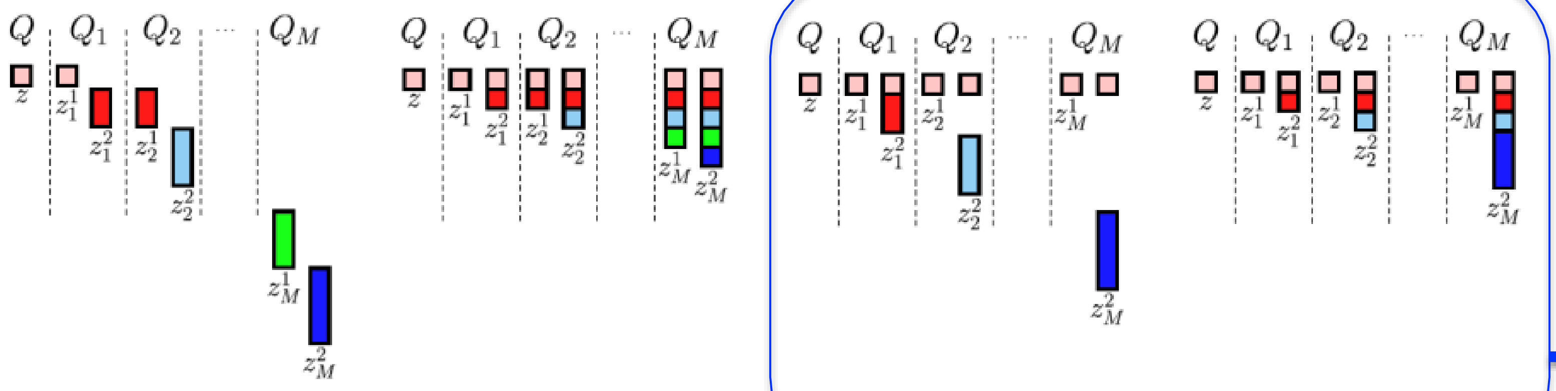
Key Ideas:

- Optimize the allocation of resources across multiple models
- Manage approximations in a principled manner: extract value without reliance
- "Fuse" data in order to obtain results that are consistent with HF but at reduced cost

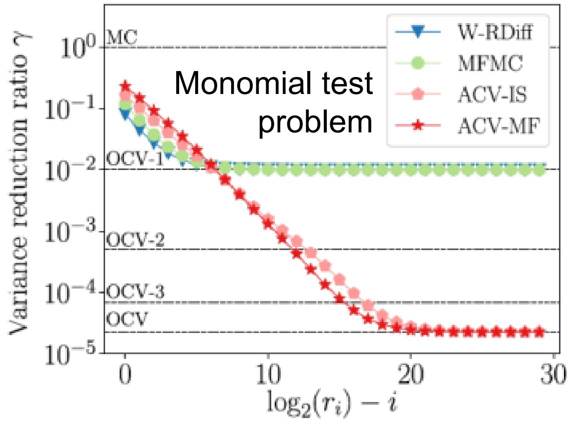
Generalized framework for multilevel / multifidelity estimators

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

Depiction of sample sets $\{z^1, z^2\}$ for model i



(a) W-RDiff sampling strat. (b) MFMC sampling strat. (c) ACV-IS sampling strat. (d) ACV-MF sampling strat.



Performance bounds for recursive vs. non-recursive

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

Estimator	Type	Sample allocation
MLMC	1D: hierarchical, recursive	Analytic
CVMC	1D: HF,LF pair	Analytic
MLCV MC	2D: HF,LF pair + resolutions	Analytic
MFMC	1D: hierarchical, recursive	Analytic, Numerical
ACV	Unordered ensemble, non-recursive	Numerical

Gorodetsky, Geraci, E., Jakeman, “A generalized approximate control variate framework for multifidelity UQ,” JCP 408 (2020)

Key mission feedbacks

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

- Extensions for complex multidimensional hierarchies → *multi-index collocation, multiphysics / multiscale*
- Investments in non-hierarchical MF methods → *ACV and MFNets*

Popular MF approaches neglect important practicalities

- "Oracle" correlations assumed → *iterated versions of MFMC, ACV* to reduce cost from pilot over-estimation
- Imperfect data → *embedded cross validation* in regression-based surrogate MF
- Dissimilar parameterizations → *shared subspaces* to link and correlate diverse models
- Stochastic simulations, simulation/surrogate error estimation → *extended error management framework*
- Heterogeneous ensemble management → *integration with HPC workflow managers, R&D in ensemble AMT*
- Free hyper-parameters in LF approximations → *model tuning*

MF methods most often utilize a fixed model ensemble determined by expert judgment

- Experts are often inaccurate in this context (intuition is often wrong as trade-offs are not obvious)
  - Physics SMEs often have high predictivity standards and tend to over-estimate the LF accuracy required
  - Leads to non-optimal correlation / cost trade-off and sub-optimal MF UQ

→ Exploration of hyper-parameter model tuning, within the context of particular estimators (ACV, MFMC, ...)

Model Tuning Approaches: All-At-Once and Bi-Level

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Model tuning performed to maximize performance *of a particular estimator* over *tunable hyper-parameters* associated with one or more low-fidelity models (HF reference is immutable)

AAO optimization (in Python):

$$\arg\min_{\theta,\mathbf{r},N} \frac{Var[Q]}{N}(1 - R^2(\theta,\mathbf{r})) \quad s.t. \quad N\left(w + \sum_{i=1}^{M} w_i(\theta) r_i\right) \le C$$

Hyper-parameters θ integrate as additional decision vars
Potential for greater efficiency: one integrated higher-D solve

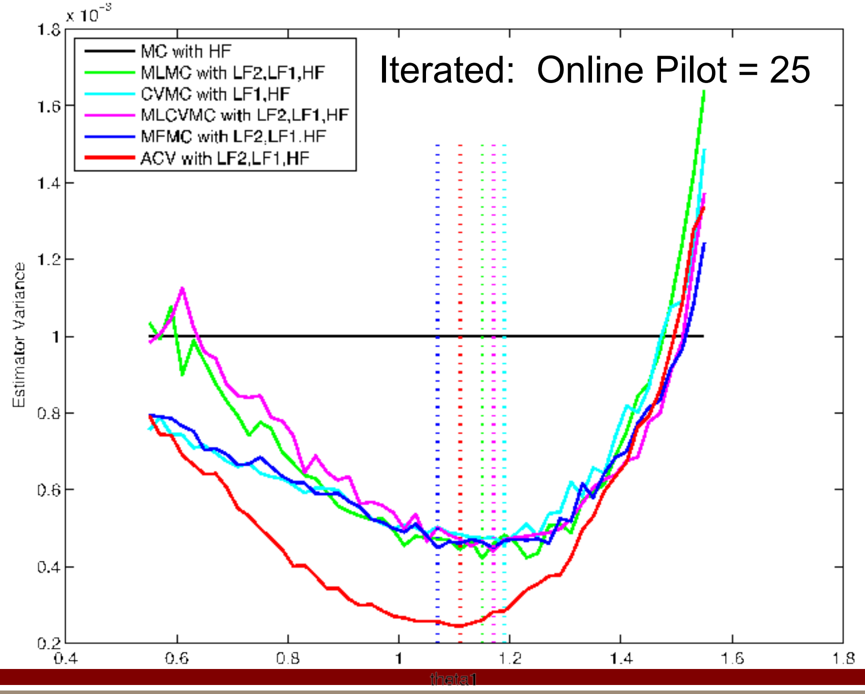
Bi-level optimization (in Dakota):

$$\arg\min_{\theta} \left[\arg\min_{\mathbf{r},N} \frac{Var[Q]}{N}(1 - R^2(\theta,\mathbf{r})) \quad s.t. \quad N\left(w + \sum_{i=1}^{M} w_i(\theta) r_i\right) \le C\right]$$

Inner loop solve for each outer loop θ iterate
Plug & play outer loop with global, surrogate-based, MINLP

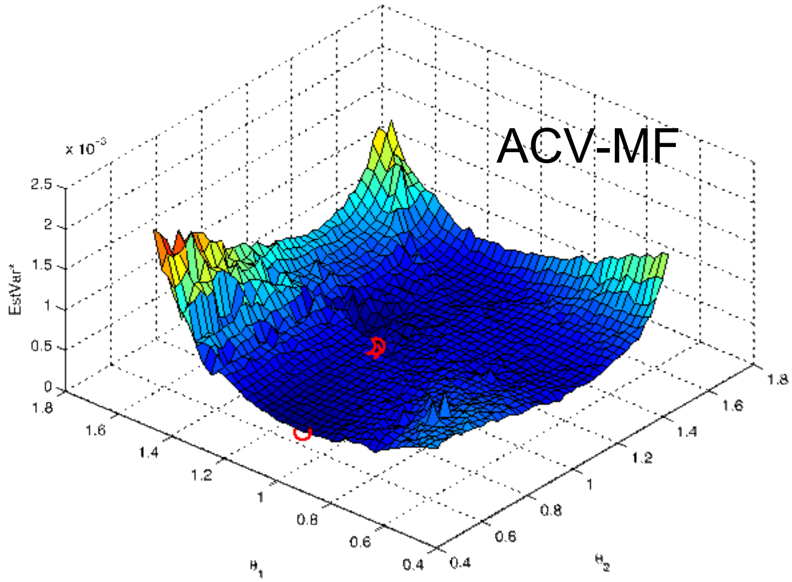
1D/2D verifications with tunable model problem:

- 5 estimators x 3 solution modes
- Optimal θ depends on estimator
- Iterated approach achieves oracle accuracy at lower cost



Efficient global optimization (EGO) navigates noisy space and locates multiple minima

- ACV flexibly adapts to model reconfiguration



E., Geraci, Portone, Gorodetsky, Jakeman, "All-at-Once (and Bi-Level) Model Tuning for Multifidelity Sampling," SIAM UQ22.