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A unified mathematical and algorithmic framework for managing multiple
information sources of multi-physics systems

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14. ABSTRACT Decision processes for complex, multidisciplinary systems draw on multiple information sources, including multi-fidelity models, historical data, operational data, experimental data, and expert opinions. In many cases there is not just a set of computational models clearly ranked in terms of fidelity; rather, there are multiple sources of information with different types of distortion of the true system. These sources are not commensurable with a scalar-valued measure of "fidelity"—they tell us different things about the problem, with their collective information being greater than the individual parts. This project comprised an integrated research program leveraging the foundations and methods of information theory, decision theory, and machine learning. These elements were brought together in new ways with multidisciplinary design optimization (MDO), multi-fidelity modeling, uncertainty quantification, and reduced-order modeling. The specific project goals were to: (1) Develop statistical approaches for defining and quantifying fidelity. (2) Establish decision-theoretic methods for optimally managing sources of uncertain multi-physics information. (3) Create reduced models with goal-driven adaptation to multi-physics interactions and with quantified uncertainty. (4) Formulate an information-theoretic approach for handling multi-physics coupling. (5) Create a scalable framework for solving multi-physics analysis and design problems under uncertainty. All goals were achieved. The MURI project made particularly high-impact contributions in developing the methods and practice of multi-information source optimization, laying the mathematical and algorithmic foundations of multi-fidelity uncertainty quantification, and advancing design and uncertainty quantification of complex multidisciplinary systems.					
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1 Project overview, goals and key accomplishments

Decision processes for complex, multidisciplinary systems draw on multiple information sources, including multifidelity models, historical data, operational data, experimental data, and expert opinions. In many cases there is not just a set of computational models clearly ranked in terms of fidelity; rather, there are multiple sources of information with different types of distortion of the true system. These sources are not commensurable with a scalar-valued measure of “fidelity”—they tell us different things about the problem, with their collective information being greater than the individual parts. This project comprised an integrated research program leveraging the foundations and methods of information theory, decision theory, and machine learning. These elements were brought together in new ways with multidisciplinary design optimization (MDO), multifidelity modeling, uncertainty quantification, and reduced-order modeling.

The specific project goals were to: (1) Develop statistical approaches for defining and quantifying fidelity. (2) Establish decision-theoretic methods for optimally managing sources of uncertain multi-physics information. (3) Create reduced models with goal-driven adaptation to multi-physics interactions and with quantified uncertainty. (4) Formulate an information-theoretic approach for handling multi-physics coupling. (5) Create a scalable framework for solving multi-physics analysis and design problems under uncertainty. All goals were achieved. The MURI project made particularly high-impact contributions in developing the methods and practice of multi-information source optimization, laying the mathematical and algorithmic foundations of multifidelity uncertainty quantification, and advancing design and uncertainty quantification of complex multidisciplinary systems.

Notable transitions made during the project include the following:

- OpenMDAO: MURI methods form the foundations of NASA’s OpenMDAO toolset, which is used by many groups around the world (<http://openmdao.org>)
- Webfoil: An online database of airfoil shapes and multi-source data, with capability for rapid design optimization (<http://webfoil.engin.umich.edu>)
- Surrogate Modeling Toolbox (SMT): An open-source Python package now being used by NASA, ONERA, and SupAero (<https://smt.readthedocs.io/en/latest/>)
- OpenAeroStruct: A wing MDO tool and scalable benchmark MDO problem used by many research groups across the world (<https://mdolab.github.io/OpenAeroStruct>)
- MURI PIs authored a highly cited survey paper on multifidelity methods [1].
- MURI multifidelity methods were transitioned to practitioners at Boeing, ExxonMobil, Uber, Facebook, Lawrence Livermore National Laboratory, AFRL, and NASA Goddard.
- Bayesian optimization algorithms, including knowledge gradient for multi-information source optimization and BayesOpt for composite functions, were implemented in Facebook’s BoTorch software package.
- Batch multi-information source Bayesian optimization software (github.com/RichardCouperthwaite/BB0-Reification)
- MIT Uncertainty Quantification Library (<http://muq.mit.edu>)
- Transport maps (including graph learning) (<http://transportmaps.mit.edu>)

- Multifidelity Monte Carlo method (<https://github.com/pehersto/mfmc>)
- Multifidelity global sensitivity analysis (mfGSA) package being used by NASA Goddard for UQ of the James Webb space telescope (github.com/elizqian/mfgsa)
- Frazier leveraged research in efficient resource allocation to play significant role in Cornell’s fall reopening; designed the targeted asymptomatic COVID-19 screening strategy that is a key part of the reopening.
- Five MURI students/postdocs became tenure-track faculty: Hwang (UCSD), Kramer (UCSD), Morrison (UC Boulder), Peherstorfer (NYU), Poloczek (U Arizona).

The MURI team were also active in dissemination and outreach. The PIs organized minisymposia at SIAM and INFORMS meetings, offered a tutorial on Bayesian optimization at the 2018 INFORMS Annual Meeting, organized MURI special sessions at AIAA Scitech 2018 and AIAA Scitech 2020, and co-organized the Workshop on Multifidelity Modeling in support of Design and Uncertainty Quantification at the 2019 AIAA Aviation Forum.

Detailed summaries of major research accomplishments are organized according to the three research thrusts (RT) of RT1: Optimal information-source management, RT2 Goal-oriented reduced-order models for the multi-source multi-physics setting, and RT3 Managing multi-physics coupling (although it should be noted that a number of the research elements crosscut multiple research thrusts).

2 RT1: Optimal Information Source Management

2.1 Beyond Greedy

Bayesian optimization (BO) sequentially builds a statistical model for the objective function and uses it as a surrogate to select the next design to evaluate. In the past, most Bayesian optimization algorithms choose the next design to evaluate by maximizing a greedy criterion. This is a suboptimal strategy because it does not account for future evaluations. We have pursued several lines of research within RT1 to understand how much is lost by this greedy strategy, and to develop strategies for obtaining improved performance through strategies that go beyond greedy. We have studied this both in traditional Bayesian optimization, where we use Gaussian processes, and in other problems that use other statistical modeling approaches.

2.1.1 Lookahead Bayesian optimization

In [2], we investigate lookahead formulations for BO that explicitly account for future evaluations. This is achieved by formulating BO as a dynamic programming instance (illustrated in Figure 1, left panel). Because the resulting formulation is intractable to solve, we explore approximate dynamic programming techniques; in particular, we employ the rollout algorithm (illustrated in Figure 1, right panel), which approximates future steps in a closed-loop fashion. The resulting algorithm achieves improved and more robust performances compared to greedy BO algorithms (Figure 2) and existing (approximate open-loop) lookahead approaches. This work has been accepted for publication in the 2016 Neural Information Processing System (NIPS) conference.

2.1.2 Going beyond greedy in constrained Bayesian optimization

The MURI team also made progress this year on methods for constrained BO. Incorporating constraints makes the optimization problem much harder to solve, but is essential if these methods

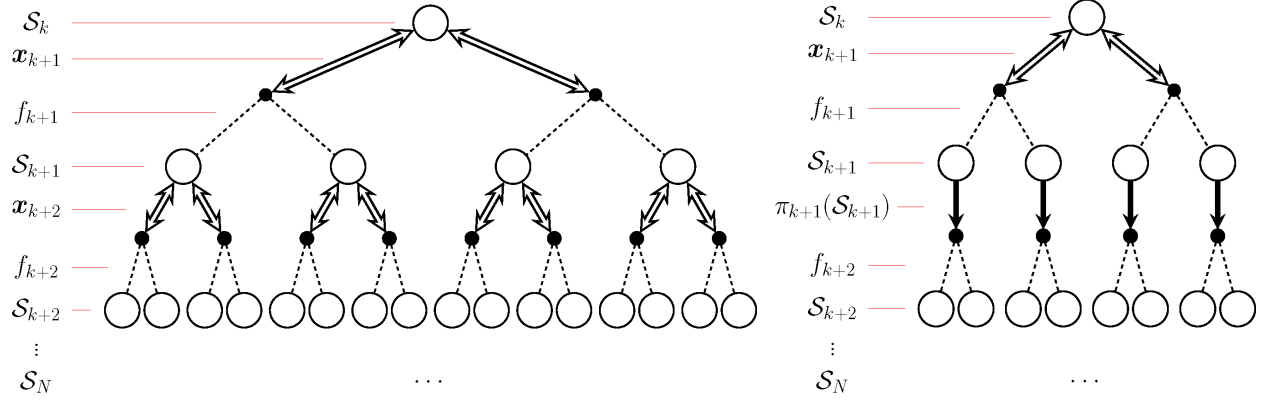


Figure 1: Graphs representing the dynamic programming (left) and the rollout (right) formulations. Note the simpler structure of the rollout graph compared to the dynamic programming one.

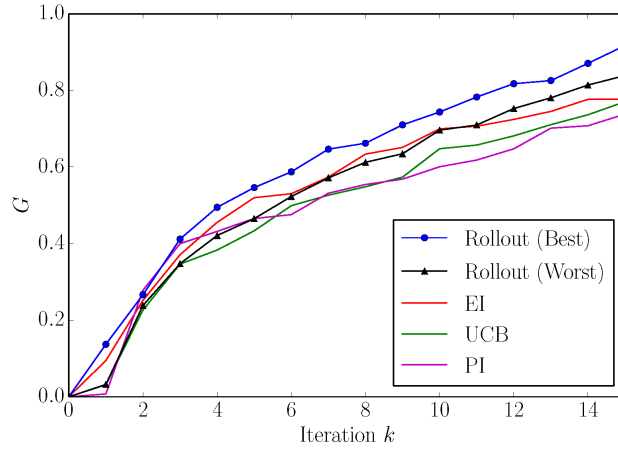


Figure 2: Normalized reduction of the objective function, G , for the rollout algorithm (best and worst configurations tested) and several greedy algorithms as a function of iteration.

are to be useful for real-world design problems. Our new method addresses optimization problems subject to inequality constraints where a finite budget of evaluations is available, a common situation when dealing with expensive models (e.g., a limited time to conduct the optimization study or limited access to a supercomputer). The method uses a lookahead BO algorithm that plans the sequence of designs to evaluate in order to maximize the improvement achieved, not only at the next iteration, but once the total budget is consumed. Incorporating lookahead is particularly important in the constrained BO setting, since it is sometimes beneficial to evaluate an infeasible design in order to gain knowledge about the location of a constraint, which will pay benefits in subsequent iterations. Existing greedy BO approaches cannot recognize this downstream benefit.

2.1.3 Two-step lookahead: fast, efficient, and practical

Accurately looking many steps ahead using reinforcement learning is computationally intensive. There are many problems where objective function evaluations are fast enough that we wish to avoid the computational overhead of these methods, but where the evaluations are slow enough that Bayesian optimization still provides substantial value over other derivative-free optimization methods. [3], published at NeurIPS 2019, addresses this need. It proposes a computationally effi-

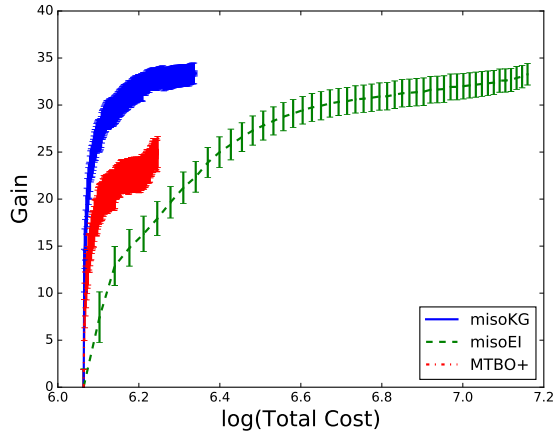


Figure 3: Our widely-used misoKG algorithm [10] significantly expanded MISO capabilities and improved performance substantially over other previously available methods.

cient algorithm that provides an accurate solution to the two-step lookahead Bayesian optimization problem in seconds to at most several minutes of computation per batch of evaluations. The resulting acquisition function provides increased query efficiency and robustness compared with previous two- and multi-step lookahead methods in both single-threaded and batch experiments. This unlocks the value of two-step lookahead in practice. We demonstrate the value of our algorithm with extensive experiments on synthetic test functions and real-world problems.

2.1.4 Exact multi-step lookahead in problems closely related to Bayesian optimization

We have also studied the value that infinite lookahead policies can provide in problems closely related to multi-information-source-optimization that have special structure that allow computing the infinite lookahead policy exactly, or that allow providing tight performance bounds. This includes work on one-dimensional feasibility determination [4], which won first place (tie) in the INFORMS Undergraduate Operations Research Prize, as well as work on coupled bisection [5], multi-armed bandits [6, 7] and multiple target localization [8, 9].

2.2 Rich Information Sources

2.2.1 Beyond independent information sources (misoKG)

In work that has received over 100 citations since its publication, and was honored with an oral presentation at NIPS (1% of submitted papers), we propose in [10] the knowledge-gradient algorithm for MISO (misoKG). This algorithm provides effective MISO and moves beyond independent information sources using two contributions. The first is a novel unified treatment of the objective function and the possible correlated information sources via Gaussian process regression, capturing explicitly uncertainties due to model discrepancy and observational noise. Second, we developed the cost-sensitive Knowledge Gradient that optimally trades off expected information gain and query cost when selecting the next information source and the design to be evaluated. An experimental evaluation in [10] demonstrates that the algorithm utilizes even heavily biased information sources effectively, thereby achieving a significant reduction in the overall optimization cost (cp. Fig. 3 (left)).

2.2.2 MISO for deep neural network hyperparameter tuning

We developed a practical code using multi-information source optimization (and in particular the misoKG algorithm) to tune hyperparameters for deep neural networks [11]. In this work, we consider the fact that the time required to evaluate the validation error for even a few hyperparameter settings remains a bottleneck. MISO promises relief using cheaper proxies to such objectives — for example, validation error for a network trained using a subset of the training points or fewer iterations than required for convergence. We propose a highly flexible and practical approach to multi-information source Bayesian optimization focused on efficiently optimizing hyperparameters for iteratively trained supervised learning models. We introduce a new acquisition function, the trace-aware knowledge-gradient, which efficiently leverages both multiple continuous fidelity controls and trace observations — values of the objective at a sequence of fidelities, available when varying fidelity using training iterations. We provide a provably convergent method for optimizing our acquisition function and show it outperforms state-of-the-art alternatives for hyperparameter tuning of deep neural networks and large-scale kernel learning. Frazier gave a plenary at the 2019 ICML workshop on AutoML based on this work.

2.2.3 Grey-box Bayesian optimization

Building on the success of MISO methods, we launched a stream of work on *grey-box* BO. In this type of MISO, we rethink the traditional approach to black-box optimization. Instead of treating the objective function as a pure black box, we allow ourselves to use some of its internal structure while treating other aspects as unknown — essentially we “look inside the box”.

One prominent example, considered in [12], is calibration problem with a time-consuming physics simulator. In such problems, we wish to find model parameters θ so that the simulator’s prediction for real-world outcomes at those parameters, $h(\theta)$, matches a vector of observed data y as well as possible in the sense of squared error. This problem is $\min_{\theta} f(\theta)$ where $f(\theta) := ||h(\theta) - y||$. A traditional black-box approach would model observations of $f(\theta)$ using a Gaussian process. Instead, we model the outcomes $h(\theta)$ using a multi-output Gaussian process and then compute a posterior on $f(\theta)$ and an associated acquisition function that leverages detailed knowledge of how $f(\theta)$ is obtained from $h(\theta)$.

More generally, [12] considers optimization of composite objective functions, i.e., of the form $f(x) = g(h(x))$, where h is a black-box derivative-free expensive-to-evaluate function with vector-valued outputs, and g is a cheap-to-evaluate real-valued function. While these problems can be solved with standard Bayesian optimization, we propose a novel approach that exploits the composite structure of the objective function to substantially improve sampling efficiency. Our approach models h using a multi-output Gaussian process and chooses where to sample using the expected improvement evaluated on the implied non-Gaussian posterior on f , which we call expected improvement for composite functions (EI-CF). Although EI-CF cannot be computed in closed form, we provide a novel stochastic gradient estimator that allows its efficient maximization. We also show that our approach is asymptotically consistent, i.e., that it recovers a globally optimal solution as sampling effort grows to infinity, generalizing previous convergence results for classical expected improvement. Numerical experiments show that our approach dramatically outperforms standard Bayesian optimization benchmarks, reducing simple regret by several orders of magnitude.

In [13, 14] we consider objectives that are the average, sum, or integral of a collection of expensive-to-evaluate functions, i.e., of the form $f(x) = \sum_i p_i h_i(x)$ and $f(x) = \int p(w)h(x, w) dw$ where p_i and $p(w)$ are known quantities and h is an expensive-to-evaluate black box. Such problems arise, for example, in hyperparameter tuning for machine learning algorithms where one seeks to minimize the cross-validation error.

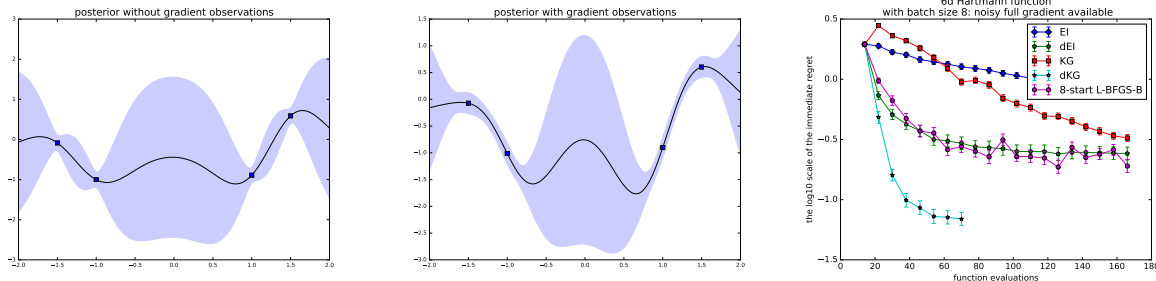


Figure 4: Utilizing observations of derivative information in BO (left and middle). Evaluation on the Hartmann benchmark (right). The accuracy of the predictive mean and uncertainty is improved significantly when taking into account observations of the gradient of the objective function. Our algorithm, the derivative-sensitive knowledge gradient (dKG), performs significantly better on the Hartmann benchmark than state of the art methods from Bayesian optimization and the gradient-based optimizer L-BFGS-B. This work was published in [15]

Work on MISO for hyperparameter tuning for deep neural networks [11] and BO with derivatives [15] described elsewhere in this report can also be considered a form of grey-box BO.

2.2.4 Bayesian optimization with derivatives

In [15] we give a Bayesian optimization algorithm that utilizes derivative information. This is especially important for solving high-dimensional problems in which derivative information is available, such as testbed aerostructural optimization problems in openMDAO. Moreover, our algorithm is capable of exploiting even noisy observations of derivative information and performs significantly better than state-of-the-art methods from Bayesian optimization and gradient-based optimizers (cp. Fig. 4). This resulted in a publication at NIPS, which was honored with a spotlight presentation (3% of submitted papers).

2.2.5 BO with interactive preference learning: the decision-maker is an information source

In [16, 17], we develop a novel formulation of multi-objective optimization in which we view the decision-maker (who will select from among the provided designs based on their attributes) as an information source. The decision-maker has a single fixed utility function over attribute vectors, but has trouble articulating it as a mathematical function. This is what prevents us from directly writing down the optimization problem as a single-objective problem. The decision-maker can, however, tell us (with some errors) which she prefers between pairs of attribute vectors found by the algorithm. Thus, the decision-maker is an information source. In [16, 17], we develop an algorithm for efficiently querying two information sources: the decision-maker and a time-consuming computer code that computes the attribute vectors associated with a design. We find that this algorithm for BO with interactive preference learning substantially outperforms other methods, especially on problems with many attributes and ones where we can form a strong prior distribution on the decision-maker’s utility function based on past interactions.

2.3 Other Advances in Bayesian Optimization

We have also contributed more broadly to Bayesian optimization during the grant.

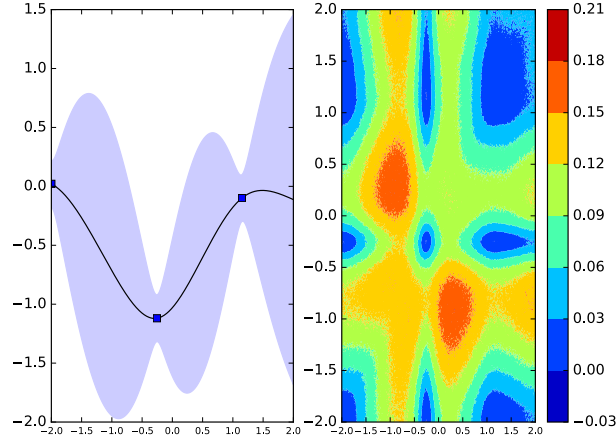


Figure 5: The Gaussian process posterior for a Bayesian optimization problem with parallel function evaluations (left); The value of information surface for measuring a pair of points in parallel, used to decide which pair of points is most valuable to evaluate in the parallel knowledge-gradient method of [19] (right).

2.3.1 Warm-starting Bayesian Optimization

In [18] we propose a BO algorithm to warm start the optimization process using knowledge acquired on previous tasks. Our experimental results indicate that this reduces the total evaluation cost required for an optimal solution significantly (see Fig. 3 (right)).

2.3.2 Parallel BO

In [19], we consider parallel optimization of expensive functions. We propose the knowledge-gradient method for parallel optimization, which is Bayes-optimal for a single batch of measurements when we can select as our final solution any point in the feasible domain. We demonstrate that this algorithm provides a significant performance improvement over the state of the art. An example of the Gaussian process posterior and the value of information surface used by this method is shown in Figure 5. This paper was accepted to appear at the 2016 Neural Information Processing System (NIPS) conference.

2.3.3 Going beyond traditional Gaussian process priors

[20] develops a new optimization algorithm that provides excellent computational efficiency in settings where one would usually employ multistart stochastic gradient ascent. This approach is a form of BO, but it goes substantially beyond the Gaussian process priors typically employed in Bayesian optimization. Stochastic gradient ascent effectively finds local optima when one can obtain noisy gradient observations, and it can be used in a multistart framework to search for a global optimum. However, multistart stochastic gradient ascent wastes computational effort when more than one start converges to the same local optimum, or when we continue to spend computational effort on one start after it becomes clear its local optimum is dominated by another. [20] develops a new Bayesian statistical model that creates a posterior distribution on the value of a start’s local optimum (based on the iterations seen thus far) and how quickly we will converge to that value. It then uses this statistical model within an acquisition function to allocate computational effort across

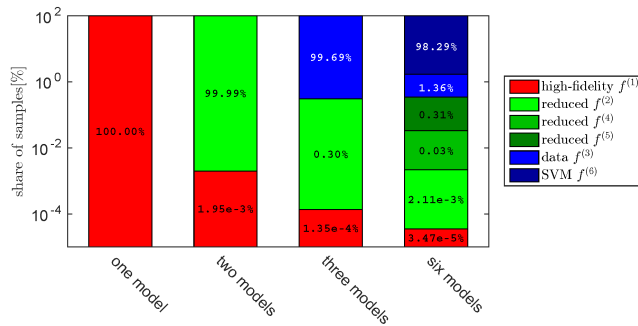


Figure 6: Our optimal model management for Monte Carlo estimation [21] provides a framework to combine an arbitrary number of models of any type for uncertainty quantification. An optimization problem balances the number of model evaluations across the high-fidelity and low-fidelity models to derive estimators that satisfy given error tolerances with minimal computational costs.

starts. This published work explores a simple 1-dimensional setting, and follow-on work planned for after the conclusion of the grant is focused on generalizing to many dimensions.

2.3.4 Improvements to the Cornell-MOE software package

The Cornell-MOE open-source software package ¹ implements Bayesian algorithms developed during this MURI, and extends the Metrics Optimization Engine (MOE) previously developed at Yelp by two of Frazier’s former PhD students. During the grant, Frazier’s group has put substantial effort toward improving this software package, focusing on ease of use and installation. Frazier’s former PhD student Jian Wu, who is the main developer on Cornell-MOE, was hired by TwoSigma to use Bayesian Optimization to tune trading algorithms. As part of his work there, TwoSigma is funding him to continue to improve and develop the software package. We also advertised this package through Frazier’s tutorial on Bayesian Optimization at the INFORMS Annual Meeting, which was attended by more than 100 people.

2.3.5 Bayesian optimization of combinatorial structures

Baptista (MIT) and Poloczek (University of Arizona) developed the BOCS algorithm that pioneers the optimization of expensive-to-evaluate functions over combinatorial structures. They showed that the algorithm has a great performance for a variety of problems in uncertainty quantification, aerospace engineering and simulation optimization. Their paper was published after peer-review at the prestigious conference ICML in 2018. This work was started when Poloczek visited the Willcox group at MIT in fall 2016.

2.4 Optimal model management for multifidelity Monte Carlo estimation

The proposed optimal model management strategy exploits multifidelity surrogate models to accelerate the estimation of statistics of outputs of computationally expensive high-fidelity models. Other acceleration methods typically exploit a multilevel hierarchy of models that follow a known rate of error decay and computational costs; however, a general collection of low-fidelity models, which may include projection-based reduced models, data-fit models, support vector machines, and simplified-physics models, does not necessarily give rise to such a hierarchy. The proposed multifidelity Monte Carlo (MFMC) approach provides a framework to combine an arbitrary number of models of any type. Instead of relying on error and cost rates, an optimization problem balances the number of model evaluations across the high-fidelity and low-fidelity models with respect to error and costs; see Figure 6. There is a unique analytic solution of the model management optimization

¹<https://github.com/wujian16/Cornell-MOE/tree/master/examples>

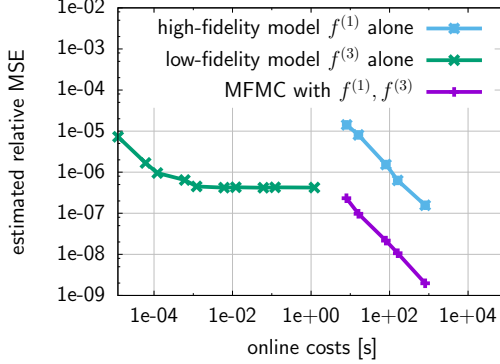


Figure 7: Uncertainty propagation in a coupled aero-structural analysis [22]: Using the low-fidelity model alone to speedup the uncertainty propagation leads to biased estimators as indicated by the leveling off of the error curve. In contrast, the proposed MFMC [21] leverages the low-fidelity model to obtain about three orders of magnitude speedup and establishes accuracy guarantees (unbiased estimator) by making occasional recourse to the high-fidelity model.

problem under mild conditions on the models. The proposed multifidelity method makes occasional recourse to the high-fidelity model; in doing so it provides an unbiased estimator of the statistics of the high-fidelity model, even in the absence of error bounds and error estimators for the low-fidelity models. Numerical experiments with linear and nonlinear examples show that speedups by orders of magnitude are obtained compared to Monte Carlo estimation that invokes a single model only; cf. Figure 7.

2.5 A transport-based multifidelity preconditioner for Markov chain Monte Carlo sampling of complex distributions

A critical task in uncertainty quantification is estimating distributions of model inputs and model parameters from data via model calibration and other inverse problems. Estimating and sampling these input distributions with, e.g., Markov chain Monte Carlo (MCMC) methods, quickly becomes computationally infeasible if the models are computationally expensive to evaluate. Replacing an expensive, high-fidelity model with a low-cost, low-fidelity model often significantly reduces computational cost; however, employing a low-fidelity model alone means that the distribution corresponding to the low-fidelity model is sampled, rather than the original distribution corresponding to the high-fidelity model. We propose a multifidelity MCMC approach [23] that combines, rather than replaces, the high-fidelity model with a low-fidelity model. First, the low-fidelity model is used to construct a transport map that deterministically couples a reference Gaussian distribution with an approximation of the low-fidelity distribution. Then, the high-fidelity distribution is explored using a non-Gaussian proposal distribution derived from the transport map. This multifidelity “preconditioned” MCMC approach seeks efficient sampling via a proposal that is explicitly tailored to the high-fidelity distribution at hand and that is constructed efficiently with the low-fidelity model; see Figure 8. By relying on the low-fidelity model only to construct the proposal distribution, our approach guarantees that the stationary distribution of the MCMC chain is the high-fidelity distribution. In our numerical examples, our multifidelity approach achieves up to $6\times$ speedups compared to single-fidelity MCMC sampling.

2.6 Information source discrepancy quantification for coupled systems

We derived necessary conditions for compatible information source discrepancy quantification models for the case of coupled, linear systems with Gaussian model discrepancies for a particular conception of model discrepancy in coupled systems. The necessary conditions relate to ensuring detailed

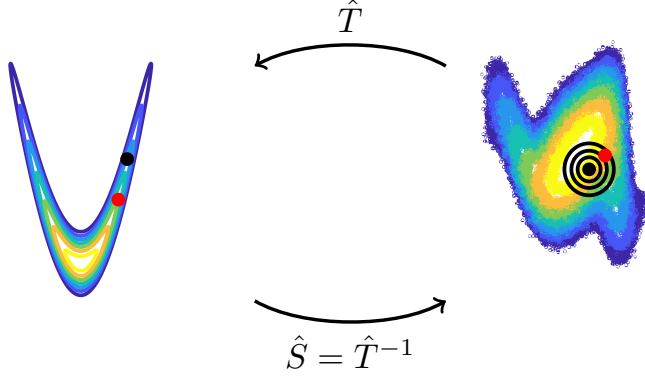


Figure 8: The proposed multifidelity MCMC [23] approach for solving Bayesian inverse problems derives a proposal distribution (right) for Metropolis-Hastings via a transport map constructed with a low-fidelity model and makes recourse to the high-fidelity model for deciding whether to accept or reject a proposal sample (right) to guarantee ergodicity of the corresponding Markov chain.

balance relations are preserved when the coupled system is viewed as a Markov chain with additive, independent, identically distributed discrepancy for each information source respectively. For nonlinear systems with Gaussian model discrepancies, we have developed a variational approach to approximating the conditions required for compatibility, which is based on steering Gaussian approximations of the joint distribution of the coupling variables toward satisfaction of the detailed balance relations.

2.7 Beyond independent information sources

We developed a model reification procedure for quantifying information source dependence prior to fusion of information from multiple models. We demonstrated this capability on the multifidelity airfoil testbed problem, where our reification procedure outperforms the covariance intersection algorithm, as well as fusion under the assumption of independent information sources. For the case of the multifidelity airfoil problem, the result of applying our reification procedure is a fused information source with lower mean square error than either SU2 or XFOIL when compared to wind tunnel data. This result is shown in Figure 9. Our fused model is built entirely from learned

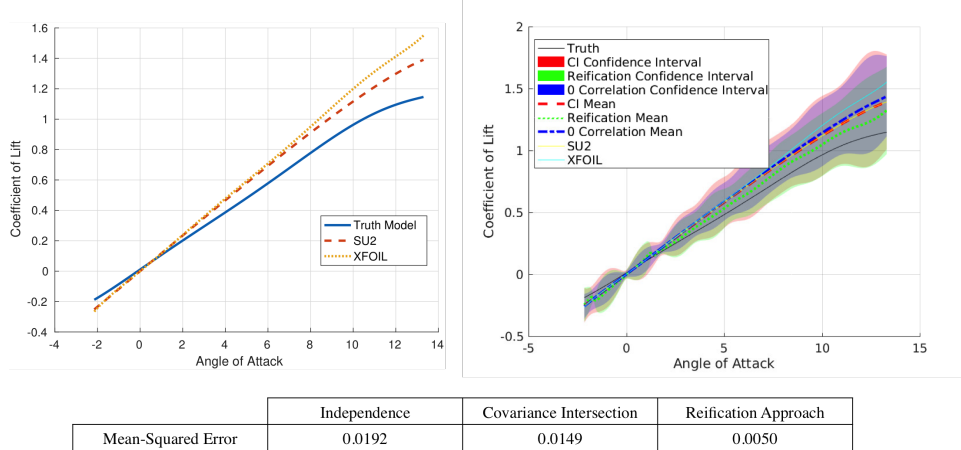


Figure 9: Information sources (left). Fused models (right). The results here show that our model reification approach fuses SU2 and XFOIL to create a better information source than either in isolation. This is achieved by taking into account the correlation of the errors in these models. The truth data is real-world NACA 0012 wind tunnel data.

correlations between the two information sources and their individual outputs. This work enables the formal study of the impact of sampling an information source in an area of the design space we know to be poor in terms of objective performance, but that may still be beneficial because of observed correlation with a more expensive information source.

2.8 Constrained multi-information source optimization

We developed an information-economic approach to the constrained optimization of a system with several available, but potentially expensive information sources. This work built off the model reification procedure for handling dependent information sources. Specifically, we developed an algorithm for choosing which information source to query and where to query it using an extension of the knowledge gradient policy and our previously developed model reification technique for fusion of information as it is acquired. A novel aspect of the work is that the query may relate to the objective or any constraint. That is, it is not required that the objective and constraint information sources be the same source, nor is it required that they be evaluated at the same location, or concurrently. We demonstrated this approach on the MURI testbed multifidelity airfoil problem.

2.9 Multi-information source framework for multi-objective optimization

We developed a multi-information source framework for enabling efficient multi-objective optimization using expected hypervolume improvement (EHVI). The framework allows for the exploitation of all available information and considers both potential improvement and cost. The framework includes ingredients of model fusion, expected hypervolume improvement, and intermediate Gaussian process surrogates. The approach is demonstrated on a test problem and an aerostructural wing design problem, where it is shown to outperform standard methods such as ParEgo and NSGA-II. The multi-information source aspect was shown in a two level demonstration to outperform a single information source approach as well.

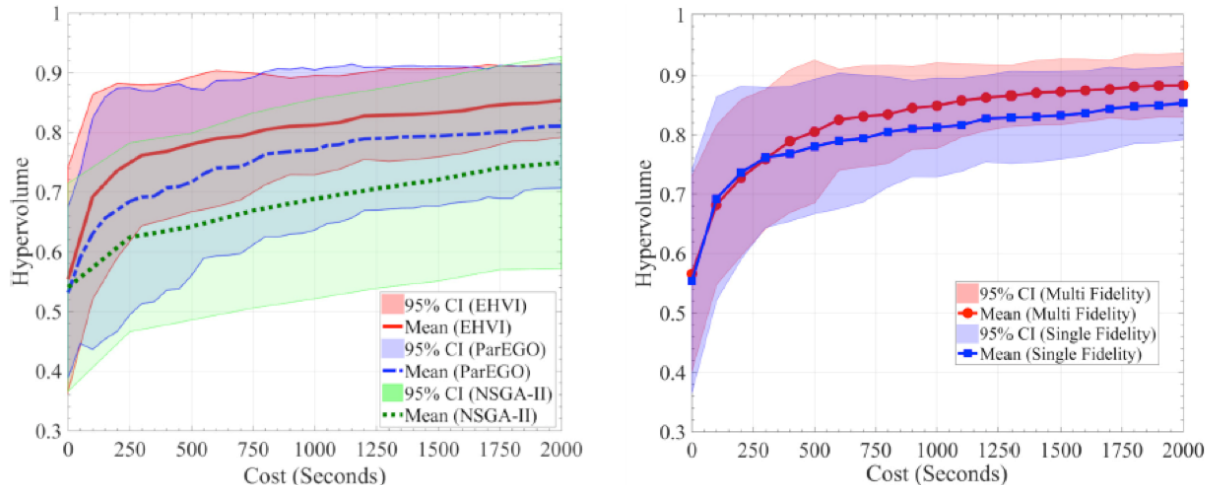


Figure 10: (Left) Our proposed approach using EHVI compared to ParEGO and NSGA-II on the OpenAeroStruct testbed problem. Shaded regions represent 95% confidence intervals. (Right) Comparison of our approach using multiple information sources versus a single source on the OpenAeroStruct testbed problem.

2.10 Multi-information source Batch Bayesian Optimization

We developed a multi-information source batch Bayesian optimization framework that creates efficiency through parallel execution of queries while also ensuring underlying stochastic processes are not over or underfit in hyperparameter space. The framework identifies next best query location and information source over a grid search of hyperparameter space. This search is rapid due to it taking place over Gaussian processes. The framework then uses k-medoids cluster analysis to identify the batch of samples to actually query based on available computational resources. The concept is shown in Figure 11, where several Gaussian processes with different hyper parameters are fit to four training points. Each different fit produces a different acquisition function shape, leading to a different preferred next query. We use k-medoids clustering to group these possible queries together in batches based on available computational resources.

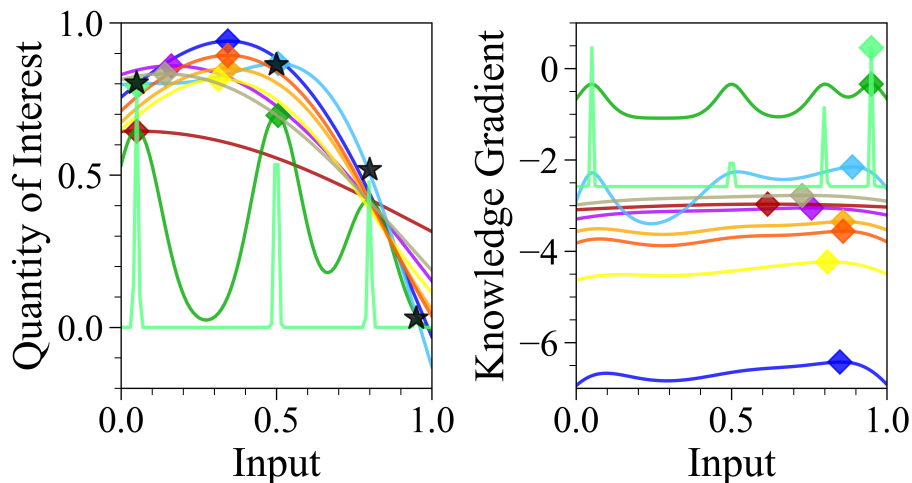


Figure 11: Gaussian Process models fit to a set of four training points (stars) using different values of the noise variance, signal variance, and length scale hyperparameter. Diamond marker indicates the location of the maximum of each Gaussian Process model in the left plot. The right-hand plot shows the knowledge gradient calculated for each GP model with the maximum indicated by a diamond marker.

2.11 Multifidelity efficient global reliability analysis through failure boundary location

This work develops mfEGRA, a multifidelity active learning method using data-driven adaptively refined surrogates for failure boundary location in reliability analysis [24]. We address the issue of prohibitive cost of reliability analysis using Monte Carlo sampling for expensive-to-evaluate high-fidelity models by using cheaper-to-evaluate approximations of the high-fidelity model. The method builds on the Efficient Global Reliability Analysis (EGRA) method, which is a surrogate-based method that uses adaptive sampling for refining Gaussian process surrogates for failure boundary location using a single-fidelity model. Our method introduces a two-stage adaptive sampling criterion that uses a multifidelity Gaussian process surrogate to leverage multiple information sources with different fidelities. The method combines expected feasibility criterion from EGRA with one-step lookahead information gain to refine the surrogate around the failure boundary. The adaptively refined multifidelity GP surrogate can then be used for computationally efficient estimate of the

probability of failure p_F . The computational savings from mfEGRA depends on the discrepancy between the different models, and the relative cost of evaluating the different models as compared to the high-fidelity model. We show that accurate estimation of reliability using mfEGRA leads to computational savings of $\sim 46\%$ for an analytic multimodal test problem and 24% for a three-dimensional acoustic horn problem, when compared to single-fidelity EGRA (see Figure 12). We also show the effect of using *a priori* drawn Monte Carlo samples in the implementation for the acoustic horn problem, where mfEGRA leads to computational savings of 45% for the three-dimensional case and 48% for a rarer event four-dimensional case as compared to single-fidelity EGRA (see Figure 13).

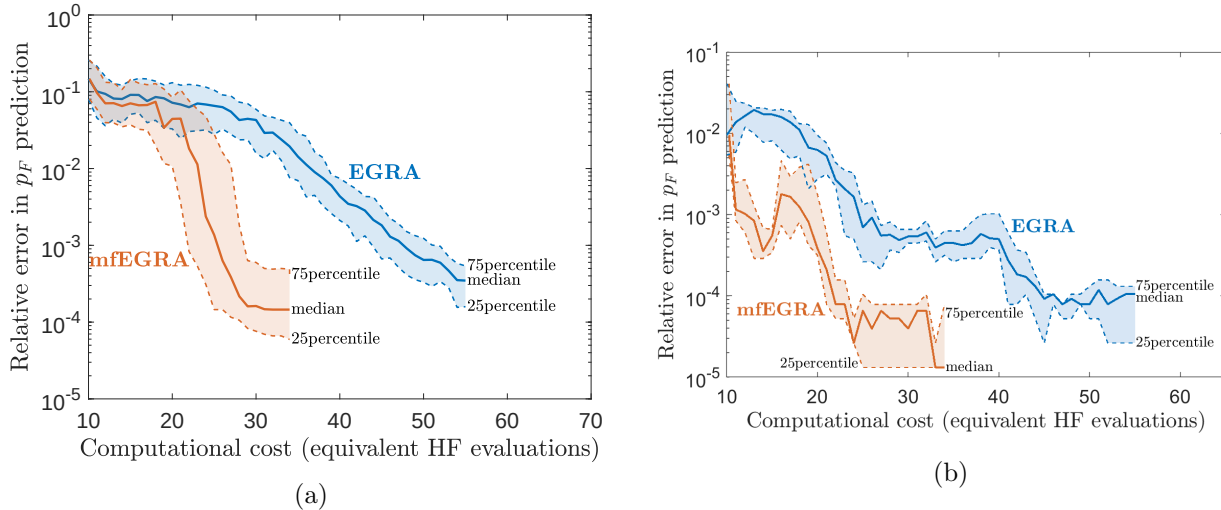


Figure 12: Comparison of mfEGRA vs single-fidelity EGRA in terms of convergence of relative error in probability of failure p_F estimate (shown in log-scale) for (a) analytic test problem using 100 different initial DOEs, and (b) three-dimensional acoustic horn using 10 different initial DOEs.

2.12 Multi-information source optimization under uncertainty

Under the MURI, we have pursued several efforts to address the prohibitive computation effort associated with optimization under uncertainty through multifidelity methods and to highlight the properties of risk-based optimization for mainstream use. We have developed methods for multi-information source robust optimization, reliability-based design optimization, and risk-averse optimization.

2.12.1 Multifidelity Robust Optimization

In [25], we developed a multifidelity method for optimization under uncertainty for aerospace problems. In this work, the effectiveness of the method is demonstrated for the robust optimization of a tailless aircraft that is based on the Boeing Insitu ScanEagle. Aircraft design is often affected by uncertainties in manufacturing and operating conditions. Accounting for uncertainties during optimization ensures a robust design that is more likely to meet performance requirements. Designing robust systems can be computationally prohibitive due to the numerous evaluations of expensive-to-evaluate high-fidelity numerical models required to estimate system-level statistics at each optimization iteration. This work uses a multifidelity Monte Carlo approach to estimate the

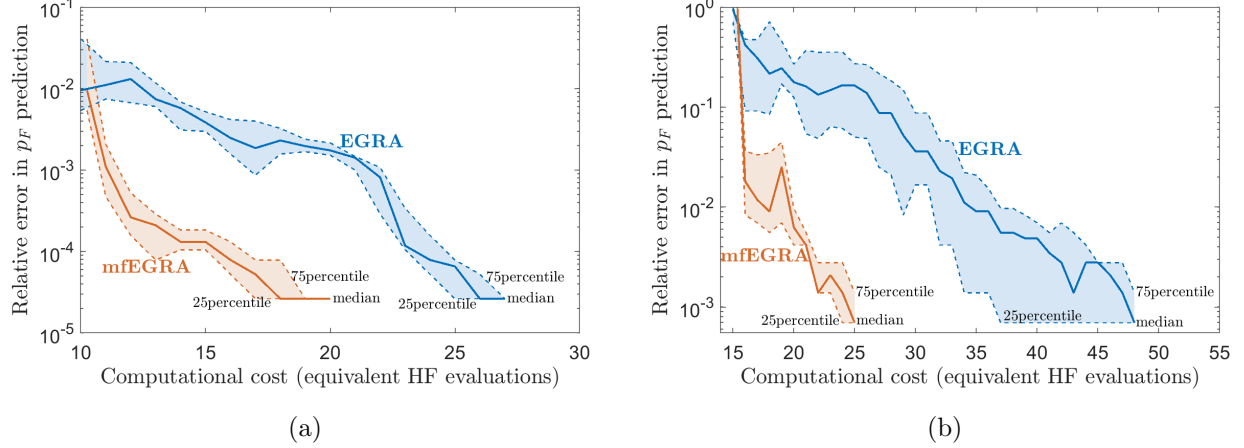


Figure 13: Comparing mfEGRA and single-fidelity EGRA in terms of convergence of relative error in probability of failure p_F estimate (shown in log-scale) by limiting the search space for adaptive sampling location to a set of Monte Carlo samples drawn from the given random variable distribution for acoustic horn problem (a) three-dimensional case, and (b) four-dimensional rarer event case using 10 initial DOEs.

mean and the variance of the system outputs for robust optimization. The method uses control variates to exploit multiple fidelities and optimally allocates resources to different fidelities to minimize the variance in the estimates for a given budget. To model the tailless aircraft we use OpenAeroStruct, an open-source aerostructural analysis and optimization tool [26]. The results for the ScanEagle application show that the proposed multifidelity method achieves substantial speed-ups as compared to a regular Monte-Carlo-based robust optimization. This is joint work between MIT and U. Michigan.

2.12.2 IRIS-RBDO: Information reuse for importance sampling in reliability-based design optimization

Reliability-based design optimization (RBDO) is a two-loop process involving an outer-loop optimization with an inner-loop reliability analysis for each optimization iteration. The reliability analysis requires estimating a probability of failure, which is typically done using Monte Carlo sampling for nonlinear systems, rendering the RBDO problem computationally prohibitive when expensive-to-evaluate models are to be used. One way to reduce computational cost is to use importance sampling, where much fewer samples are needed from a biasing density. However, as is well known, finding a good biasing density in importance sampling is challenging.

In [27], we proposed a new importance-sampling-based RBDO method that reuses information from past optimization iterations for computationally efficient estimation of the reliability constraint. At the core of the **IRIS-RBDO** (Information **R**euse for **I**mportance **S**ampling in **R**BDO) method, we propose to build a good importance sampling biasing density by reusing data from previous optimization iterations. The proposed method reduces the computational time for probability of failure estimates in each RBDO iteration through two levels of information reuse:

1. At the current design iteration, once the reliability estimate is computed via importance-sampling based Monte Carlo sampling, we reuse the current batch of samples from the reliability estimate to form an *a posteriori* biasing density. The *a posteriori* biasing density is

built in an optimal way by minimizing the Kullback-Leibler (KL) divergence measure to the optimal (zero-variance) biasing density.

2. At the next design iteration, we reuse the available *a posteriori* biasing densities from nearby designs explored in the past iterations to construct a mixture density at the current iteration. The motivation for this is that nearby designs are likely to have similar failure regions, and hence reusing the *a posteriori* biasing densities from the existing nearby designs can lead to efficient biasing densities.

We demonstrate the efficiency of the proposed IRIS-RBDO method for the RBDO benchmark of a speed reducer problem and the reliable design of a combustion engine problem. For the speed reducer problem, the total number of samples used for probability of failure estimate with a given accuracy in each optimization iteration in IRIS-RBDO compared to importance sampling with no reuse and subset simulation is shown in Figure 14(a). When no designs are nearby, our method builds a biasing density from scratch, hence the marker for IRIS overlaps with no reuse case. Otherwise, IRIS-RBDO always outperforms the other methods. Note that we are showing the plots for the same designs in each RBDO iteration for both cases. In this case, IRIS-RBDO leads to overall computational savings of around 51% compared to using importance sampling with no reuse and subset simulation throughout the optimization. For the combustion engine problem, IRIS-RBDO leads to computational savings of around 76% compared to importance sampling with no reuse as seen in Figure 14.

2.12.3 Reusing information for multifidelity active learning in RBDO

This work develops a multifidelity method to reuse information from optimization history for adaptively refining surrogates in RBDO. As noted above, RBDO can be computationally prohibitive due to numerous evaluations of the expensive high-fidelity models to estimate the probability of failure of the system in each optimization iteration. In this work, the high-fidelity model evaluations are replaced by cheaper-to-evaluate adaptively refined surrogate evaluations in the probability of failure estimation. The method reuses the surrogates from past optimization iterations as an information source for devising an efficient multifidelity active learning (adaptive sampling) algorithm to refine the surrogates that best locate the failure boundary at current iteration. We implement the information-reuse method using a multifidelity extension of efficient global reliability analysis (mfEGRA) that combines the expected feasibility function with a weighted lookahead information gain criterion to pick both the next sample location and information source used to evaluate the sample. We use a multifidelity Gaussian process (GP) as the surrogate for the limit state function that combines information from the available information sources. The adaptively refined multifidelity GP surrogates can then be used for computationally efficient reliability analysis in each RBDO iteration and stored for future reuse.

We use an acoustic horn problem to demonstrate the effectiveness of reusing surrogates from past optimization iterations as an extra information source in mfEGRA for efficient refinement of surrogates in RBDO. Figure 16(a) shows the computational cost for building the adaptive surrogates using the proposed mfEGRA with information-reuse method as compared to using EGRA with only the high-fidelity model at each optimization iteration. In this case, we reduce the overall computational cost by almost 60% by building the adaptive surrogates through the proposed information-reuse method. The low computational cost through the mfEGRA method is due to the reuse of extremely cheap surrogates from previous optimization iterations as an information source. The allocation of resources to the cheaper low-fidelity model (reused GP model from RBDO history)

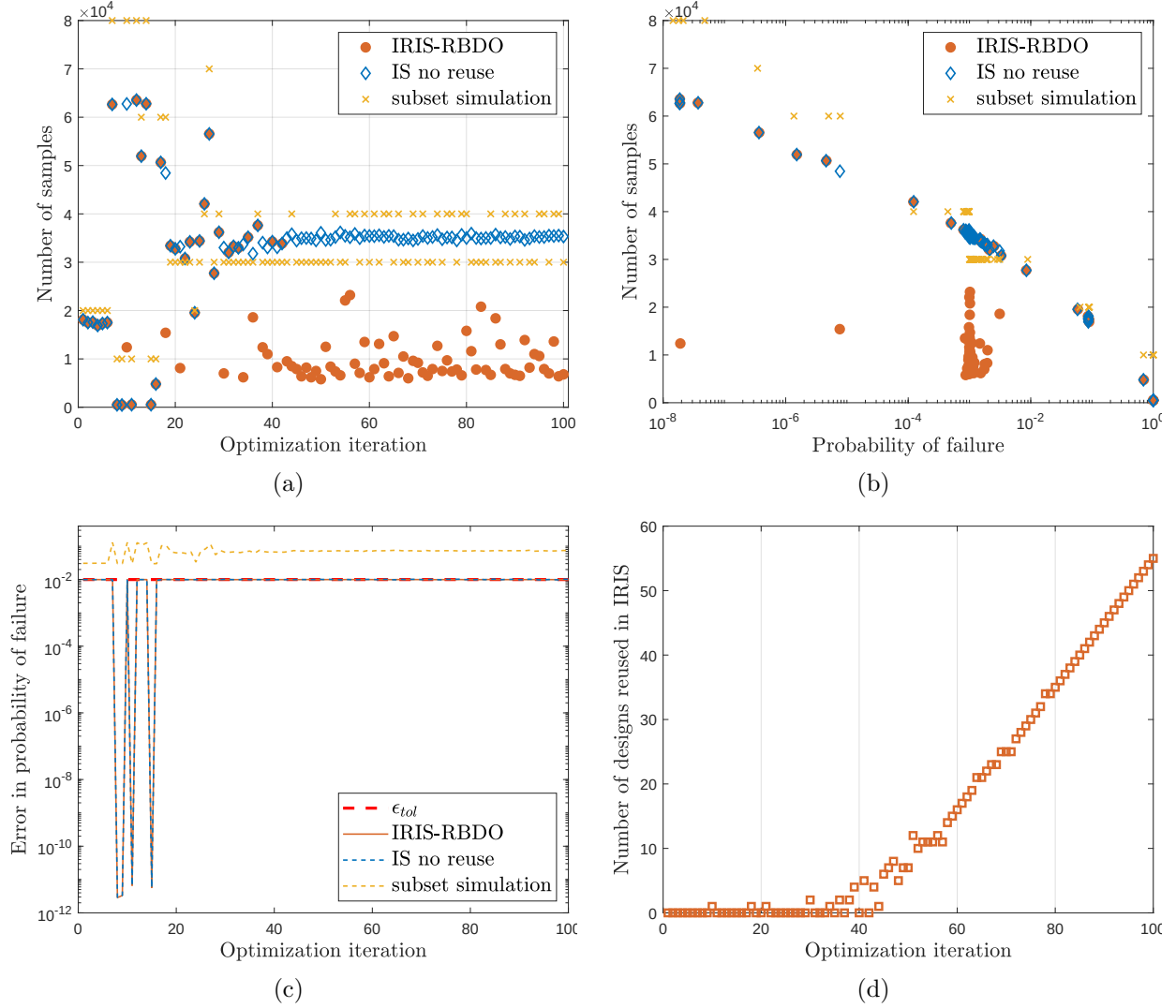


Figure 14: Comparison of IRIS, importance sampling (IS) with no reuse and subset simulation for the same designs showing (a) number of samples required in each optimization iteration, (b) number of samples required to calculate the corresponding probabilities of failure, (c) error in probability of failure estimate (quantified by the coefficient of variation) in each optimization iteration, and (d) number of designs reused in IRIS in each optimization iteration for the speed reducer problem.

as shown in Figure 16(b), which takes around 10^{-4} seconds/evaluation, in mfEGRA leads to substantial reduction in computational cost compared to running EGRA that uses only the high-fidelity model, which takes around 0.3 seconds/evaluation.

2.12.4 Certifiable risk-based engineering design optimization

Reliable, risk-averse design of complex engineering systems with optimized performance requires dealing with uncertainties. A conventional approach is to add safety margins to a design that was obtained from deterministic optimization. Safer engineering designs require appropriate cost and constraint function definitions that capture the *risk* associated with unwanted system behavior in the presence of uncertainties. In [29], we propose two notions of certifiability. The first is based on accounting for the magnitude of failure to ensure data-informed conservativeness. The second is the ability to provide optimization convergence guarantees by preserving convexity. Satisfying these notions leads to *certifiable* risk-based design optimization (CRiBDO). In the context of CRiBDO, risk measures based on superquantile (a.k.a. conditional value-at-risk) and buffered probability of failure are analyzed. CRiBDO is contrasted with reliability-based design optimization (RBDO), where uncertainties are accounted for via the probability of failure, through a structural and a thermal design problem. A reformulation of the short column structural design problem leading to a

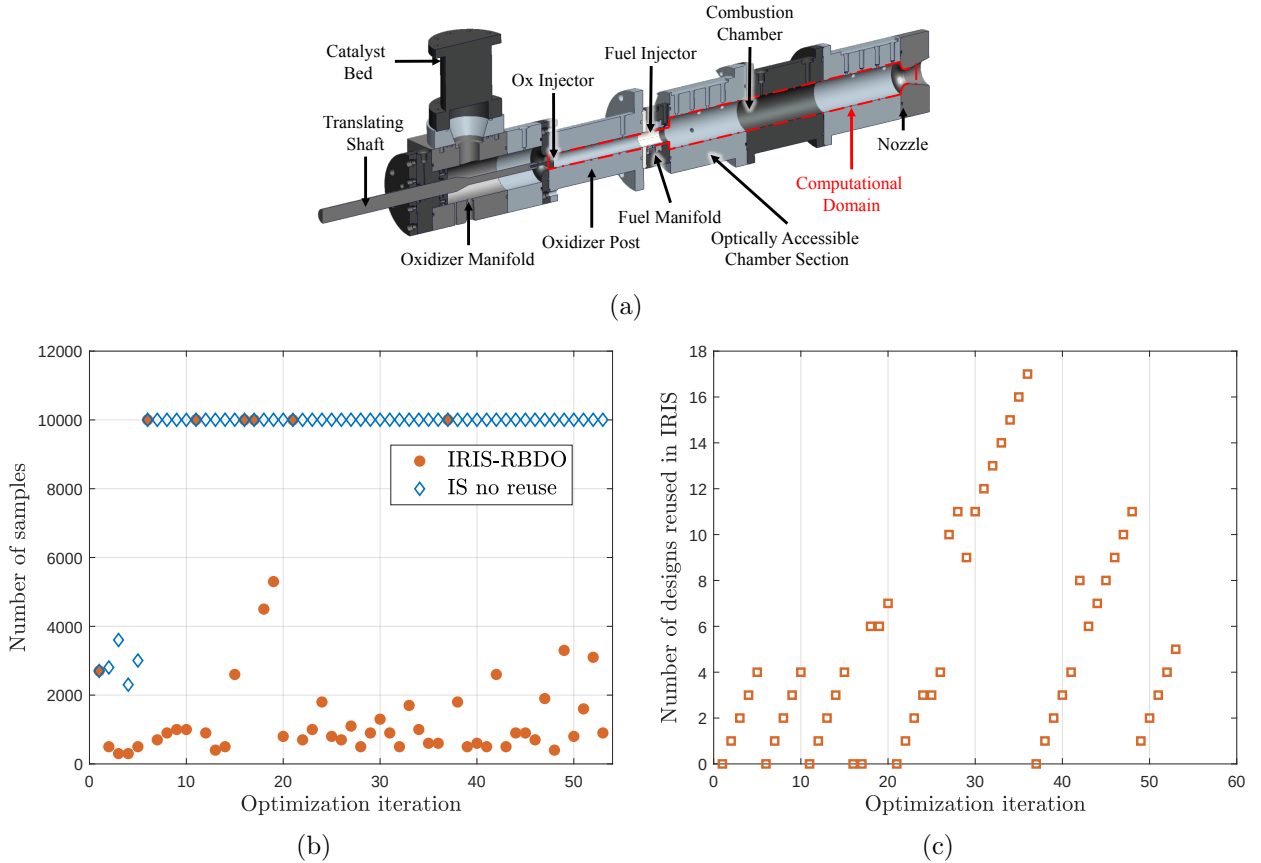


Figure 15: (a) Continuously variable resonance combustor (CVRC) experimental configuration from [28], (b) comparison of IRIS and importance sampling (IS) with no reuse for the same designs showing (a) number of samples required in each optimization iteration, and (c) number of designs reused in IRIS in each optimization iteration for the combustion engine problem.

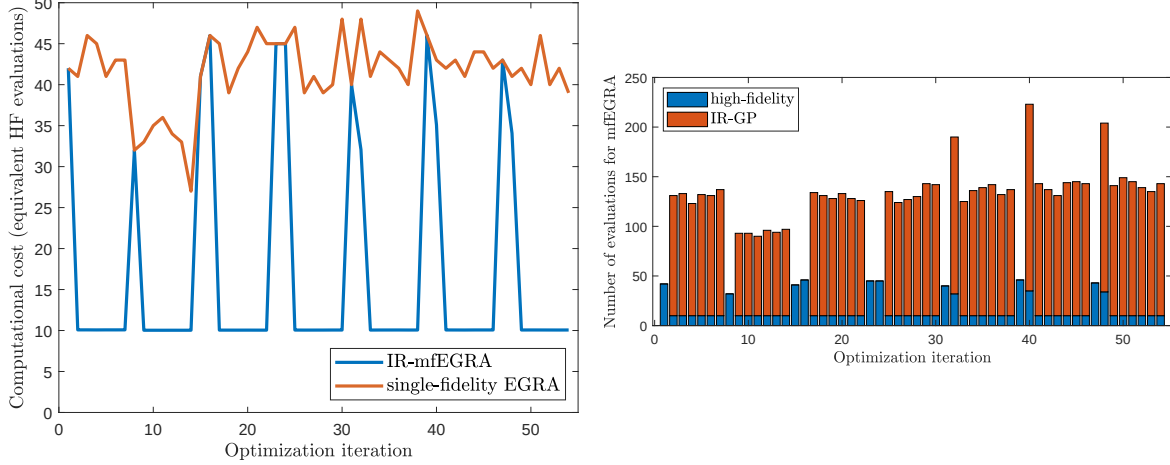


Figure 16: (a) Comparison of the computational cost for building adaptive surrogates using mfEGRA with information reuse (IR-mfEGRA) vs using single-fidelity EGRA at each optimization iteration. (b) Number of evaluations required by mfEGRA from the high-fidelity model and the reused GP model (IR-GP) in each RBDO iteration for the acoustic horn problem.

convex CRiBDO problem is presented. The CRiBDO formulations capture more information about the problem to assign the appropriate conservativeness, exhibit superior optimization convergence by preserving properties of underlying functions, and alleviate the adverse effects of choosing hard failure thresholds required in RBDO.

3 RT2: Goal-oriented reduced-order models for the multi-source multi-physics setting

3.1 Multifidelity dimension reduction via active subspaces

We developed a multifidelity approach to identify subspaces of low dimension capturing most of the variations of a function of interest. Our approach builds on the gradient-based active subspace methodology, seeking the computation of the active subspace matrix H defined as the second moment matrix of the gradient function. The proposed approach overcomes computational cost limitations of Monte Carlo methods used to estimate this matrix, by using a low-fidelity, cheap-to-evaluate gradient approximation as a control variate. The performance improvements of the resulting MF estimator H_{MF} are demonstrated on two engineering examples governed by partial differential equations: a high-dimensional linear elasticity problem defined over more than three thousand input variables and an expensive shape optimization problem defined over 50 input variables.

Analysis of the performance of the multifidelity technique yields error bounds for the matrix error $\|H - H_{MF}\|$ both in expectation and with high probability. These error bounds depend on the intrinsic dimension of the problem, which is related to the spectral decay of the active subspace matrix. When a function varies along a few directions, the intrinsic dimension is low. This suggests that, in such a case, approximating H requires a small number of gradient evaluations. This was confirmed empirically by a parametric study conducted on two analytical problems: lower intrinsic dimension led to lower matrix error for the same number of high-fidelity evaluations.

The performance improvements of the multifidelity approach are threefold. First, we showed

that the MF estimator reduces the cost of performing dimension reduction. This was illustrated on the linear elasticity problem where the multifidelity approach needed about 43% less computational resources than its single-fidelity counterpart to achieve the same relative error. Second, we showed that the multifidelity approach was able to recover singular vectors qualitatively similar to the exact ones. Third, the MF estimator led to better estimates of the spectral decay of H . On the linear elasticity problem, which is characterized by a low intrinsic dimension (≤ 5), the multifidelity approach led to better estimates, especially for smaller singular values. On the shape optimization problem, which is characterized by a higher intrinsic dimension (≈ 9), the MF estimator led to better estimates for all singular values. This is in contrast to the single-fidelity method that overestimated the leading singular values and underestimated the lower singular values, thereby underestimating the intrinsic dimension of H and overestimating the spectral decay.

Recovering the spectral decay of H is particularly important since one popular way of choosing the dimension r of the active subspace is based on the spectral gap between consecutive singular values. If the spectral decay is overestimated, r might be chosen too small to correctly capture the behavior of the high-fidelity function. By providing a better estimate of the spectral decay, the MF estimator reduces this risk. The dimension of the active subspace can also be chosen in order to control a functional error bound. We showed that the approximation of this bound, which depends on the unknown H , improves as the matrix error decreases. Because the MF estimator reduces the matrix error with fewer high-fidelity evaluations, the proposed multifidelity approach leads to a better selection of the active subspace dimension r .

This work is joint between the Willcox and Marzouk groups and was published in *SIAM J. Scientific Computing* [30].

3.2 Uncertainty Modeling and Management in ROMs

3.2.1 Background

The use of reduced order models in the propagation of system uncertainty to system response can be carried out in two different ways. The first proceeds with the uncertainty modeling at the full order model (FOM) level, e.g., finite element model, by specifying certain material and/or material properties and/or boundary conditions to be uncertain and adopting specific, probabilistic here, models for them. For each of the full order samples generated one can proceed with the reduced order modeling and thereby obtain the system response. This effort can be quite expensive if the construction of the reduced order model is computationally demanding as is the case for example in ROMs for the nonlinear geometric response of structures.

A faster, more desirable approach would be to introduce the uncertainty directly at the level of the ROM without returning to the full order model. In the problems considered here, i.e., uncertainty in the coupled thermal and structural ROMs for heated structures, such an effort is challenging because there are physical constraints that the coefficients of the ROM must satisfy and which must absolutely be guaranteed by every sample of the uncertain ROMs. Such constraints also exist in the FOM but they are typically obvious, e.g., geometrical dimensions are positive and so are material properties (Young's modulus, conduction coefficient, etc.).

A breakthrough in the modeling of uncertainty at the ROM level was made by Soize in 2000 [31] through the formulation and ensuing development of the maximum entropy (MaxEnt) approach in which the joint probability density function of the ROM parameters is determined as a constraint optimization problem. Specifically, this distribution is selected to maximize the corresponding entropy under the constraints that: (a) all physically derived requirements on them are satisfied, (b) the mean of the uncertain ROM equals the baseline, deterministic ROM, and (c) the overall uncertainty level equals its specified value.

The MaxEnt approach was initially derived for linear structural dynamics problems for which it is well known that the ROM (or modal) mass, stiffness, and damping matrices must be positive definite. It is accordingly on satisfying these properties for every sample that Soize focused on his original work. In ensuing extensions of the MaxEnt approach, other physical constraints were encountered that also led to positive definite matrices, i.e., in structural-acoustic problems [32], nonlinear geometric ROMs [33], rigid body dynamics [34], and rotordynamics [35, 36].

It should be noted that the introduction of uncertainty at the ROM level, especially using the MaxEnt principle, allows the introduction in the system of not only aleatoric uncertainty but also some epistemic one, see [37, 38] for some discussion, which represents a very positive feature of the approach.

3.2.2 Uncertainty Modeling for Problems with Localized Response

Early efforts in this investigation to model the uncertainty in the conductance and capacitance properties of heated structures using the MaxEnt principle recognized that the corresponding ROM matrices must be positive definite. However, it was also found that this property may not be sufficient to obtain physically expected samples of the temperature distribution. In fact, it was recognized that the temperature distribution may, depending on boundary conditions, exhibit a localization, i.e., may not diffuse over the entire structure but rather stay localized near the heated zone. A similar situation is encountered in some structural problems, e.g., the deflections of the annulus shown in Fig. 17(a) under a unit transverse loading in the zone highlighted in yellow, is localized to the region of excitation, see Fig. 17(b).

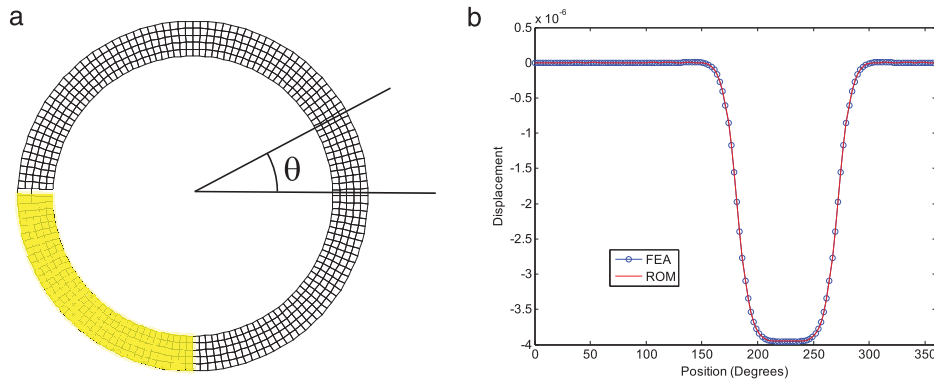


Figure 17: (a) The annulus and its finite element model with the loading domain highlighted in yellow. (b) Static transverse displacement at the periphery, full finite element (FEA) and reduced order (ROM) models.

In general, the "standard" MaxEnt approach does not induce this property and the resulting uncertainty exhibits a "globalization" as shown in Fig. 18(a), i.e., the response also extends to zones where it was zero/negligible for the mean model. This behavior was studied in [39] and it was demonstrated that the localization results from the existence of eigenvalues of the stiffness matrix that are very closely spaced. Moreover, the relative positioning of these eigenvalues is the feature of the system that induces the localization. Based on that observation, a modified MaxEnt approach was formulated that maintains the relative positioning of the closely spaced frequencies, allowing them to jointly increase or decrease while performing normally on the eigenvalues that are distant from each other. This process maintains the localization of every sample of the response as demonstrated on Fig 18(b).

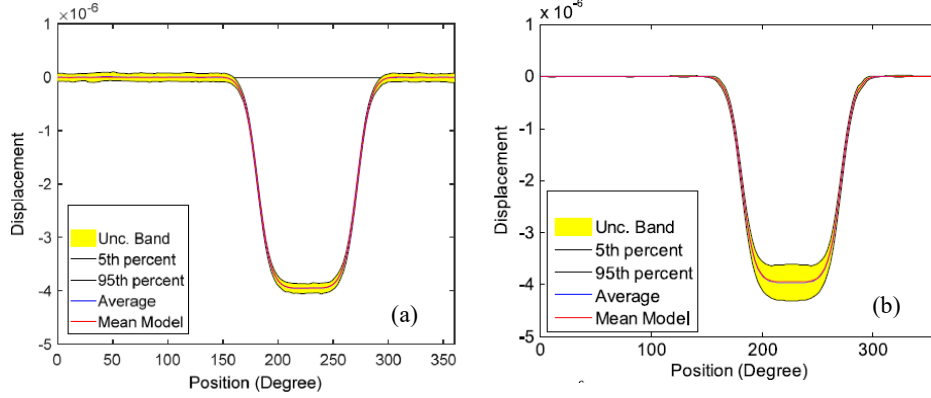


Figure 18: 5th-95th Percentiles uncertainty bands on the static response of the annulus. (a) "Standard" MaxEnt approach. (b) Modified MaxEnt approach.

3.2.3 Uncertainty Modeling in Nonlinear structural-thermal ROMs

The consideration of uncertainty in heated structures brings, in addition to the uncertainties on the structural and thermal problems alone, the need to consider the uncertainty on the coupling mechanism, i.e., the coefficient of thermal expansion. To understand how the modeling of this uncertainty must be carried out at the ROM level, the derivation of the ROM equations for heated structures derived earlier [40] were considered and it was demonstrated first that the structural ROM parameters and those coupling the structural ROM with the temperature one *must* be considered *together* in the modeling. Moreover, it was demonstrated that the structural parameters and the stiffness and thermal force terms originating from the temperature effects must be regrouped in a single, larger size matrix which must be positive definite. Additional, punctual challenges also arise in this modeling process that are resolved in [41] (see paper for details). This work then provides a fully consistent approach to introduce uncertainty in ROMs of hot structures exhibiting nonlinear geometric (or linear when reduced) effects.

The application of this novel methodology was carried out on the oscillating flux testbed problem and shown in Fig 19 are the uncertainty bands on the temperature and structural response under different conditions. In Fig 19 (a) and (b), the uncertainty is only on the thermal problem, i.e., the conductance matrix. The uncertainty on the structural response is thus induced by the uncertainty on the temperature and this effect is seen in Fig 19 (b) to be very large, much larger than the level of uncertainty on the temperature itself. Introducing uncertainty on the structural-thermal coupling terms, see Fig 19 (c), or on structural only terms, see Fig 19 (d) leads to significantly less uncertainty on the structural response. These coupled analyses are computationally very expedient owing to the small structural and thermal ROMs and the direct inclusion of uncertainty at the ROM level.

3.3 More Economical/Flexible Uncertainty Modeling Approaches

3.3.1 MaxEnt Strategies at the Elemental Level

Since its inception in [31], the ROM-based MaxEnt approach has been shown to be powerful: computationally efficient as it relies on ROMs and extendable to a broad array of different types of single- and multi-physics problems, as discussed above and see [37, 38] for reviews. The global character of the ROM employed in the above applications leads naturally to computational efficiency but renders difficult the control of the uncertainty at the "local" level, e.g., introducing more

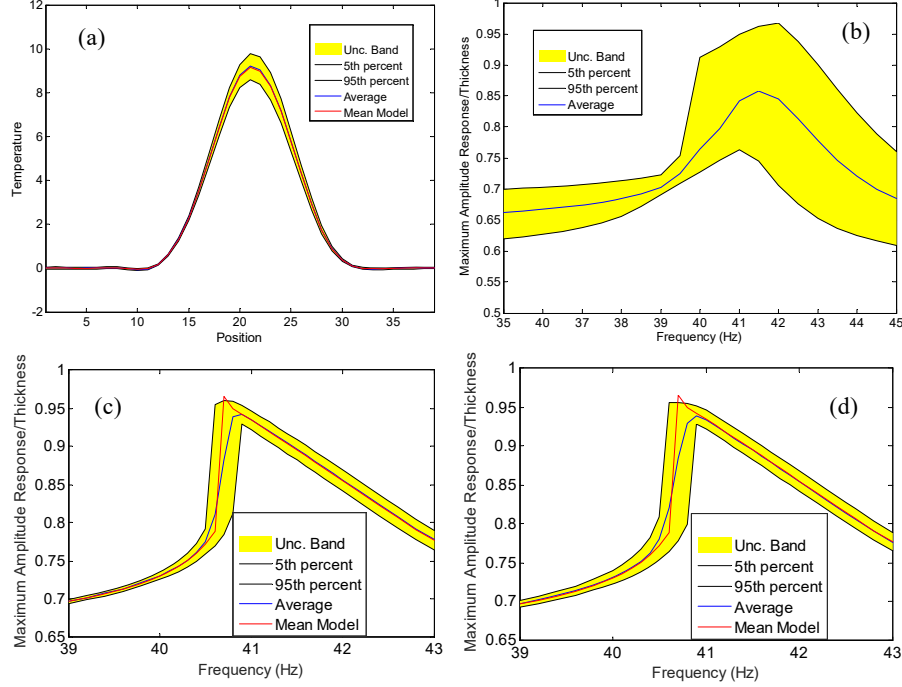


Figure 19: 5h-95th Percentiles uncertainty bands. (a) On a snapshot of the temperature. (b)-(d) On the amplitude of peak structural (transverse) response as a function of the flux oscillating frequency. (a), (b) Uncertainty on conductance. (c) Uncertainty on thermal-structural coupling parameters only. (d) Uncertainty on structural parameters only.

uncertainty on some parts of the structure than on others. Moreover, its extension to new problems and/or physical properties that do not simply reduce to the positive definiteness of a matrix may be challenging as discussed above [39]. It is finally noted that the ROM basis must be general enough to capture the response of not only the mean model but the uncertain ones as well, a requirement that may be difficult to meet when the changes in physics induced by uncertainty are complex, i.e., not predictable in advance.

For these situations, one can certainly return to the detailed uncertainty modeling at the FOM level where the MaxEnt principle is still applicable for material properties e.g., to introduce the uncertainty on the elasticity tensor, see [37, 38]. However, any potential uncertainty on the geometry would have to be addressed separately. The capability of the MaxEnt formulation to capture some epistemic uncertainty would also be curtailed.

These observations have led the ASU group to investigate the potential of a "middle of the road" or mesoscale uncertainty modeling fitting between the macroscale approach of the global ROM and the microscale strategy of uncertainty modeling at the FOM level. Such an approach is in fact possible and proceeds at the level of each *element* using the MaxEnt approach by recognizing that the finite element discretization and interpolation process provides in fact a reduced order modeling of the continuum within the element. The corresponding ROM matrices are the elemental matrices, mass, stiffness, and damping in the case of structure undergoing small (linear) motions.

The overall perspective on this elemental MaxEnt approach is thus to apply the strategies developed in context with global ROMs, see [37, 38, 41] to the governing equations of each element. However, while there is only one stiffness matrix say at the global ROM level, there are many such matrices - one per element - when proceeding at the elemental level. Moreover, these various

matrices are added together in the finite element assembly process. Expecting the variations of material and geometrical properties to be smooth over the structure, it is thus necessary to enforce a correlation between the elemental matrices of neighboring elements. Moreover, it is also required that the ordering of the degrees of freedom in different elements be consistent with each other.

These challenges were resolved in [42] for linear structural or thermal problems and in [43, 44] for heated structures. The exemplification of these new approaches to the annulus of Fig. 17(a) is shown in Fig. 20 in the purely structural case and in Fig. 21 in the presence of temperature. In Fig. 20, the annulus is subjected to a unit static load in the yellow zone, exactly as in Fig. 18(b), and it is seen that localization does indeed take place as well, see Fig. 20(c) but there was no need here to impose the localization through a coordinated variation of eigenvalues, it occurred naturally as a result of the assembly of the finite element model. This finding is one of the expected benefits of operating at the elemental level. The drawback is clearly that each element must be randomized and that the assembly of the finite element model must be performed for each sample.

It should be noted that the application of the MaxEnt principle has led to the introduction in the response of epistemic uncertainty. Indeed, note that the response to the transverse only load does generate in plane displacements as well, see Fig. 20(a) and (b). A similar observation would have been found from the global ROM approach if in plane modes had been included in the basis.

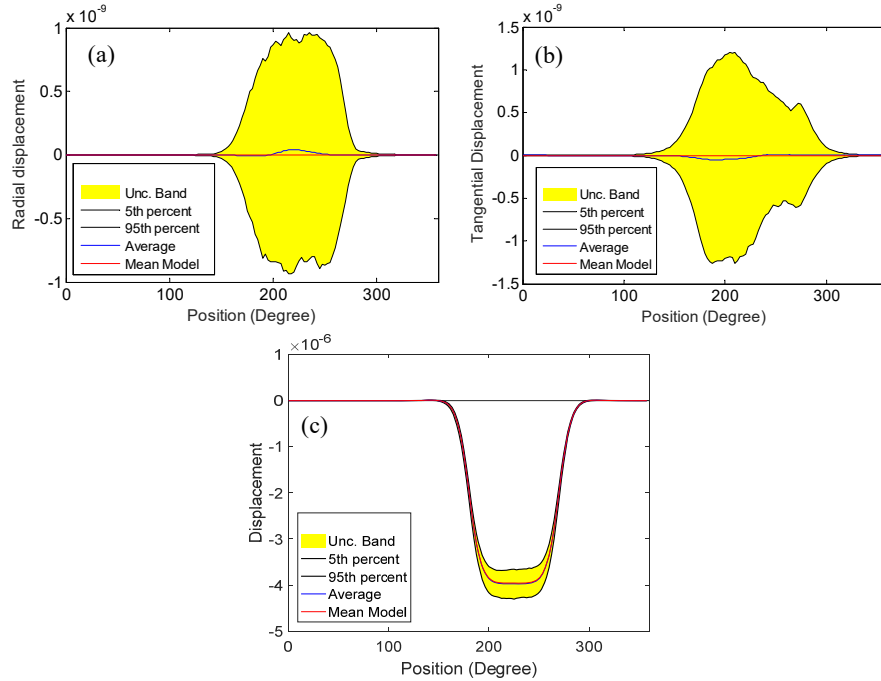


Figure 20: Displacements (in m) at the periphery of the mean annulus (in red) and 5th-95th percentile uncertainty band in (a) transverse, (b) radial and (c) tangential direction. Unit load, no temperature.

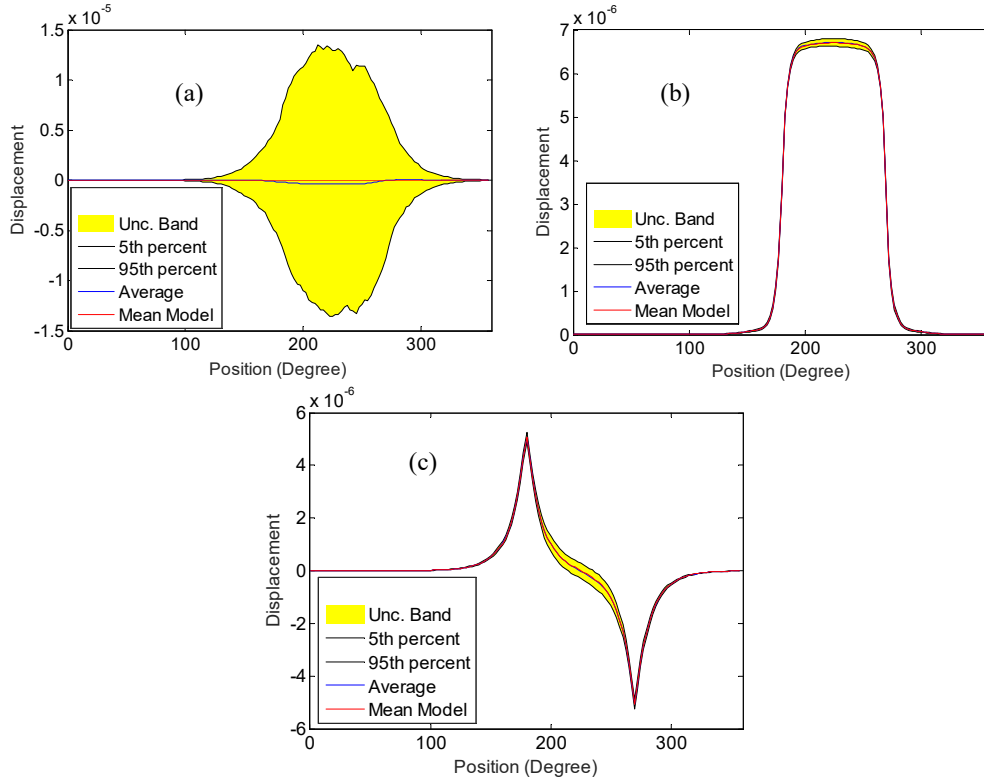


Figure 21: Displacements (in m) at the periphery of the mean annulus (in red) and 5th-95th percentile uncertainty band in (a) transverse, (b) radial and (c) tangential direction. Uncertainty on stiffness. No load, unit temperature.

Consider next the deformations of the annulus under a unit temperature rise in the yellow zone without any force applied, see Fig. 21 when the uncertainty is on the structural (stiffness) properties of the annulus. Note again that the localization of the response does take place and that transverse displacements also take place when uncertainty is present while none do for the mean model, see Fig. 21(a), demonstrating again the presence of epistemic uncertainty. The displacements induced when the uncertainty is on the structural-thermal coupling terms are similar to those of Fig. 21 except that the transverse displacements remain zero which is expected since the corresponding (mean) structural model does not have any transverse - in plane coupling.

It should finally be noted that the methodology developed for heated structures is also applicable to unheated ones with active piezoelectric components owing to the "thermal analogy" of the piezoelectric effects. This possibility was implemented and validated in a collaborative effort with Prof. Liao, see [45].

3.3.2 Compressed Principal Component Analysis

A standard approach for modeling the uncertainty in finite element models is to rely on the Karhunen-Loeve expansion (or Principal Component Analysis, PCA) which expresses the random deviations of the vector, process or field of interest in terms of the eigenvectors and eigenvalues of its correlation structure. For a n -component random vector $\mathbf{X}$, this representation is

$$\mathbf{X}_{PCA}^m = \mathbf{m}_X + \sum_{\alpha=1}^m \sqrt{\lambda_{\alpha}} \Gamma_{\alpha} \varphi^{\alpha}, \quad (1)$$

where $m \leq n$, and for $\alpha = 1, \dots, n$, λ_α and $\boldsymbol{\varphi}^\alpha = (\varphi_1^\alpha, \dots, \varphi_n^\alpha)$ are the eigenvalues and eigenvectors of its covariance matrix $[C_{\mathbf{X}}]$. Owing to the symmetry of this matrix, the eigenvectors $\boldsymbol{\varphi}^1, \dots, \boldsymbol{\varphi}^n$ form an orthonormal basis of $\mathbb{R}^n$. In addition, Γ_α are zero mean, unit variance *uncorrelated* random variables.

One of the challenges of the PCA is in fact that the random variables Γ_α are only uncorrelated and not independent when the random vector $\mathbf{X}$ is not jointly Gaussian. Accordingly, these random variables are usually expressed through a Polynomial Chaos (PC) expansion which enables their modeling but at the cost of a large to very large number of coefficients when the number of terms, m , in Eq. (1) becomes large.

In the present effort, an alternate, approximate representation of the vector $\mathbf{X}$ was sought in the form

$$\mathbf{X}_{CPCA}^N = \mathbf{m}_{\mathbf{X}} + \sqrt{\frac{\mu}{N}} \sum_{\alpha=1}^N H_\alpha \boldsymbol{\varphi}^{J_\alpha}, \quad (2)$$

where N is a parameter of the approximation, which can be less than, equal to, or greater than m

$$\mu = \sum_{\alpha=1}^m \lambda_\alpha, \quad (3)$$

and the real-valued random variables $\{H\}_\alpha$ have zero mean, unit variance and are uncorrelated. Finally, $\mathbf{J} = (J_1, \dots, J_N)$ denotes a random vector that is independent of $\mathbf{H}$ and for which the components $J_1, \dots, J_N$ are N independent copies of a random variable J with values in the set $\{1, \dots, m\}$ of integers and with distribution

$$\text{Prob}\{J = \alpha\} = \frac{\lambda_\alpha}{\mu} \quad \text{for } \alpha = 1, \dots, m. \quad (4)$$

Some properties of the above approximation are key in understanding its usefulness and completing its definition. More specifically, it can be shown [46] that:

- (i) the compressed principal component approximation has the same first two moments as its standard PCA counterpart, and
- (ii) in approximating a given random vector $\mathbf{X}$ in the form of Eq. (2), it is sufficient to consider random vectors $\mathbf{H}$ with a probability density function $\mathbf{H} \mapsto p_{(\mathbf{H})}$ continuous on $\mathbb{R}^N$ that is a *sym-metric function* with respect to $h_1, \dots, h_N$, the components of $\mathbf{H}$.

This second property is particularly useful because it enables to represent the vector $\mathbf{H}$ in terms of a small number of deterministic parameters. Specifically, it is shown in [46] that

$$\mathbf{H} = \sum_{k=1}^M z_k \boldsymbol{\psi}^k(\boldsymbol{\Xi}) \quad (5)$$

in which $\boldsymbol{\psi}^k(\boldsymbol{\Xi})$ is a set of vector-valued symmetric polynomials depending on the canonical Gaussian random vector $\boldsymbol{\Xi} = (\Xi_1, \dots, \Xi_N)$, see [46] for construction, and where the coefficients of the representation are gathered in vector $\mathbf{z} = (z_1, \dots, z_M)$. It should be noted that the number M of polynomials $\boldsymbol{\psi}^k(\boldsymbol{\Xi})$ is in fact quite small and converges to a constant value when N becomes equal to $n_d + 1$, n_d being the order of the polynomials. For $n_d=3$, the maximum number of such polynomials is only 13!

The representation of Eq. (2)-Eq. (5) is referred to here as the Compressed Principal Component Analysis (CPCA) approximation of the vector $\mathbf{X}$. Owing to the small number of polynomials, the CPCA is a very compact approximation of the vector $\mathbf{X}$.

The identification of the parameters z_k from samples of the vector $\mathbf{X}$ is discussed in details in [46] and completes the construction of the CPCA approximation. Its assessment was done in [46] on a notably non-Gaussian random vector $\mathbf{X}$ of 729-components for which the number of retained PCA eigenvalues and eigenvectors was found to be $m=15$. Shown in Fig. 22 is a typical comparison of the probability density functions of the original process, its PCA and CPCA approximations as well as a Gaussian one. It is seen from these figures that the CPCA matching is very good, especially in the tail of the distribution and is obtained with only cubic polynomials and thus 13 coefficients. These results are extremely encouraging. Additional analysis, validation, and extension of the CPCA modeling is currently in progress.

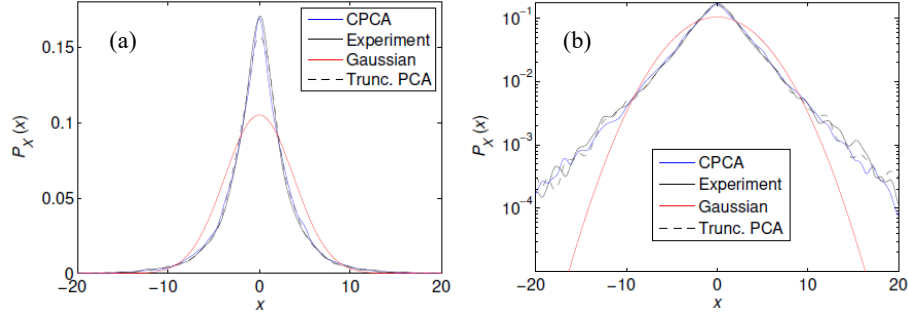


Figure 22: Probability density functions $p_X(x)$, of variable X_{329} , (a) linear scale, (b) logarithmic scale. Original data ("Experiment"), PCA truncated to $m=15$ terms ("Trunc. PCA"), its Gaussian approximation, and CPCA approximation.

3.4 Acceleration of Uncertain ROM Computations

While the computational effort to determine the system response using ROMs is much faster than it is for FOMs, the CPU time for transient computations carried out over long trajectories may still be significant, especially when multiphysics effects are present and/or when such analyses are performed in a Monte Carlo framework to assess the effects of uncertainty. This is in particular the case for the fully coupled aero-structural-thermal testbed for which the nonlinear structural ROM has 44 modes while the thermal one has 42 basis functions.

In such cases, it is highly desirable to define strategies complementary of the existing ROM formulations that provide an additional reduction in the computational effort. Two such strategies were investigated in the present effort the first one of which seeks to reduce the number of ROM basis functions by adapting these functions to the features of the response [47]. The second strategy focuses on reducing the cost induced by Monte Carlos simulation by using multifidelity concepts, e.g., see [48, 25, 21]. These two strategies are presented in detail below.

3.4.1 Reduced ROMs (RROMs) Formulation and Application

The potential for large bases is particularly clear in multiphysics problem. Owing to the interaction of the various physical components of the system, its response is likely to be difficult to narrow down to a small number of a priori basis functions and thus a large basis is adopted to ensure a good representation of the FOM solution. A strategy to reduce the basis can nevertheless be devised by "learning" from the solution as it proceeds and adjusting the basis accordingly. That is, the ROM solution with the large basis can be computed for a certain number of time step, then this data is analyzed through a Proper Orthogonal Decomposition to (i) optimally rotate the basis and (ii)

shrink it so that the resulting "reduced ROM" would still capture the full ROM solution to within a given error.

The system's response is then computed using the reduced ROM but periodic checks are carried out to ensure that this solution and the one that would be computed from the full ROM remain within the stated tolerance. If/once that check fails, the solution is backtracked to the last "good point" and the full ROM is marched again for an appropriate length to provide data for a new reduced ROM to be learned from, see Fig. 23 for the flowchart of the strategy.

This process was implemented for the fully coupled aero-structural-thermal testbed and the results are shown in Fig. 24. Note on these figures that the blue zones are full ROM learning solutions while red ones correspond to RROM predictions. It is seen that rather long periods of RROMs predictions occur even though the response of the panel is undergoing dramatic changes through the trajectory. The number of structural and thermal basis functions in the 4 RROM zones were found to be (15,5), (30,10), (21,7), and (30,9) all of which correspond to very significant reductions over the (44,42) of the full ROM. The total computational effort associated with the full ROM learning and RROMs computations was overall less than 50% of the original one, most of it being associated with full ROM learning phases.

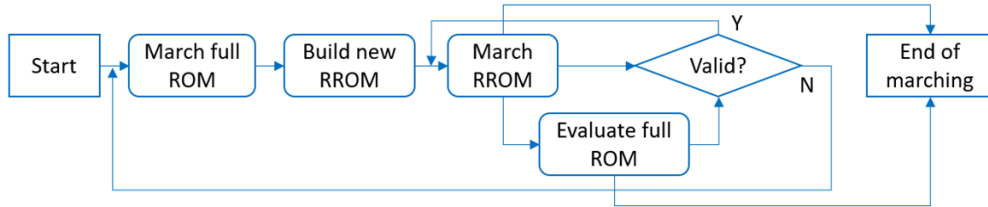


Figure 23: Flowchart of the RROM construction and adaptation processes.

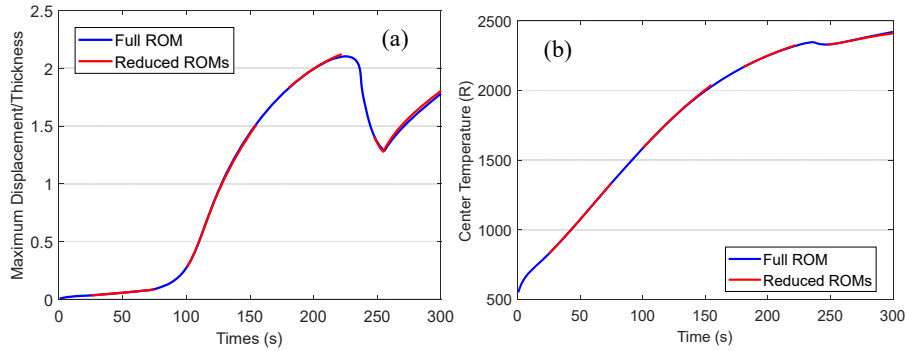


Figure 24: Predictions of (a) the maximum transverse displacement and (b) the temperature of the panel center by the full ROM and the Reduced ROMs. Blue zones are full ROM learning solutions while red ones correspond to RROM predictions.

3.4.2 Multifidelity Reduced Order Modeling

In the last few years, it has been successfully demonstrated, e.g., see [48, 25, 21], that predictions from models of different fidelities can be successfully combined to obtain accurate estimates of the mean and standard deviation of statistics of the response. This framework, referred to as Multifidelity Monte Carlos (MFMC) simulation, is perfectly suited for ROMs where fidelity is naturally

associated with basis size. This observation prompted us to assess the potential of combining multifidelity concepts and reduced order modeling, in what is referred to here as multifidelity reduced order modeling, for the prediction of the mean and standard deviation of some responses.

Since such an approach would be most useful with models with large basis, the target application was the fully coupled aero-structural-thermal testbed. Moreover, to optimize the computational gain, it was decided to combine this multifidelity prediction with the reduced ROM approach of the previous section. That is, different reduced ROMs were considered with number of structural and thermal basis functions equal to (9,3), (12,4), and (15,5) in the first blue-red interval of Fig. 24. The results of this analysis are shown in Fig. 25, it is seen that the multifidelity predictions are indeed accurate in comparison to the much more expensive full ROM computations, even for the variance which is very small and thus hard to capture well. Computational details and additional examples presented in [49] clearly demonstrate the strong potential of combining ROMs, potentially RROMs, and multifidelity concepts to estimate the statistics of the uncertain response in a computationally very efficient manner.

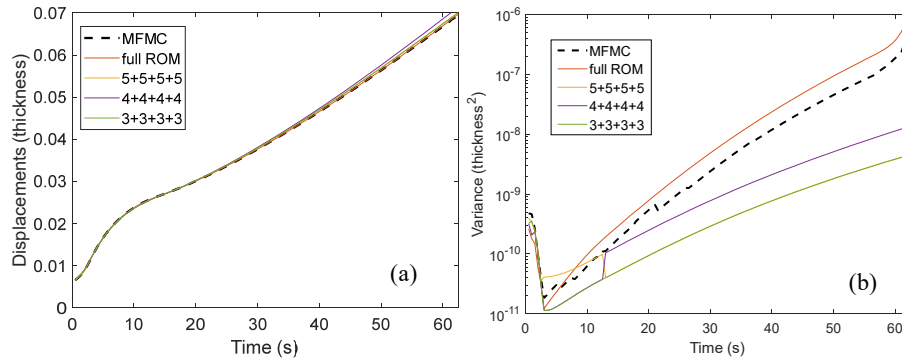


Figure 25: (a) Mean and (b) variance of the maximum transverse response vs. time as predicted from the MFMC approach and the three different ROMs.

3.5 Multifidelity estimation for managing uncertainty in complex simulations

For complex multi-discipline simulations, there are typically many options for deriving reduced models, which vary greatly with respect to fidelity, stability, and other criteria. Which of the reduced models is the most appropriate one for the current task at hand is often unclear, except in certain limited settings where error bounds for the reduced models can be derived. Therefore, the selection of a reduced model is often ad-hoc and based on engineering judgment, manual fine-tuning, and domain expertise. For example, reduced models of convection-dominated phenomena are typically stabilized with closure terms, which are derived in an ad-hoc manner from physical insights. Which closure term yields the most accurate reduced model depends on many aspects such as parameter configurations, inputs, and other properties of the problem, and therefore selecting the closure term that leads to a reduced model with minimal error, or another desired property, is challenging. We introduce in [50] a multifidelity uncertainty quantification approach for estimating failure probabilities that uses all given reduced models and so avoids the problem of selecting one out of many available reduced models. We show that our multifidelity approach provides estimators with mean-squared errors that are up to a constant lower than the mean-squared errors of the corresponding estimators that use any of the given reduced models alone—even in settings where no information about the approximation qualities of the reduced models is available. Therefore, our multifidelity approach avoids the problem of selecting the reduced model that leads to the estimator

with the lowest mean-squared error. The mathematical analysis shows that even if many of the given reduced models fail to provide accurate approximations, our multifidelity approach still provides an accurate failure probability estimate because it uses all reduced models. We demonstrated our multifidelity approach on numerical examples that develop shocks. We derived reduced models with different closure terms and combined all of them with our multifidelity approach. Even though many of the reduced models were unstable, our multifidelity estimator provided accurate results, and so avoided the problem of manually selecting a reduced model that leads to stable behavior.

3.6 Multi-fidelity preconditioning of the cross-entropy method for rare event simulation and failure probability estimation

Accurately estimating rare event probabilities with Monte Carlo can become costly if for each sample a computationally expensive high-fidelity model evaluation is necessary to approximate the system response. Variance reduction with importance sampling significantly reduces the number of required samples if a suitable biasing density is used. MIT and U. Wisconsin developed a multifidelity approach that leverages a hierarchy of low-cost surrogate models to efficiently construct biasing densities for importance sampling. Our multi-fidelity approach is based on the cross-entropy method that derives a biasing density via an optimization problem. We approximate the solution of the optimization problem at each level of the surrogate-model hierarchy, reusing the densities found on the previous levels to precondition the optimization problem on the subsequent levels. With the preconditioning, an accurate approximation of the solution of the optimization problem at each level can be obtained from a few model evaluations only. In particular, at the highest level, only few evaluations of the computationally expensive high-fidelity model are necessary. Our numerical results demonstrate that our multi-fidelity approach achieves speedups of several orders of magnitude in a thermal and a reacting flow example compared to the single-fidelity cross-entropy method that uses a single model alone.

3.7 Towards context-aware learning: Monte Carlo estimation with adaptive low-fidelity models

Multifidelity Monte Carlo (MFMC) estimation combines low- and high-fidelity models to speedup the estimation of statistics of the high-fidelity model outputs. MFMC optimally samples the low- and high-fidelity models such that the MFMC estimator has minimal mean-squared error for a given computational budget. In the setup of MFMC, the low-fidelity models are static, i.e., they are given and fixed and cannot be changed and adapted. In contrast, a context-aware approach learns/adapts low-fidelity models based on the current context at hand: the proposed adaptive MFMC (AMFMC) method [51] splits the computational budget between adapting the low-fidelity models to improve their approximation quality and sampling the low- and high-fidelity models to reduce the mean-squared error of the estimator. The AMFMC approach derives the quasi-optimal balance between adaptation and sampling in the sense that an upper bound of the mean-squared error is minimized, instead of the error directly. The quasi-optimal number of adaptations of the low-fidelity models is bounded even in the limit case that an infinite budget is available. This shows that adapting low-fidelity models in MFMC beyond a certain approximation accuracy is unnecessary and can even be wasteful. In contrast, the proposed AMFMC approach takes the context given by MFMC into account and trades-off adaptation and sampling and so avoids over-adaptation of the low-fidelity models. Besides the costs of adapting low-fidelity models, AMFMC also accounts for the costs of the initial construction/learning of the low-fidelity models (“offline costs”), which is critical if low-fidelity models are computationally expensive to build such as reduced models

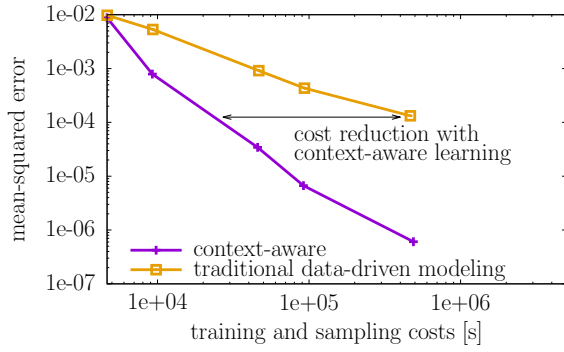


Figure 26: Numerical results with the AMFMC method demonstrate that training and sampling costs of context-aware learning are up to one order of magnitude lower compared to traditional data-driven modeling. For the same costs, context-aware learning provides a two orders of magnitude more accurate outer-loop result because it balances the computational budget more efficiently between training and sampling [51].

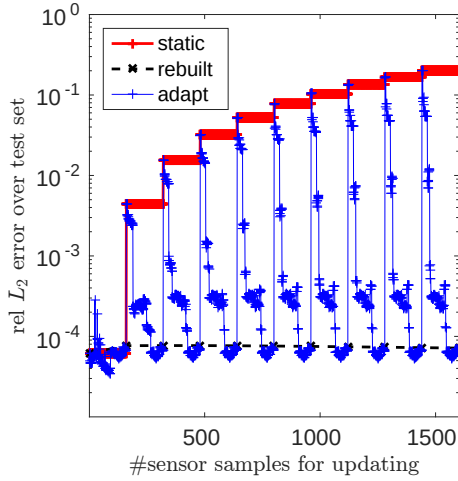


Figure 27: Our online adaptive model reduction approach updates the reduced basis and the reduced operators of reduced models from incomplete data and so dynamically adapts reduced models to changes and new dynamics of the system of interest.

and data-fit surrogate models. Numerical results demonstrate that AMFMC achieves orders of magnitude speedups compared to MFMC estimators with static, context-free low-fidelity models and compared to Monte Carlo estimators that use the high-fidelity model alone; see Figure 26.

3.8 Online adaptation of reduced models of systems that undergo dynamic changes

Classical model reduction constructs a reduced model of a large-scale system in an offline phase and then keeps the reduced model unchanged during the evaluations in an online phase; however, the system might develop dynamics online that cannot be anticipated during the construction of the reduced model in the offline phase, and therefore the reduced model may fail to make accurate predictions of the system behavior. Consider for example a multi-discipline system, where for each discipline a reduced model is derived separately offline. By coupling the reduced models online, dynamics may develop that were not anticipated when building the reduced models separately. Rebuilding the reduced models from scratch online is often too expensive in time-critical and real-time environments. We introduced a dynamic data-driven adaptation approach [52] that adapts the reduced models from incomplete data samples (sensors) obtained from the system during the online computations. Such incomplete data may be obtained by occasionally querying the high-fidelity components of the multi-discipline system, instead of the reduced models. The updates to the reduced models are derived directly from the incomplete data, without recourse to a full-system analysis. Our adaptivity approach approximates the missing values in the incomplete data with gappy proper orthogonal decomposition. These approximate data are then used to derive low-rank

updates to the reduced basis and the reduced operators of the reduced models. In our numerical examples, incomplete data with 30-40% known values are sufficient to recover the reduced models that would be obtained via rebuilding from scratch; see Figure 27.

3.9 Active subspaces in Bayesian Global Optimization

For both scalability and efficiency, we developed a novel two-step knowledge gradient policy that exploits potential active subspaces of the available underlying information sources as part of our multi-information source optimization framework. In our approach, with previously queried data, the active subspace method is used to map the problem to one of smaller dimension based on directions of greatest variability of the true function. Exponentially fewer alternatives are required on this smaller dimensional problem and the knowledge gradient can readily be applied. The solution to the problem on the active subspace is then mapped to the original space where a second knowledge gradient is applied to a hyperplane orthogonal to the active subspace. The result is a method that enables the application of the alternatives-based knowledge gradient policy to moderately high dimensional problems. Further, due to the fact that the initial knowledge gradient step is focused in directions defined by the largest variability of the true function, our method is significantly more efficient than direct application of the knowledge gradient to the true function. That is, exploiting the active subspace, when one exists, can lead to significant gains in terms of iterations required for convergence. We have demonstrated this approach on an aeroelastic testbed problem. A depiction of the general approach is shown in Figure 28.

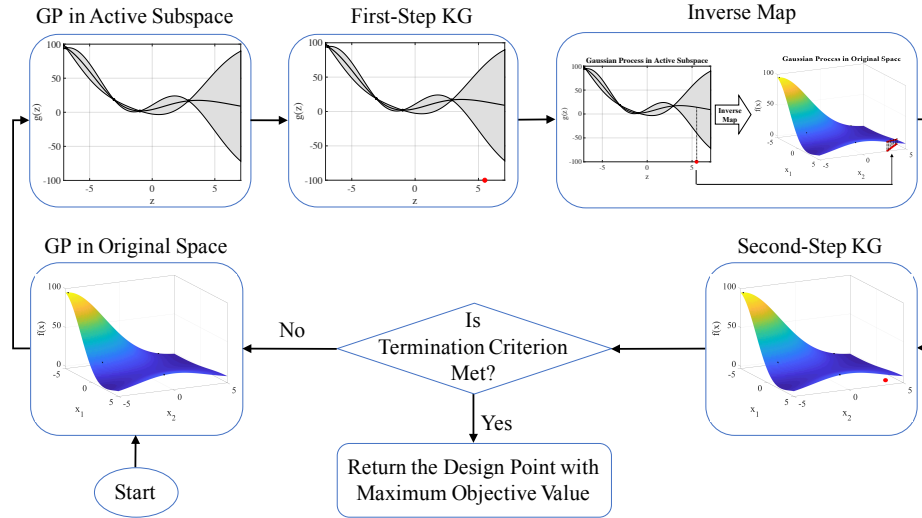


Figure 28: A depiction of our proposed approach for fast sequential optimization using active subspaces for Bayesian global optimization.

4 RT3: Managing multi-physics coupling

4.1 Multifidelity uncertainty propagation in coupled multidisciplinary systems

The focus of this research is on devising methods for efficient uncertainty propagation for feedback-coupled multidisciplinary systems. This research lies at the intersection of RT2 and RT3. Fixed

point iteration (FPI) is a common strategy to handle interdisciplinary coupling within a feedback-coupled multidisciplinary analysis. For each coupled analysis, this requires a large number of disciplinary high-fidelity simulations to resolve the interactions between different disciplines. When embedded within an uncertainty analysis loop (e.g., with Monte Carlo sampling over uncertain parameters) the number of high-fidelity disciplinary simulations quickly becomes prohibitive, since each sample requires a fixed point iteration and the uncertainty analysis typically involves thousands or even millions of samples. In [53], we developed a method for uncertainty analysis in feedback-coupled systems that leverages adaptive surrogates to reduce the number of cases for which fixed point iteration is needed. The multifidelity coupled uncertainty propagation method is an iterative process that uses surrogates for approximating the coupling variables and adaptive sampling strategies to refine the surrogates. The adaptive sampling strategies explored in this work are residual error, information gain, and weighted information gain. Rigorous convergence analysis shows that under certain conditions, the use of the proposed adaptive surrogate refinement leads our method to recover the results that would be obtained using high-fidelity FPI on all samples. Yet, the results indicate that the method can lead to significant reductions in computational cost (shown in Figure 29 for an analytic test problem). This method identifies the entire distribution of the system output of a feedback-coupled multidisciplinary system and can be used for estimating any statistical moments and risk measures.

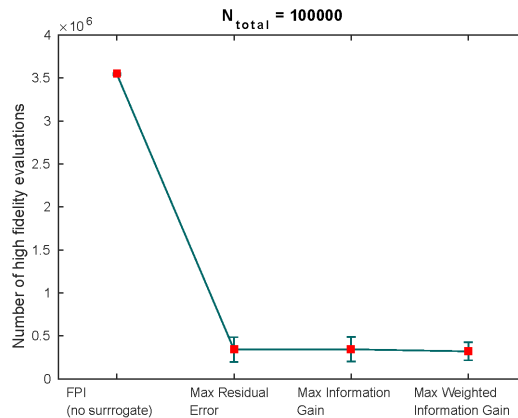


Figure 29: Comparing mean number of high-fidelity evaluations required for uncertainty propagation using 10^5 samples for an analytic test problem [53]. Error bar indicates twice the standard deviation of 10 trials.

4.2 Optimal coupling in multidisciplinary models

In the design of engineering systems, the coupling among disciplines contributes significantly to the computational cost of analyzing the system. For many models, however, disciplines are weakly coupled and the interactions can be neglected without significantly impacting the accuracy of the system’s output. While typical practice derives model couplings in an ad hoc manner based on domain specific knowledge, this work proposes a new approach to identify the optimal model couplings. In the context of systems that depend on uncertain model parameters, we formulate an optimization problem to find the model that reduces the number of couplings between disciplines while keeping the output variables close in distribution to the original system. The optimization uses sequential Monte Carlo to efficiently search the combinatorial model space that grows exponentially in size with the number of disciplines. In addition, we propose the use of model linearizations to estimate

the distance between the output distributions of competing models. In [54], the algorithm is applied to two commonly used engineering systems: a fire-detection satellite and a model for turbine engine cycle analysis. In both cases, the algorithm finds an optimal set of models that trades-off accuracy with the complexity of the model by incrementally removing weak discipline connections. These resulting models are close in distribution and average absolute error to the original model, making them cost-effective for uncertainty quantification or design optimization. An example of the optimal satellite model is displayed below where dashed lines indicate decoupled connections. The joint distributions for the system outputs of the original and decoupled models are also presented below.

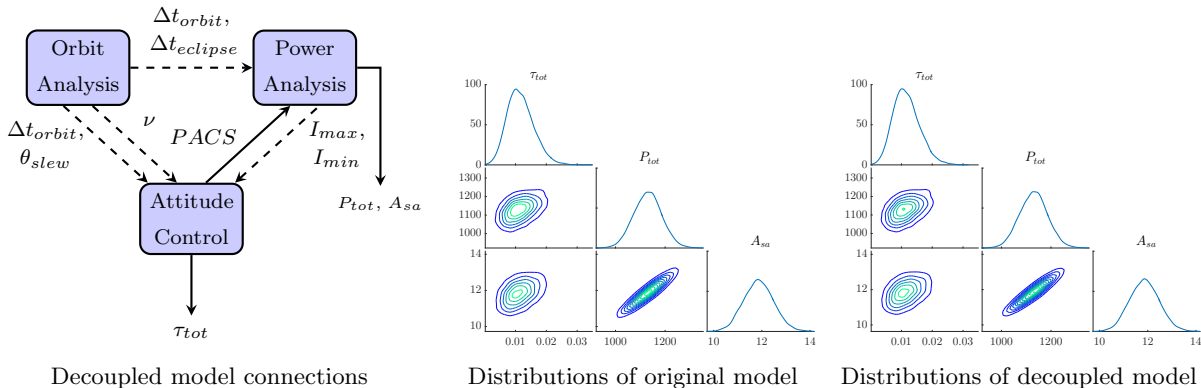


Figure 30: Decoupling of a fire-detection satellite model

4.3 Structure learning in non-Gaussian distributions

Multidisciplinary engineering systems with many sources of uncertainty typically involve state and output variables that follow high-dimensional and non-Gaussian probability distributions. In general, these multidisciplinary systems are constructed by coupling mathematical models from different physical domains. In order to build more efficient and parsimonious models, we investigate the connection between the necessary coupling among domains and the joint distribution of the state and output variables. This connection is revealed by the *conditional independence* (CI) properties of the distribution. These properties can be encoded by the edges in an undirected graphical model (also known as a Markov random field) where each node corresponds to a random variable and the lack of an edge denotes conditional independence between the corresponding variables. In this setting, our goal is to learn the edges of this graph given a limited number of samples from the joint distribution.

To learn the graphical model underlying a continuous non-Gaussian distribution from samples, we developed an algorithm called SING (Sparsity Identification in Non-Gaussian distributions). The approach relies on a connection between the sparsity of the graph and the sparsity of the transport map that represents the corresponding distribution, as described in the section above. Estimating the parameters of the transport map yields a representation for the distribution which then enables computation of its properties including CI. In SING, CI is represented by the sparsity of a matrix known as the *generalized precision*. This matrix is adaptively thresholded to identify a sparse graph. The graph structure is then used to learn the parameters with lower variance estimates due to a sparser transport map, thereby improving the estimates for the CI. These steps are repeated until the set of discovered edges converges.

To validate the SING algorithm, we applied it to various generated non-Gaussian datasets including a so-called butterfly distribution and a stochastic volatility problem. In our recent paper (NIPS

2017), existing algorithms that make Gaussian assumptions on the underlying data-generating process were shown to fail in these cases. On the other hand, the SING algorithm recovered the true graph structure. In the context of the MURI testbed problems, we applied the SING algorithm to data from the fire-detection satellite model (figure 31) that was also analyzed in other RT3 efforts. Previous work had identified the distribution of the model’s quantities of interest to be closely approximated by a candidate model with fully decoupled disciplines. As seen in figure 32, SING automatically identified the strong edges between variables of each discipline (denoted in blue), and learned a disconnected graph over the different disciplines.

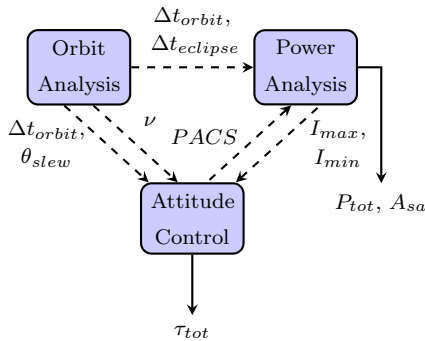


Figure 31: Coupling in satellite model. Dashed lines indicated non-necessary couplings as found in previous RT3 work.

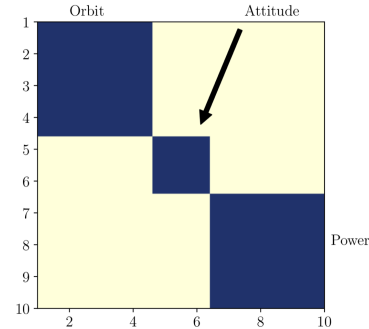


Figure 32: Edges recovered by SING. Disconnected blocks correspond to the three physical domains.

4.4 Learning sparse transport maps

Transport maps provide a rich means of expressing complex probability distributions by transforming simple reference distributions. To characterize a high dimensional distribution π , one approach is to learn a transport map from samples drawn from π . When the ambient dimension of the distribution is large relative to the number of available samples, however, one must exploit low-dimensional structure to accurately estimate the distribution.

Some of our recent theoretical results show that the Markov structure associated with π yields a lower bound on the sparsity pattern of the map (i.e., the functional dependence of each component of the map on the random variables). As a result, knowledge of the conditional independence properties of π allows for the estimation of a sparse map using fewer samples. Although in practice it may be difficult to know *a priori* the exact sparsity pattern, it has been observed that these map components are often approximately sparse with many parameters being near zero. In this setting, we can formulate a regularized optimization problem (that resembles a sparse regression or LASSO problem for linear maps) to estimate the unknown parameters.

Our efforts have connected optimization of linear transport maps to sparse linear regression. In this way, we showed that the ℓ_2 error of numerically computed linear maps depends on the number of samples n , the sparsity of the map s , and weakly on the dimension d , with n only scaling as $s \log(d)$. This makes the estimation of high-dimensional transport maps feasible in a heavily undersampled regime.

4.5 Adaptive transport maps and structure learning for non-Gaussian graphical models

Undirected graphical models are probabilistic models where the graph represents the conditional dependencies, or Markov properties, of a collection of random variables. Knowing the sparsity of this graph is valuable for modeling multivariate probability distributions and for performing inference and prediction tasks. While learning the graph structure from data has been studied extensively for certain parametric families of distributions, most existing methods fail to consistently recover the graph for non-Gaussian data.

Continuing our previous years' work under this MURI, we have been advancing algorithms for learning the Markov structure of continuous and non-Gaussian distributions. We propose a new score based on the expected Hessian of the joint log-density, and have recently proved that this score upper bounds conditional mutual information for a general class of distributions. To compute the score, our algorithm SING estimates the density using a deterministic coupling, known as a transport map, and iteratively exploits sparse structure in the map to reveal the sparsity in the graph. For certain non-Gaussian datasets, we can show that our algorithm recovers the graph structure even with a biased approximation to the density.

Related to this question of structure learning problem is the problem of *adaptively* learning sparse transport maps from data. Given a finite sample from a non-Gaussian distribution, one would like to identify, from these data alone, how to efficiently and stably learn a map representing this distribution. To this end, we have developed an adaptive semi-parametric approach that iteratively chooses which basis functions to add to the map representation. Based on an adaptation of gradient boosting and ideas from high-dimensional approximation that search for features in the *reduced margin* of a downward-closed index set, our algorithm identifies which nonlinearities to add to a map, and in which variables. Moreover, it balances the bias of an incomplete map representation with the variance due to estimating this representation from finite samples. The result is an automated procedure for identifying *sparse* nonlinear transport maps from data, and thus efficiently representing non-Gaussian probability distributions exploiting their conditional independence structure.

4.6 Safe predictions using generalized Bayesian inference

The predictive models used in decision making under uncertainty are often calibrated from observed data using Bayesian parameter inference. The risk associated with a decision is defined in terms of the posterior distribution, which describes the uncertainty in the model via uncertainty in its parameters. In standard Bayesian inference, the posterior distribution concentrates near the *single* most-likely parameter value as the number of data points increases. Likewise, the posterior predictive distribution concentrates onto the *single* most-likely model output. When the model is well-specified—there exists a single parameter value that adequately describes *all* of the observed data—this concentration is often desirable and the resulting uncertainty estimates are meaningful. However, when the model is misspecified, the resulting predictive distribution may not resemble the data and may grossly under-represent predictive uncertainty.

To address the over-concentration issue, we introduce a *generalized* posterior distribution by modifying the likelihood function of the original predictive model to achieve the following:

1. Local concentration onto *multiple* parameter values consistent with *subsets* of the data.
2. Robustness to outliers by discounting observations that are inconsistent according to our model.

3. Proportional representation: the probability ratio between two parameter values is proportional to the fraction of data consistent with each parameter value.
4. Interpretability and portability: by leaving the predictive model untouched, the generalized posterior remains compatible with downstream applications such as prediction and decision making.

We achieve local concentration and robustness to outliers by introducing data weights $w_i(\theta)$ that are functions of the model parameters and describe how consistent observation y_i is under the model with parameter value θ . We use the likelihood function $p(y_i|\theta)$ as a proxy for model consistency and introduce two tuning parameters, $0 \leq \tau_1 < \tau_2 < \infty$, which describe likelihood thresholds of model-data consistency:

$$w_i(\theta) = \begin{cases} 1 & p(y_i|\theta) > \tau_2 & \text{(fully consistent)} \\ \frac{p(y_i|\theta) - \tau_1}{\tau_2 - \tau_1} & \tau_1 \leq p(y_i|\theta) \leq \tau_2 \\ 0 & p(y_i|\theta) < \tau_1 & \text{(not consistent)} \end{cases}$$

Finally, by pre-multiplying by the sum of weights and normalizing, we can achieve the desired proportional representation. The generalized posterior, in relation to the standard posterior, is summarized in the following equation:

$$\underbrace{p(\theta|y)}_{\text{posterior}} \propto \underbrace{p(\theta)}_{\text{prior}} \underbrace{\prod_{i=1}^n p(y_i|\theta)}_{\text{likelihood}} \rightarrow \underbrace{\pi(\theta; y)}_{\text{generalized posterior}} \propto \underbrace{\pi(\theta)}_{\text{prior}} \underbrace{\left[\frac{1}{Z(\theta)} \sum_{i=1}^n w_i(\theta) \right] \prod_{i=1}^n [p(y_i|\theta)]^{w_i(\theta)}}_{\text{modified likelihood}}$$

We demonstrate the effectiveness of our approach on a regression problem where we calibrate a linear model against data from (i) a mixture of linear models and (ii) a nonlinear (quadratic) function. In Figures 33 and 34, we see that the generalized posterior distribution, even for a large number of observations ($N = 100$) does not concentrate onto a single parameter value, but instead concentrates onto multiple plausible parameter values. The resulting generalized posterior predictive distributions also have much better coverage of the observations, even though the predictive model itself is unchanged.

In summary, decisions that depend on uncertainty in the posterior distribution resulting from Bayesian inference are sensitive to model misspecification. The uncertainty captured in the generalized posterior produces *safer*, more conservative predictions especially when multiple values of the model parameters are locally consistent with the data—a common form of misspecification.

Our ongoing work extends these ideas to dynamical models (e.g., as described by ordinary differential equations) and the associated real data sets, and addresses the computational challenges of simulating from the generalized posterior in higher dimensions.

4.7 Importance weight ensemble Gibbs sampling for coupled multiphysics systems.

We developed an efficient information source discrepancy propagation technique for coupled multiphysics systems. Our approach is based on offline independent evaluation of information sources via Monte Carlo simulation followed by online synthesis of offline results that does not require evaluations of the coupled system. The online synthesis is conducted via importance weighted ensemble Gibbs sampling, which iteratively recomputes the joint distribution among coupling variables in the system via sample re-weighting. Numerical results demonstrate that for compatible information source discrepancies, the unique joint distribution of the coupling variables in the system can be

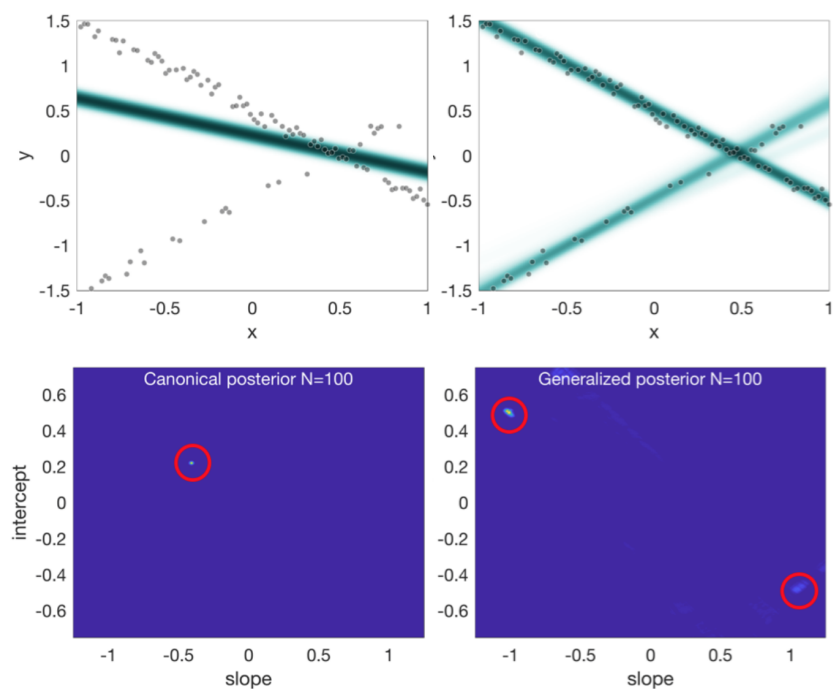


Figure 33: Comparison of the standard posterior and its predictive (left) and the generalized posterior (right) on a linear regression task with nonlinear data.

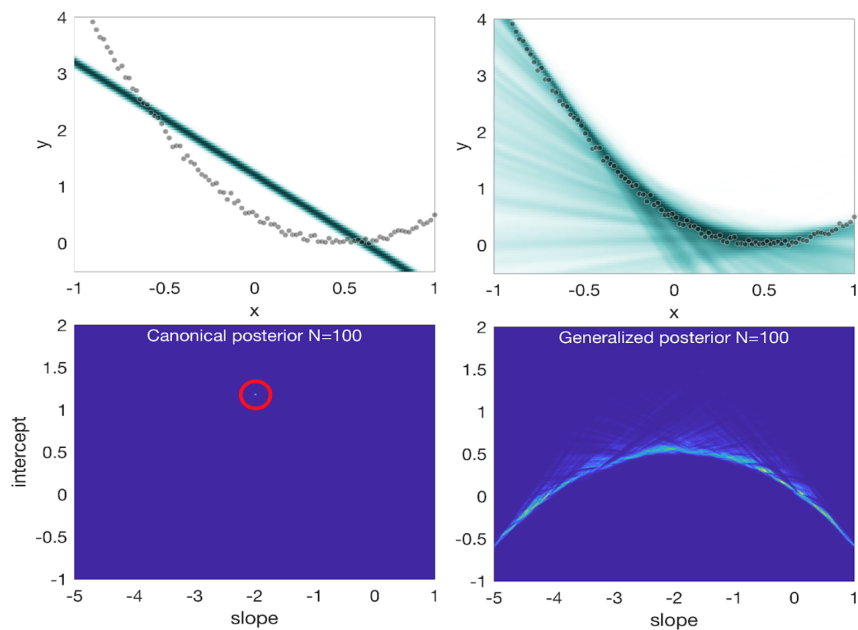


Figure 34: Comparison of the standard posterior and its predictive (left) and the generalized posterior (right) on a linear regression task with nonlinear data.

recovered without ever evaluating the coupled system. This capability addresses the important task of how to update or replace an information source in an integrated system without having to re-evaluate the entire integrated system. The process is depicted in Figure 35.

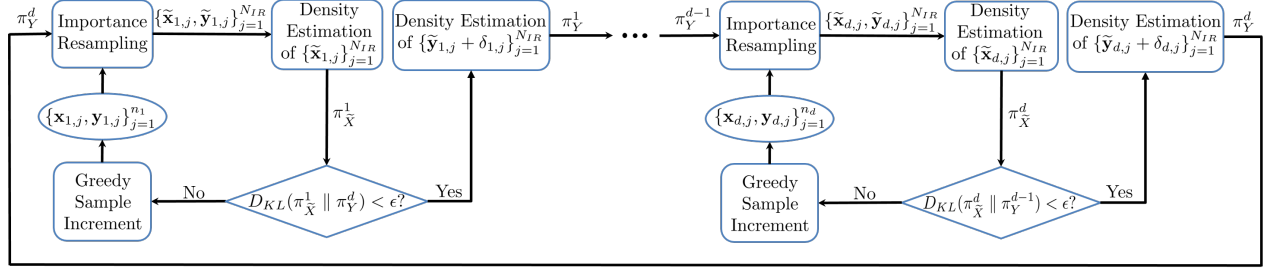


Figure 35: A depiction of our approach for uncertainty propagation in a multidisciplinary system containing d disciplines. The methodology consists of a Gibbs sampling procedure that is enabled by iteratively re-weighting the samples available for each discipline, $\{\mathbf{x}_{i,j}, \mathbf{y}_{i,j}\}_{j=1}^{n_i}$, through a combination of density estimation and sequential importance resampling. The approach includes a greedy sample increment process which adds samples to the available samples adaptively based on the Kullback-Leibler divergence, D_{KL} . Note that π_Y^d is initialized as π_0 .

4.8 Efficient Propagation of Uncertainty in Coupled Systems

Building on our importance weighting work, we developed an efficient computational methodology for converging to appropriate, detailed balance satisfying joint distributions in coupled systems. Our approach incorporates sequential importance resampling techniques in Gibbs sampling iterations to ensure we never have to evaluate a full coupled system. The approach handles model discrepancy as well as parametric uncertainty using a greedy sample increment strategy to maintain proper marginal distributions of the parametric uncertainties while converging on the detailed balance satisfying joint distribution of the quantities of interest. Figure 36 demonstrates the effectiveness of our approach in the case of a parametrically uncertain variable and two coupled information sources with model discrepancy. Our approach is provably convergent for any number of uncertain parameters or models.

4.9 Coupled Uncertainty Propagation

We developed algorithms for enabling the rapid propagation of information through expensive to evaluate coupled multiphysics systems. These algorithms can be used for tasks such as uncertainty analysis and design. Our approach consists of offline discipline level analyses followed by an online synthesis that results in accurate approximations of full coupled system level analyses. Coupling is handled by an efficient procedure for approximating the map from system inputs to fixed point sets that makes use of ℓ_1 -minimization techniques and cut high dimensional model representations (cut-HDMR). We have demonstrated the methodology on a standard analytic numerical example and the MURI testbed fire detection satellite system.

4.10 Formulation and Solution of Multi-Physics Analysis and Design Problems

Existing formulation and solution methods for multi-physics systems are limited in that the decomposition and coupling is pre-determined along disciplinary boundaries, consider only single fidelity models, and are deterministic. We have finalized the core of the new algorithmic framework, MAUD (modular analysis and unified derivatives), by parallelizing it to take advantage of

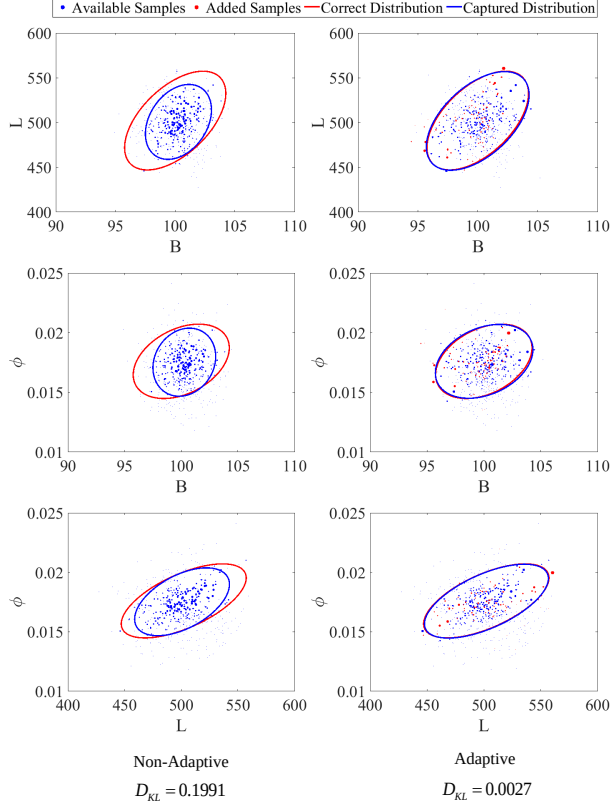


Figure 36: 95% confidence interval of tri-variate joint distribution captured by adaptive and non-adaptive approaches represented by blue contours. Red contours show 95% confidence interval of joint distributions captured by Monte Carlo simulation. D_{KL} is the Kullback-Leibler divergence between the joint distributions captured by MCS and each of adaptive and non-adaptive approaches.

high performance computing clusters. This algorithmic framework has been implemented in the open source framework OpenMDAO, which is available as open source software. We are now implementing our high-fidelity aerodynamic and structural models within this framework to support some of the testbed problems. We have also developed a new surrogate model approach that is able to interpolate scattered multivariate data, and we are now adapting this approach to utilize multiple sources of information.

4.10.1 Modular Multifidelity Framework for Design Optimization of Multi-Physics Systems

The modular analysis and unified derivatives (MAUD) algorithmic framework was finalized, and has since been implemented as the core set of algorithms and data structure in OpenMDAO. The code was transitioned to AFRL using the publicly available link ². The framework was used to develop the new low-fidelity wing design optimization problem, which provides not only a testbed problem, but serves as an introduction to MAUD. This code was used successfully to in a graduate class to introduce students to both wing design and state of the art multi-physics algorithms.

²<http://www.openmdao.org>

4.10.2 Scalable Multifidelity Surrogate Models

Surrogate models are useful in optimization and uncertainty quantification when costly high-fidelity simulations are involved, and can be constructed using multi-fidelity information. However, there are currently no surrogate modeling techniques that scale well with the number of independent variables while maintaining sufficient accuracy.

To address this issue, we developed a new surrogate modeling approach: gradient-enhanced kriging with partial least squares regressions (GEKPLS). This approach is built on the recently developed PLS and shows promise. For a desired accuracy, the GEKPLS approach is orders of magnitude faster than conventional kriging, as shown in Fig. 37.

For high-dimensional problems, using a standard kriging model is computationally expensive because we must invert a large covariance matrix several times to estimate the hyperparameters. The KPLS model addresses this issue by constructing a covariance kernel that depends on only a few parameters. This kernel is constructed based on information obtained from the partial least squares method. In addition, the kriging models can be extended to utilize gradient information when available, which improves the accuracy of the model, reduces the number of observation, or both. While effective for many problems, the gradient-enhanced kriging methods still suffer from a number of weaknesses. The GEKPLS model is a recently developed approach that exploits the gradient information without increasing the size of the covariance matrix while reducing the number of hyperparameters.

The KPLS and GEKPLS approaches will be made available through the surrogate model toolbox (SMT), which also includes least square regression, square polynomial, inverse distance weighting and kriging-based surrogate models.

4.11 Surrogate Modeling Toolbox-enabled Webfoil v1.0

4.11.1 Gradient-Enhanced Surrogate Modeling

Gradient-enhanced kriging has the potential to reduce the number of function evaluations for the desired accuracy when efficient gradient computation, such as an adjoint method, is available. However, current gradient-enhanced kriging methods do not scale well with the number of sampling points due to the rapid growth in the size of the correlation matrix, where new information is added for each sampling point in each direction of the design space. Furthermore, they do not scale well with the number of independent variables due to the increase in the number of hyperparameters that needs to be estimated. To address this issue, we developed a new gradient-enhanced surrogate model approach that drastically reduced the number of hyperparameters through the use of the partial-least squares method that maintains accuracy. In addition, this method is able to control the size of the correlation matrix by adding only relevant points defined through the information provided by the partial-least squares method. To validate our method, we compared the global accuracy of the proposed method with conventional kriging surrogate models on two analytic functions with up to 100 dimensions, as well as engineering problems of varied complexity with up to 15 dimensions. We show that the proposed method requires fewer sampling points than conventional methods to obtain a desired accuracy, or provides more accuracy for a fixed budget of sampling points. In some cases, we get models that are over three times more accurate than previously developed surrogate models for the same computational time, and over 3200 times faster than standard gradient-enhanced kriging models for the same accuracy. This work was submitted to a journal and was recently accepted subject to minor revisions. We have also applied it to wing aerodynamic shape optimization.

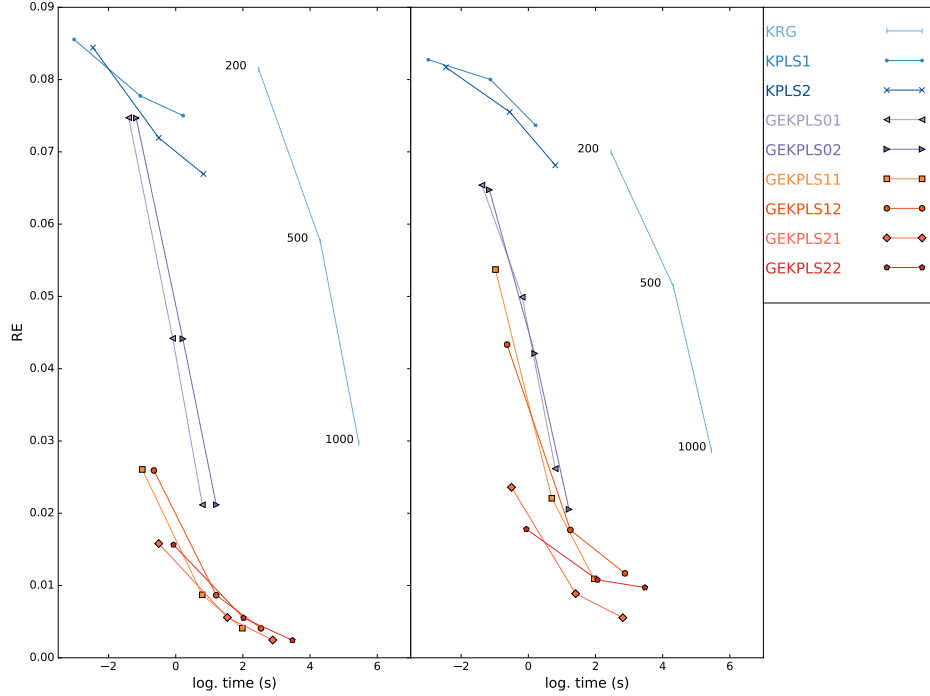


Figure 37: RE versus CPU time using the 9 surrogate models involved for 100-dimensional functions y_1 (left) and y_2 (right) based on 30 trials. Three points are plotted for each surrogate model corresponding to the number of sampling points: 200, 500, 1000, respectively.

4.11.2 SMT: Surrogate Modeling Toolbox

The surrogate modeling toolbox (SMT) is a Python package that contains a collection of surrogate modeling methods, sampling techniques, and benchmarking functions. This package aims to provide a library for surrogate modeling that is simple, both to use and to implement a new method. SMT is different from existing surrogate modeling libraries because of its emphasis on derivatives, including training derivatives used for gradient-enhanced modeling, prediction derivatives, and derivatives with respect to the training data. It also includes new surrogate models that are not available elsewhere: kriging by partial-least squares reduction (GE-KPLS) and energy-minimizing spline interpolation. SMT is documented using custom tools for embedding automatically-tested code and dynamically-generated plots, to produce high-quality user guides with minimal effort for contributors. It is distributed under the New BSD license and is available from GitHub³. New methods are being developed as mixture of experts and multifidelity models using a bridge function. We are currently preparing a paper on this toolbox .

4.11.3 Surrogate-based Airfoil Design Optimization

Since the MURI topic calls for multiple sources of information, we decided that airfoil design was a great application because of the large amount and variety of data that is available. This provided

³<https://github.com/SMTorg/SMT>

a way to demonstrate the gradient-enhanced surrogate modeling that we developed.

Airfoils are of great importance in aerodynamic design, and there is a need for tools that can evaluate and optimize their performance. Existing tools are usually either accurate or efficient, but not both. This paper presents a tool that can analyze airfoils in both subsonic and transonic regimes in about one hundredth of a second, and optimize airfoil shapes in a few seconds. We use camber and thickness mode shapes derived from over one thousand existing airfoils to parameterize the airfoil shape, which reduces the number of design variables. More than one hundred of thousand RANS evaluations associated with different airfoils and flow conditions (M , α) are selected in a well-defined way to obtain aerodynamic coefficients (C_l , C_d and C_m) and their gradients. The gradients for the RANS evaluations are computed using an adjoint method. This data is used to train a surrogate model that combines gradient-enhanced kriging, partial least squares (GE-KPLS), and mixture of experts. Two global models composed of dozens of GE-KPLS models are constructed in the subsonic and transonic regimes. These surrogate models provide fast aerodynamic analysis and gradient computation, which are coupled with a gradient-based optimizer to perform rapid airfoil shape design optimization. In a validating test of 2741 airfoils and 989 airfoils in the subsonic and transonic regimes, the mean differences of the surrogate models from RANS evaluations in the drag coefficient are 0.09 and 0.8 counts, respectively. We also validate the airfoil optimization for various cases by comparing with drag minimization based on direct RANS analysis. The largest differences in C_d are 0.04 counts for subsonic cases, and 2.5 counts for transonic cases. This approach opens the door for interactive airfoil analysis and design using any modern computer or mobile device.

Figure 38 shows a planned interactive airfoil design optimization tool using any modern computer or mobile device is in construction. On the other hand, this tool could be considered as one level of fidelity and used jointly with other airfoil design tools into a multifidelity framework. Furthermore, other source information in addition to the gradient would be integrated to improve the accuracy of surrogate models. We presented this work at the AIAA SciTech Conference.

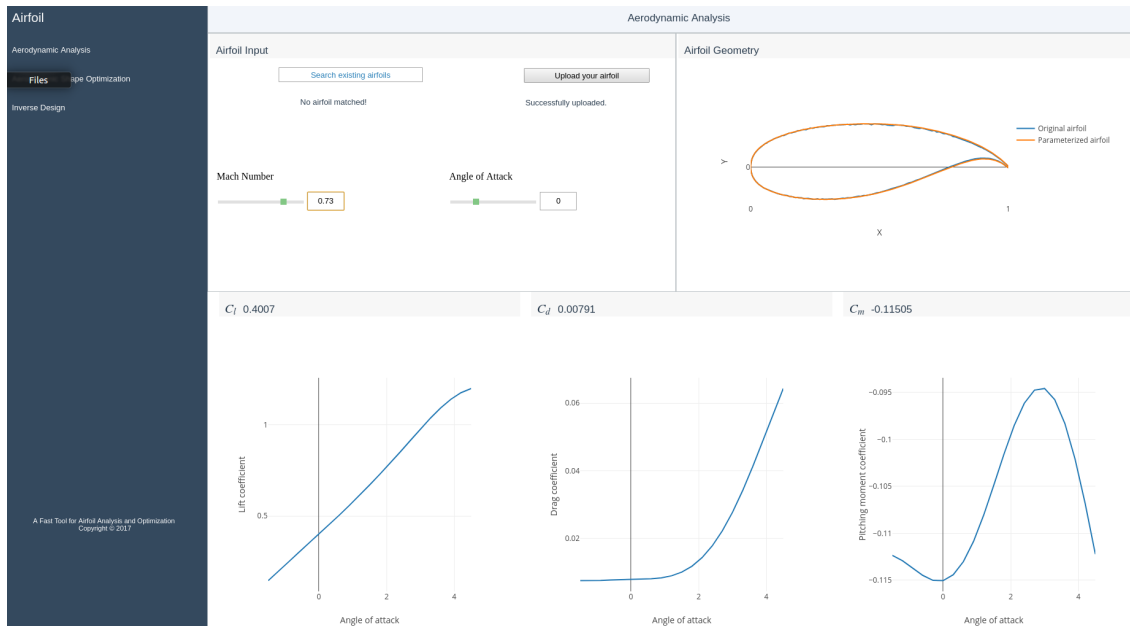


Figure 38: Airfoil design optimization tool graphical user interface.

4.11.4 MDO Benchmark

To perform research on multidisciplinary design optimization (MDO), it is useful to have accessible software that runs quickly, allowing hands-on exploration of coupled systems and optimization methods. Open-source software exists for low-fidelity aerodynamic or structural analysis, but there is no existing software for fast tightly coupled aerostructural analysis and design optimization. To address this need, we present OpenAeroStruct, an open-source low-fidelity aerostructural analysis and optimization tool developed in NASA’s OpenMDAO framework. It uses the coupled adjoint method to compute the derivatives required for efficient gradient-based optimization. OpenAeroStruct combines a vortex lattice method and 1-D finite-element analysis to model lifting surfaces, such as aircraft wings and tails, and uses the coupled-adjoint method to compute the aerostructural derivatives. We use the Breguet range equation to compute on-design aerostructural performance and do not consider off-design or maneuver conditions. OpenAeroStruct has proved effective both as an educational tool and as a benchmark for researching new MDO methods. There is much more potential to be exploited as the research community continues to develop this tool.

This work was submitted to a journal and is it currently accepted subject to minor revisions. OpenAeroStruct has been used in various applications within the MURI, including work on multi-fidelity optimization under uncertainty of a tailless aircraft in collaboration with MIT presented at the AIAA SciTech Conference.

4.12 Deep Neural Networks-enabled Webfoil v2.0

4.12.1 Multi-Fidelity Surrogate-Based Airfoil Design Optimization

In CFD-based airfoil shape optimization, different sources of information, including both experimental and simulation data, are available. Therefore, airfoil shape optimization problems are an excellent example for multiple information source optimization (MISO). In addition, gradient information can be calculated efficiently for the simulation data using adjoint methods, which provides and additional set of information. We demonstrated the performance of a novel gradient-enhanced surrogate modeling method on airfoils design and analysis problems for both subsonic and transonic regimes. When comparing the surrogate-based optimization with optimization based on direct RANS evaluations (ADflow, CFD-RANS, coupled with pyOptSparse), the largest differences in minimum C_d are 0.04 counts for subsonic cases and 2.5 counts for transonic cases. We then created an interactive application for airfoil analysis and design. This work has been published as a conference paper and as a peer-review journal paper.

To extend this application to multi-fidelity airfoil design and analysis problems we developed an web application, Webfoil, that serves as an airfoil database with both experimental and numerical results. Webfoil is available at <http://mdolab.engin.umich.edu/webfoil/analysis/>. The numerical results use three different models: Xfoil, ADflow, and an ensemble of gradient-enhanced surrogate models using a clustering technique. Figure 39 shows the interactive airfoil design tool results for three models. Many airfoils also have experimental data collected from various sources, which are also available in Webfoil.

In order to optimize airfoil shapes using all these available information sources, we are working on building a new multi-fidelity optimization framework that exploits the reification method of and new techniques based on machine learning and deep learning. The idea is to use the correlation coefficients of each CFD data computed through the reification method, and integrate them into a loss function that is used for training a deep neural network (DNN). Those coefficients will weight the influence of each training sampling point in the loss function with respect to its correlation to the experimental data. We are using the Sobolev training method that has proved its capability

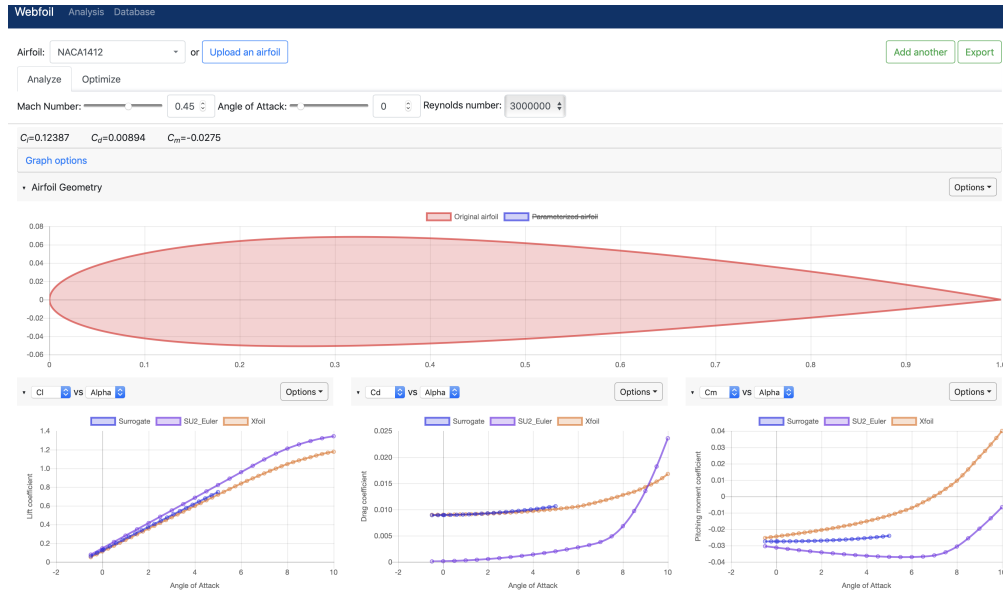


Figure 39: Webfoil is an airfoil database and design optimization tool with a graphical user interface containing three different information sources (<http://mdolab.engin.umich.edu/webfoil/analysis/>).

in training DNN using different kind of information sources. The Sobolev algorithm has been successfully used for training a DNN for both subsonic and transonic cases using two different information sources: the CFD coefficients and their respective gradients. In subsonic case, Figure 40 shows an improvement of two orders of magnitude, in terms of relative error, using DNN with Sobolev training method on the C_d coefficient compared to the GE-KPLS model.

4.12.2 Extension of the Toolbox SMT to Multi-Fidelity Surrogate Modeling

In a previous review for the MURI project, we presented a new Python surrogate modeling toolbox (SMT), which is available at <https://github.com/SMTorg/SMT>. The main distinguishing feature of SMT compared to existing packages is its emphasis on derivatives, including training derivatives used for gradient-enhanced modeling, prediction derivatives, and derivatives with respect to the training data.

Recently, SMT has been extended to multi-fidelity and more complex surrogate modeling using a simple and unique interface. To this end, we created a new interface “extension” into SMT that implements new surrogate modeling techniques: mixture of experts (MOE), which combines several surrogate models together, variable-fidelity modeling (VFM) and multi-fidelity kriging (MFK), which support multi-information sources. These new models implement derivative functions which are of great importance for multi-fidelity optimization problems. A journal manuscript based on this work has been prepared and submitted.

4.12.3 Multi-Fidelity Insitu Scan-Eagle Test Case

To facilitate the exploration and assessment of the methods developed under the MURI project, we developed a multi-fidelity test case bases on the Insitu Scan-Eagle aircraft. Initial work with this model was conducted in OpenAeroStruct. OpenAeroStruct(OAS) is an open-source aerostructural analysis code that uses vortex lattice methods to model the aerodynamics and a beam finite element

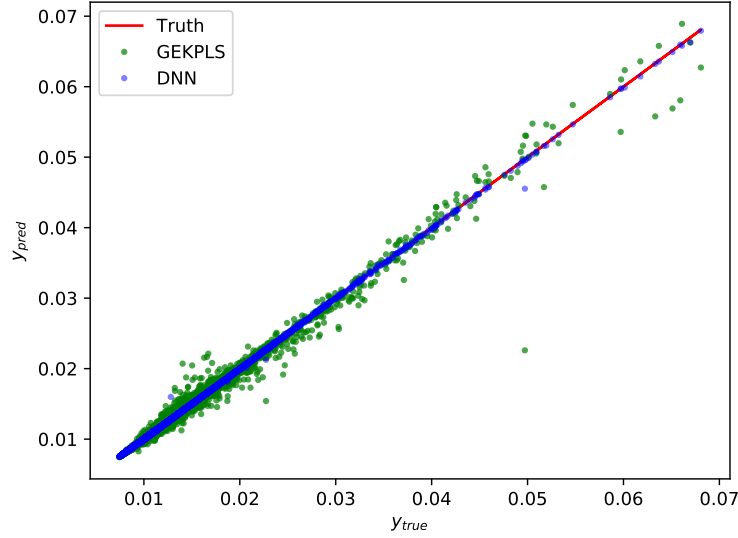


Figure 40: Comparison of the DNN and GE-KPLS models on the C_d coefficient in subsonic case. We observed an improvement in terms of accuracy with DNN: the relative error is 0.488% (DNN) vs 2.923% (GE-KPLS).

code to model the structure. This allows the computations to be light-weight and accessible to a wide variety of research groups. Using this code, we developed a series of models with varying mesh densities. These models were then used to study the methodology for optimization under uncertainty proposed by Chaudhuri.

This work was presented early this year and is now being prepared for submission to a journal. A sample of this work is shown in Figure 41.

Following on this work, we developed a high-fidelity version of the model for the MACH framework. This model, shown in Figure 42 with its key geometric parameters, uses RANS CFD to simulate the flow over the aircraft and shell finite elements to simulate a tubular spar in the wing.

An initial study was conducted with this model and the optimization under uncertainty method of. Initial results from this work, shown in Figure 43 demonstrated that it was possible to run about 20 high-fidelity simulations per optimization iteration. This is far less than the thousands of samples needed to converge the Monte-Carlo uncertainty methods used in the optimization, which highlights the need for a multi-fidelity method. Work is currently underway to extend this work to a full multi-fidelity optimization including both the MACH and OAS models.

4.13 Deep Neural Networks-enabled Webfoil v3.0

Webfoil⁴ is a web-based airfoil design tool that also serves as a database that contains information and numerical data for each airfoil. We built up the Webfoil v1.0 using the gradient-enhance kriging with partial least squares surrogate models, and upgraded it to the Webfoil v2.0 enabled by deep neural networks which achieved a higher level of accuracy. We recently made the new sets of surrogate models ready for the next generation of Webfoil, Webfoil v3.0. In addition to the functionality of the previous versions, Webfoil v3.0 increases the number of geometric design variables for higher flexibility (especially in the transonic regime), incorporates continuous Reynolds number of a broad range and adds the new feature of predicting pressure coefficient distributions of

⁴<http://webfoil.engin.umich.edu>

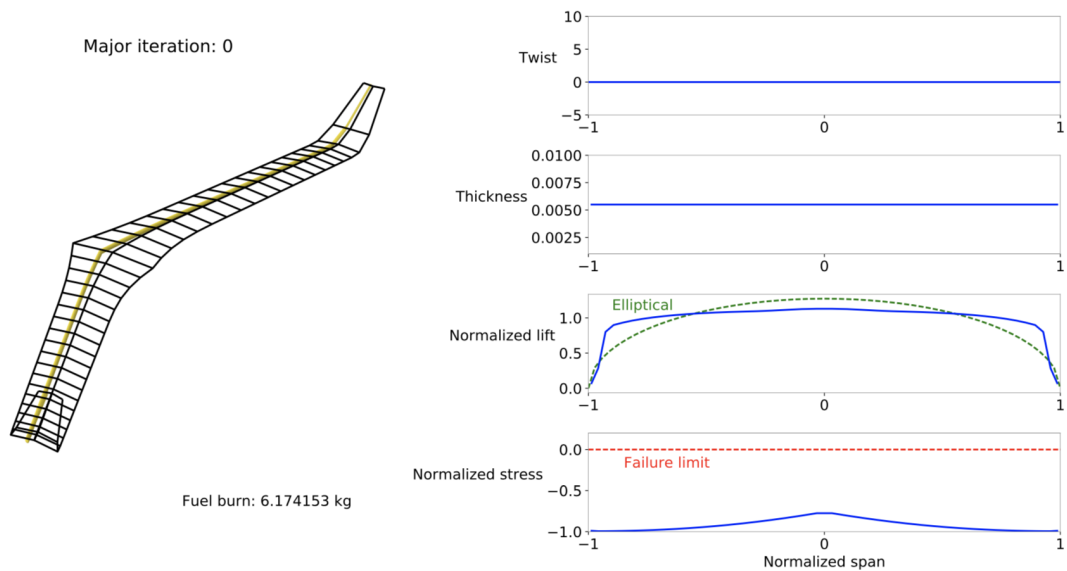


Figure 41: Sample results from the OAS study using the optimization under uncertainty method of.

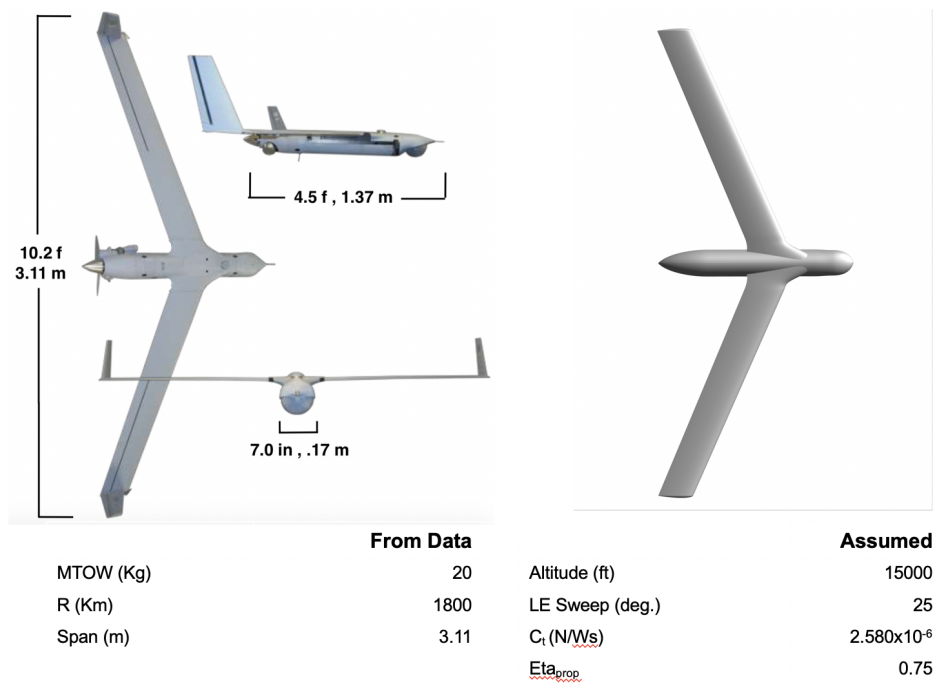


Figure 42: Overview of the geometry for the MACH Scan Eagle model.

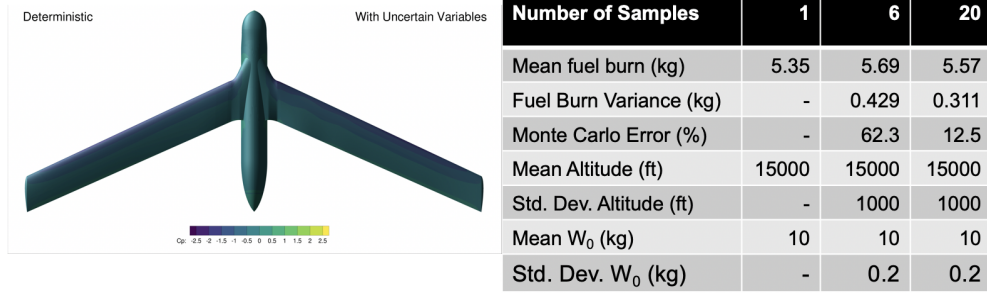


Figure 43: Initial high-fidelity results from the MACH Scan Eagle model.

baseline and optimal designs. To achieve these goals, we developed and implemented the following techniques as summarized in the remainder of this section.

4.13.1 B-Spline-based Generative Adversarial Networks

We developed the unique B-spline-based generative adversarial networks (BSplineGAN) to intelligently parameterize airfoil shapes (Fig. 44). Specifically, BSplineGAN generates only realistic airfoils after the simultaneous training of the generator and discriminator. The generator reads user-defined input parameters $\mathbf{c}$ (each element follows $\mathcal{U}(0, 1)$) and $\mathbf{z}$ (each element follows $\mathcal{N}(0, 0.5^2)$) and generates random airfoil shapes ($\mathbf{g}$). The discriminator reads $\mathbf{g}$ and existing airfoil shapes ($\mathbf{e}$) of a post-processed airfoil database and output the probability of $\mathbf{g}$ coming from the existing database ($\mathbf{p}_g$), the probability of $\mathbf{e}$ from the existing database, and the distribution ($Q_{c|e}$) for approximating the real distribution $P_{c|e}$. The training of the generator aims at leading $\mathbf{p}_g$ to $\mathbf{1}$ by tuning $\mathbf{w}_g$ such that $\mathbf{g}$ have very similar data pattern as $\mathbf{e}$. In contrast, the training of the discriminator targets at leading $\mathbf{p}_g$ to $\mathbf{0}$ (tuning $\mathbf{w}_g$) and $\mathbf{p}_e$ to $\mathbf{1}$ (tuning $\mathbf{w}_d$) such that the discriminator can successfully differentiate $\mathbf{g}$ and $\mathbf{e}$. The competition between the generator and the discriminator results in the $\mathbf{p}_g$ and $\mathbf{p}_e$ values of $\mathbf{0.5}$ within the whole $\mathbf{c} - \mathbf{z}$ space meaning that the discriminator cannot differentiate $\mathbf{g}$ and $\mathbf{e}$ because they have very similar data patterns. The distribution $Q_{c|e}$ formulates the lower bound of the mutual information between $\mathbf{c}$ and $\mathbf{e}$

$$L_1(\mathbf{w}_g, \mathbf{w}_d) = \mathbb{E}_{\mathbf{g} \sim P_G(\mathbf{c}, \mathbf{z})} [\mathbb{E}_{\mathbf{c}' \sim P(\mathbf{c}|\mathbf{e})} [\log Q(\mathbf{c}'|\mathbf{e})]] + \text{const}, \quad (6)$$

where $P_{G(\mathbf{c}, \mathbf{z})}$ is the distribution of generated airfoil shapes. Thus, we maximize the mutual information between $\mathbf{c}$ and $\mathbf{e}$ by maximizing the lower bound such that $\mathbf{c}$ exert the most global control on the airfoil shapes while $\mathbf{z}$ add minor effects (Fig. 45).

Note that the generator has a B-spline layer as the last one layer to guarantee smoother generated airfoil shapes. In particular, we use two B-spline curves to separately parameterize the airfoil upper and lower surfaces. Such parameterization is capable of fixing the positions of leading and trailing edges at the coordinates of $(0, 0)$ and $(1, 0)$, respectively. A parametric study shows that a trained BSplineGAN with 16-element $\mathbf{c}$ and 10-element $\mathbf{z}$ combined with two 18-th order B-spline curves can achieve a mean relative l^1 fitting error of within 1% to reconstruct the airfoils in the existing database. This guarantees the variability of the BSplineGAN model within the $\mathbf{c} - \mathbf{z}$ input space. In the meantime, Fig. 46 shows an obvious parameterization advantage of the trained BSplineGAN model over the direct B-spline parameterization since the BSplineGAN model generates only realistic airfoil shapes.

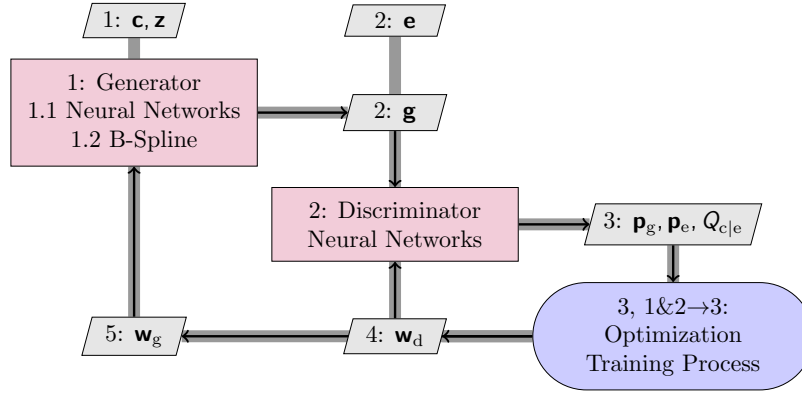
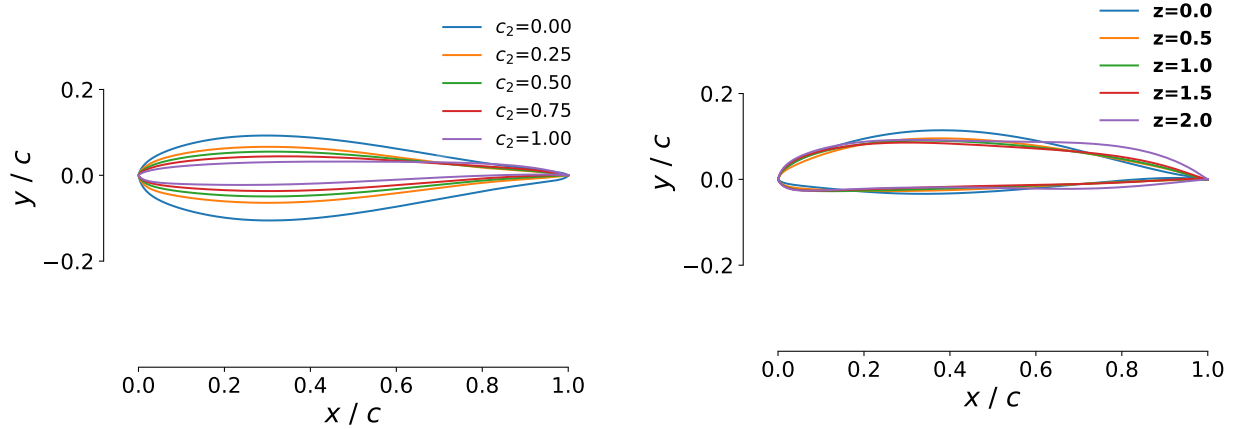


Figure 44: The BSplineGAN model captures salient structured semantic features by maximizing mutual information between existing data and latent variables ($\mathbf{c}$). The B-spline layer within the generator guarantees smooth airfoils. The diagonal nodes are process components and the off-diagonal nodes are the data transferred between components. The thick gray lines represent the data flow, while the black lines represent the processflow.



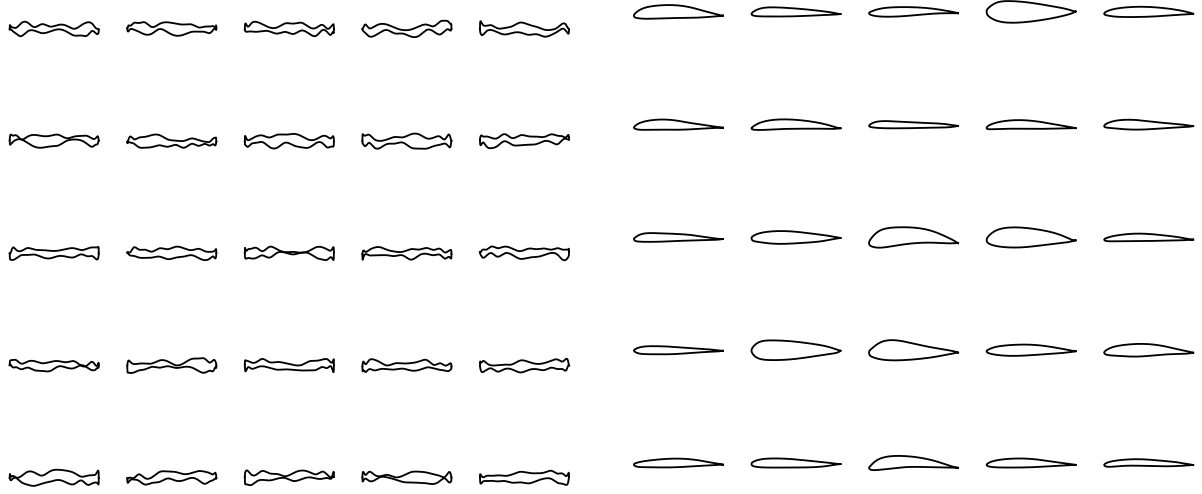
(a) c_2 captures the airfoil thickness variable ($c_0 = c_1 = 1.0, \mathbf{z} = \mathbf{0}$)

(b) $\mathbf{z}$ slightly change the airfoil shapes, but when all elements are greater than 1, the geometric effects are still obvious ($\mathbf{c} = \mathbf{0.5}$)

Figure 45: We train an example BSplineGAN model with $\mathbf{c}$ (3 elements) and $\mathbf{z}$ (10 elements) to investigate the effects on the generated airfoil shapes. We decide to consider both $\mathbf{c}$ and $\mathbf{z}$ when constructing the surrogate models.

4.13.2 Gaussian Copula Dependence Sampling & Infilled Sampling

We investigated the practically used Mach (M) and Reynolds (Re) numbers of typical aircraft (Table 1) and implemented Gaussian copula dependence sampling to address correlation (Fig. 47). Gaussian copula strategy reduces the $M - Re$ space by avoiding unrealistic $M \& Re$ pairs. Plus, Gaussian copula maps standard uniform space into probability space identified by pre-assigned cumulative distribution functions (CDF) via the inverse Nataf transformation process. This feature provides correlation between M and Re and allows each to have any type of probabilistic distribu-



(a) Randomly generated airfoils by B-spline curves of 18-th order with 18 control points on each airfoil surface. (b) Randomly generated airfoils by a BSplineGAN model. We use 18-th order B-spline curves (18 control points on each airfoil surface) as the last one layer of the generator networks.

Figure 46: Comparison of randomly generated shapes between B-spline and BSplineGAN.

tion instead of having to assume Gaussian marginal distributions to apply multivariate Gaussian distributions. In this work, we assign M as $\mathcal{U}(0.3, 0.7)$ and $\log(Re)$ as $\mathcal{U}(4, 10)$. Another flight condition considered is the angle of attack which is set as an independent parameter following the distribution $\mathcal{U}(0.0, 3.0)$ and sampled by Latin hypercube sampling (LHS). Infill sampling extends the small data set while keeping the characteristics of LHS (Fig. 48). Thus, we can enlarge the training data set by an arbitrary number anytime without wasting any completed training sample points. We use the function `augmentLHS` within the R package `lhs` for infilled sampling.

Table 1: Flight condition (M, Re) pairs for a wide range of aircraft.

Aircraft	M	Re	Aircraft	M	Re
Boeing 747	0.67	2×10^9	Cirrus SR22	0.285	4.7×10^6
Airbus A350	0.72	9×10^6	Model airplane	0.105	2.5×10^5
Airbus A320	0.71	2.7×10^6	Jonker JS-3 Rapture	0.087	1.6×10^6
Embraer E190	0.74	2.8×10^6	Paper airplane	0.001	4.7×10^4
Cessna 425	0.426	6.3×10^6			

4.13.3 Deep Neural Network Surrogate Modeling

We constructed two separate sets of deep neural network surrogates for the M ranges of $[0.3, 0.6]$ and $[0.6, 0.7]$. Each set of the deep neural networks contains separate surrogates for drag coefficient (C_d), lift coefficient (C_l), and pressure coefficient distribution (C_p). Specifically, we use multilayer

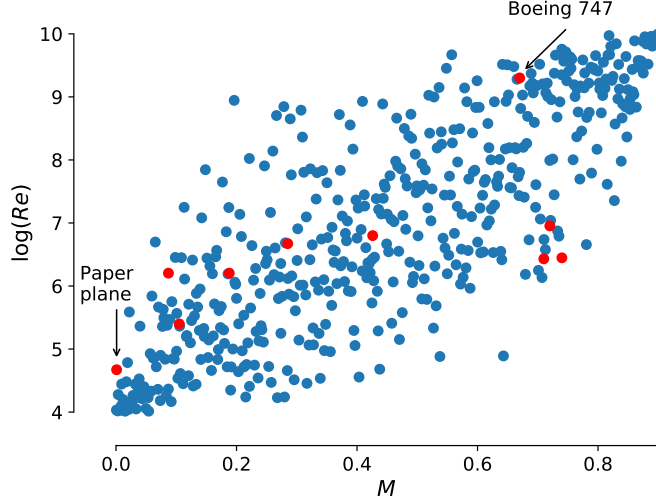
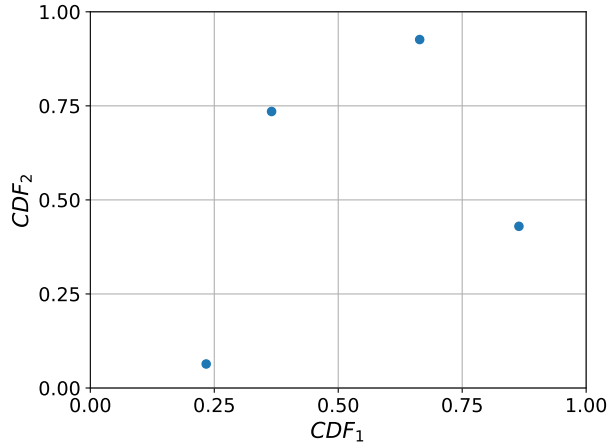
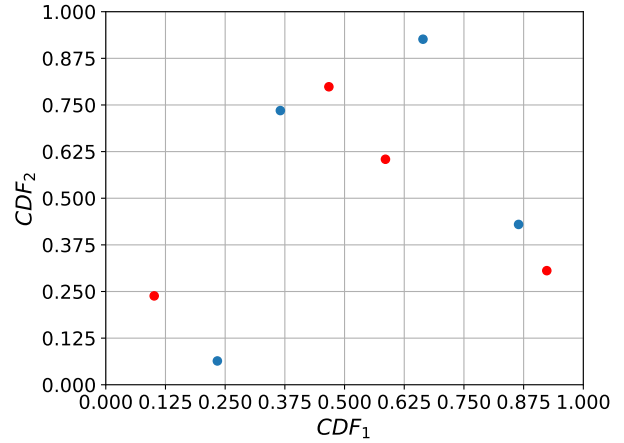


Figure 47: Gaussian copula-generated samples (blue) with a pre-assigned correlation of 0.85 covers typical (M, Re) pairs (red) adequately.



(a) Four initial LHS sample points



(b) Four augmented LHS sample points added to the initial samples

Figure 48: Augmented LHS adds four new LHS points (red) to initial LHS points (blue) by sweeping through columns of the $(4+4) \times (4+4)$ matrix and by generating a random value within an arbitrary empty row at each column sweep as normal LHS method.

perceptron to predict C_d and C_l and long short-term memory recurrent neural networks to predict C_p . We verify the surrogates by calculating the root mean squared error (RMSE) and comparing it with the standard deviation of the testing data set (σ_{test}). We also calculate the relative l^2 error (ϵ) for C_d and C_l and the mean relative l^1 error ($\bar{\epsilon}$) for C_p . Table 2 shows the neural network surrogates of $(C_d$ and $C_l)$ in the subsonic regime match well simulation results and achieve ϵ values of around 2%. The C_p surrogate achieves a RMSE of around 8σ and a $\bar{\epsilon}$ of around 6% which is slightly higher than the C_d and C_l surrogates. This is because the order of the magnitude of C_p is at the level of 1 making the relative error higher, but a closer look into the random C_p predictions in the testing data set shows a good agreement (see Figure 49).

Table 3 shows the surrogate predictive performance in the transonic regime. The predictions

Table 2: Errors for the subsonic surrogate model.

	C_d	C_l	C_p
σ_{test}	56.91	236.00	0.44
RMSE	2.77	12.90	0.0372
$\epsilon / \bar{\epsilon}$ (%)	2.26	2.34	6.13

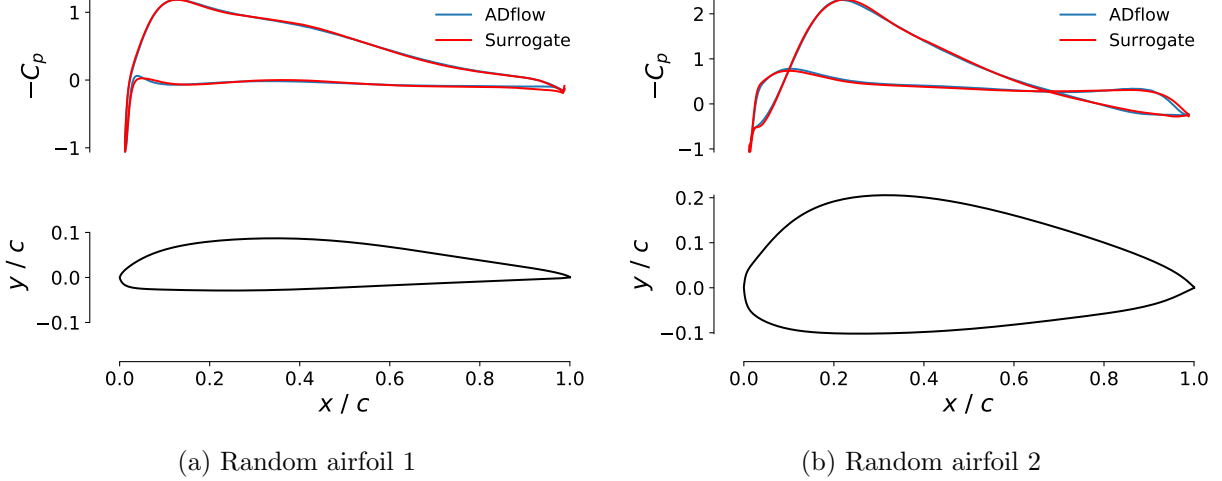


Figure 49: C_p comparison between simulation results and surrogate predictions for random airfoils in testing data set.

on C_d and C_l reach a satisfactory accuracy in terms of RMSE and relative errors, but are not as good as the subsonic surrogates. This is because the high M range ($[0.6, 0.7]$) introduces more nonlinear characteristics into aerodynamic quantities of interest (C_d and C_l). The C_p predictions have a relative error of around 11% which is also larger than the subsonic surrogate. Figure 50 shows that the surrogate model matches well with the simulation results in general but slightly smooths out shock wave.

Table 3: Errors for the transonic surrogate model.

	C_d	C_l	C_p
σ_{test}	126.67	238.74	0.51
RMSE	8.76	16.13	0.084
$\epsilon / \bar{\epsilon}$ (%)	4.65	2.87	11.72

4.13.4 Numerical Examples of Aerodynamic Optimization

We tested a series of aerodynamic optimization cases to verify the surrogate-based optimization and obtained good agreement on optimal designs and corresponding predictions of aerodynamic quantities. Here we show a subsonic case and a transonic case as examples (Table 4). Both cases minimize C_d by varying BSplineGAN variables and angle of attack under a Re of 6.5×10^6 . The subsonic case has a C_l^* of 0.4, M of 0.6, and six thickness constraints evenly distributed within the x coordinates $[0.01, 0.99]$. In contrast, the transonic case targets at $C_l^* = 0.6$ with $M = 0.7$ and sets 100 evenly distributed thickness constraints.

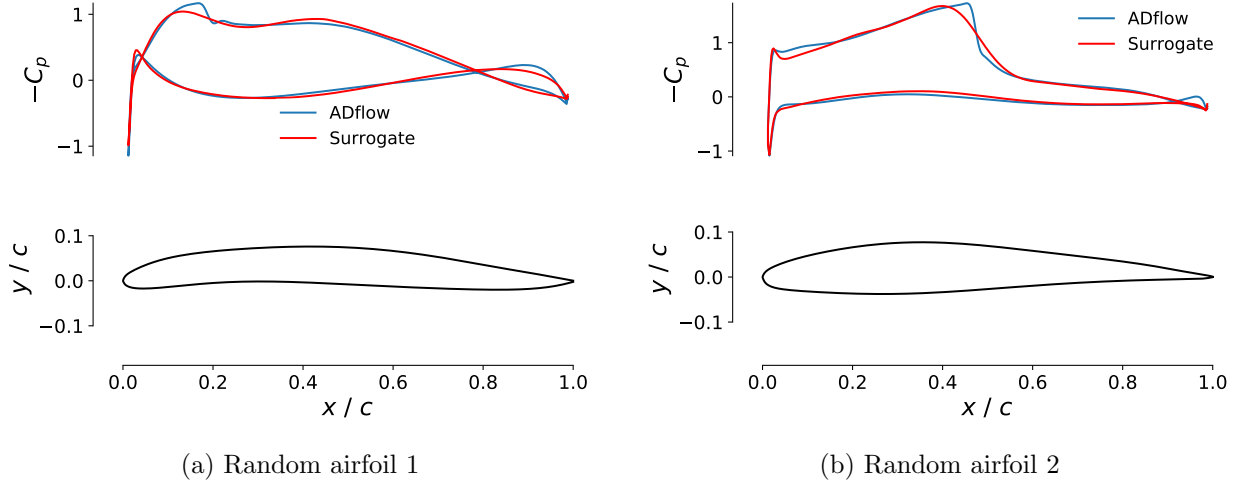


Figure 50: Transonic regime C_p comparison between simulation results and surrogate predictions for random airfoils in testing data set.

Figure 51 shows that surrogate-based optimization finds almost the same optimal design as the direct-simulation-based optimization. Plus, the surrogate prediction on the baseline shape (NACA 0012) has a ~ 0.4 count difference with the simulation results (Table 5). And the difference on the optimal design obtained by the surrogate-based optimization is ~ 2.2 counts. Both predictive differences match the RMSE calculated during verification. The C_p distribution predictions of baseline and optimal designs match very well with simulations results and provide richer optimization information (Fig. 52).

The surrogate-based optimization and C_p prediction takes around three seconds using one-processor on a personal desktop computer. In contrast, the simulation-driven optimization integrated with adjoint solver for gradient information requires around one hour using 48 processors on a high-performance computing (HPC) cluster.

In the transonic case, Fig. 53 shows a good match on the optimal designs between the surrogate-based and the direct-simulation-based optimizations. We can obtain a supercritical optimal airfoil shape to improve the aerodynamic performance (lower drag and weaker shock) under a M of 0.7. Table 6 shows that the differences between the surrogate-predicted and simulation-based C_d ($C_l^* =$

Table 4: Airfoil optimization problem formulation.

	Function or variable	Description	Quantity
minimize	C_d	Drag coefficient	
w.r.t.	$\mathbf{x}$	BSplineGAN variables	26
	α	Angle of attack	1
		Total design variables	27
subject to	$C_l^* = 0.4, 0.6$	Lift-coefficient constraint	1
	$0.8\mathbf{t}_{\text{base}} \leq \mathbf{t} \leq 3.0\mathbf{t}_{\text{base}}$	Thickness constraints	6 or 100
		Total constraints	7 or 101
Conditions	$M = 0.6, 0.7$	Mach number	
	$Re = 6.5 \times 10^6$	Reynolds number	

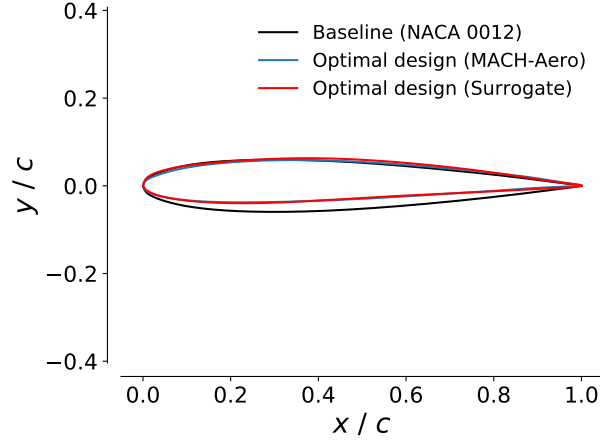


Figure 51: Comparison of optimal airfoils for the surrogate-based and direct-simulation-based optimizations starting from a NACA 0012 baseline.

Table 5: Comparison of baseline and optimized C_d and C_l computed by surrogates and simulation of the subsonic case (1 count = 10^{-4}).

	C_d (counts)	C_l
Baseline (Surrogate)	87.98	0.4
Optimized (Surrogate)	79.59	0.4
Baseline (Simulation)	88.34	0.4
Optimized (Simulation)	81.75	0.4

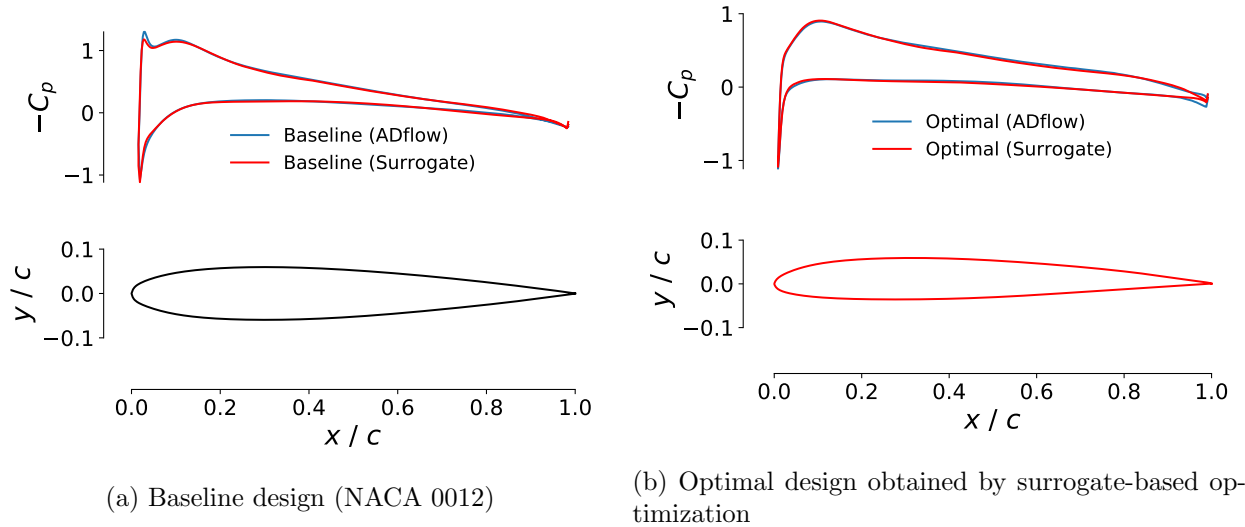


Figure 52: Comparison of C_p distributions for simulation and surrogate for this subsonic case.

0.6) on the baseline and optimal designs are 4.5 counts and 1 count, respectively. The predictive performance agrees with the verification RMSE of the testing data set, but is not as good as the subsonic case because of the nonlinearity in the transonic regime. The C_p prediction shows good agreement with the simulation results along the lower airfoil surface and most parts of the upper

surface. The minor differences happen on the upper airfoil surface near the fore section because shock normally happens in that region. The general predictive performance of the subsonic surrogates is sufficient to achieve satisfactory optimal designs, although the predictive accuracy is not as good as subsonic surrogates due to the nonlinearity.

Similarly as the subsonic surrogate-based optimization and C_p prediction, the whole process takes only around three seconds using one core on a desktop machine. In contrast, the simulation-based optimization integrated with adjoint solver for gradient information requires twice as much time as the subsonic case (around two hours using 48 processors on an HPC cluster).

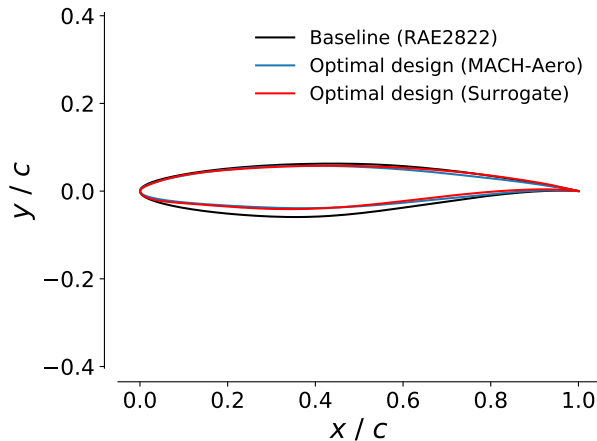


Figure 53: Optimal airfoils for the surrogate-based and direct-simulation-based optimizations both starting from a RAE 2822 baseline are compared.

Table 6: Comparison of baseline and optimized C_d and C_l computed by surrogates and simulation of the transonic case (1 count = 10^{-4}).

	C_d (counts)	C_l
Baseline (Surrogate)	117.66	0.6
Optimized (Surrogate)	85.55	0.6
Baseline (CFD)	113.11	0.6
Optimized (CFD)	86.55	0.6

4.14 Multifidelity method for locating aeroelastic flutter boundaries

In [55], we introduce a multifidelity method that can produce accurate estimates of the flutter boundary at a reduced cost by combining information from low- and high-fidelity aeroelastic models. Estimating the flutter boundary in the presence of non-linear aerodynamic phenomena is challenging because high-fidelity aeroelastic models are expensive to evaluate, and flutter analysis requires many model evaluations. On the other hand, relatively inexpensive approximate aeroelastic models (low-fidelity models) exist and are routinely applied to reduce the cost of estimating flutter, albeit with lower accuracy. The multifidelity method introduced here uses an active learning algorithm to leverage information from low-fidelity models. A multifidelity statistical surrogate is used to fit damping coefficient estimates computed with different aeroelastic models. This surrogate is used to estimate the uncertainty in the prediction of the flutter boundary, which drives the selection of new

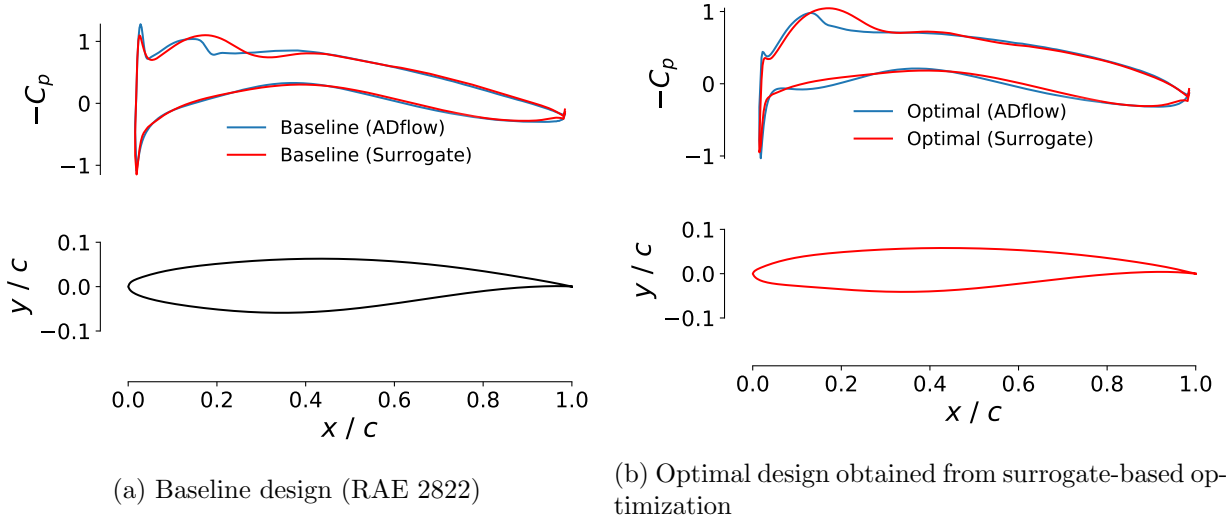


Figure 54: Comparison of C_p distributions from CFD and surrogate model for this transonic case.

evaluations. The multifidelity method proposed here is based on CLoVER (**C**ontour **L**ocation **V**ia **E**ntropy **R**eduction) [56], an active learning algorithm that combines information from multiple models to locate the zero contour of an expensive-to-evaluate function. In the case of aeroelastic flutter analysis, one wants to locate the flutter boundary, which corresponds to the zero contour of the aeroelastic damping coefficient.

The effectiveness of the multifidelity method is demonstrated by estimating the aeroelastic flutter boundary of a typical section model at a cost 85% lower when compared to the bisection method. Four aeroelastic models are considered: three models (including the high-fidelity model) use a computational fluid dynamics solver based on the Euler equations, whereas one model uses a two-dimensional doublet-lattice method. The evolution of the predicted flutter boundary with sequential sampling through the multifidelity method is shown in Figure 55.

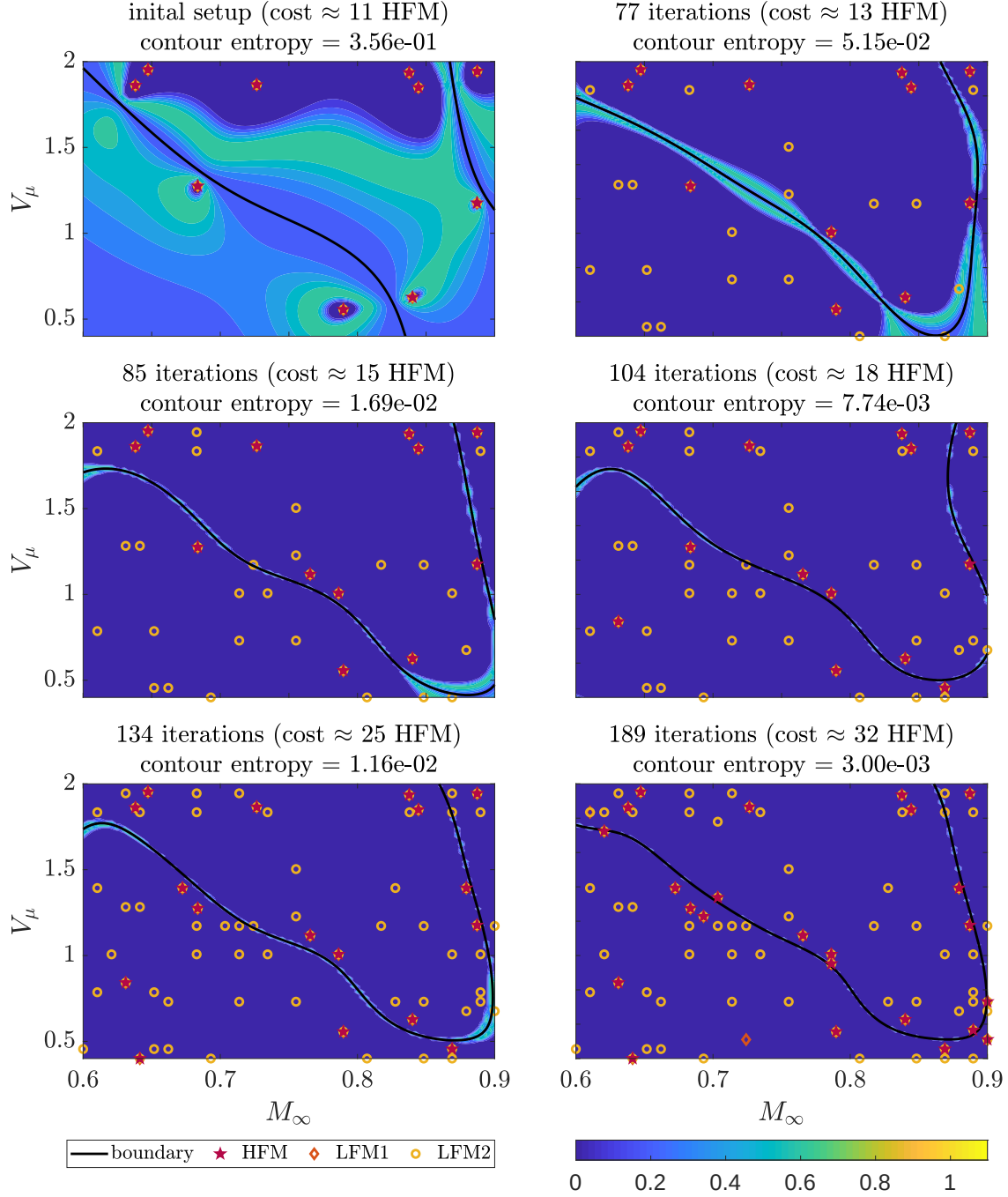


Figure 55: Locating the flutter boundary of the Isogai case A problem. Each plot shows the estimates of the multifidelity method for different iterations. The solid black line is the aeroelastic flutter boundary estimated by the multifidelity method. The contours show the local value of the entropy $\mathbf{H}(\mathbf{W}_x)$. The symbols are evaluations made with the different aeroelastic models.

5 Publications

5.1 Journal papers accepted or appearing during reporting period

2021

- Chaudhuri, A., Marques, A., Willcox, K., mfEGRA: Multifidelity Efficient Global Reliability Analysis through Active Learning for Failure Boundary Location, Structural and Multidisciplinary Optimization, 2021 (to appear).
- Kramer, B., and Willcox, K., Balanced Truncation Model Reduction for Lifted Nonlinear Systems. In Realization and Model Reduction of Dynamical Systems, Springer, 2021 (to appear).
- Mignolet, M.P., and Soize, C., Compressed Principal Component Analysis of Non-Gaussian Vectors, To appear, SIAM/ASA Journal on Uncertainty Quantification.
- Song, P., Wang, X.Q., and Mignolet, M.P., Applications of Multifidelity Reduced Order Modeling To Single And Multiphysics Nonlinear Structural Problems, Applications in Engineering Science, Vol. 5, pp. 100035.1-100035.11, 2021.
- Wang, X.Q., Liao, Y., and Mignolet, M.P., Uncertainty Analysis of Piezoelectric Vibration Energy Harvesters Using a Finite Element Level-Based Maximum Entropy Approach, ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems Part B: Mechanical Engineering, Vol. 7, pp. 010906-1 - 010906-15, Mar. 2021.

2020

- Benner, P., Goyal, P., Kramer, B., Peherstorfer, B. & Willcox, K. Operator inference for non-intrusive model reduction of systems with non-polynomial nonlinear terms. Computer Methods in Applied Mechanics and Engineering, 372, 2020.
- Bouhlel, M. A., He, S. and Martins, J. R. R. A. Scalable gradient-enhanced artificial neural networks for airfoil shape design in the subsonic and transonic regimes. Structural and Multidisciplinary Optimization. 61:1363–1376, March 2020. doi: 10.1007/s00158-020-02488-5.
- Cook, L.W., Willcox, K.E. and Jarrett, J.P., Design optimization using multiple dominance relations. International Journal for Numerical Methods in Engineering, 121(11), pp.2481-2502, 2020.
- Chaudhuri, A., Kramer, B. and Willcox, K.E., Information Reuse for Importance Sampling in Reliability-Based Design Optimization. Reliability Engineering & System Safety, 201, p.106853, 2020.
- Couperthwaite, R., Molkeri, A., Khatamsaz, D., Srivastava, A., Allaire, D., and Arroyave, R., Materials Design Through Batch Bayesian Optimization with Multisource Fusion, JOM, 72(12):4431-4443, 2020.
- Khatamsaz, D., Peddareddygar, L., Friedman, S., and Allaire, D., Bayesian Optimization of Multi Objective Functions Using Multiple Information Sources, AIAA Journal, accepted for publication, 2020.

- Khatamsaz, D., Molkeri, A., Couperthwaite, R., James, J., Arroyave, R., Allaire, D., and Srivastava, A., Efficiently Exploiting Process-Structure-Property Relationships in Material Design by Multi-Information Source Fusion, *Acta Materialia*, accepted for publication, 2020.
- Lam, R., Zahm, O., Marzouk, Y., Willcox, K.E., Multifidelity dimension reduction via active subspaces. *SIAM Journal on Scientific Computing*, 42(2), pp.A929-A956, 2020.
- Marques, A., Lam, R., Chaudhuri, A., Opgenoord, M., Willcox, K., A multifidelity method for locating aeroelastic flutter boundaries, *AIAA Journal*, 58(4), pp. 1772-1784, 2020.
- Qian, E., Kramer, B., Peherstorfer, B., and Willcox, K., Lift & Learn: Physics-informed machine learning for large-scale nonlinear dynamical systems. *Physica D: Nonlinear Phenomena*, Volume 406, May 2020, 132401.
- Song, P., Wang, X.Q., Murthy, R., Matney, A.K., and Mignolet, M.P., Nonlinear Geometric Thermoelastic Response of Structures with Uncertain Thermal and Structural Properties, *AIAA Journal*, Vol. 58, No. 8, pp. 3639-3652, 2020.
- Swischuk, R., Kramer, B., Huang, C., and Willcox, K., Learning physics-based reduced-order models for a single-injector combustion process. *AIAA Journal*, Vol. 58, No. 6, June 2020, pp. 2658-2672. Also in *Proceedings of 2020 AIAA SciTech Forum & Exhibition*, Orlando FL, January, 2020.
- J. Wang, S.C. Clark, E. Liu, and P.I. Frazier. Parallel Bayesian Global Optimization of Expensive Functions. *Operations Research*, 2020.

2019

- Bouhlel, M. A., Hwang, M. A., Bartoli, N., Lafage, R., Morlier, J. and Martins, J. R. R. A. A Python surrogate modeling framework with derivatives. *Advances in Engineering Software*, 135:102662, September 2019. doi:10.1016/j.advengsoft.2019.03.005.
- Bouhlel, M. A. and Martins, J. R. R. A. Gradient-enhanced kriging for high-dimensional problems. *Engineering with Computers*, 35:157–173, January 2019. doi: 10.1007/s00366-018-0590-x.
- Cook, L., Mishra, A., Jarrett, J. Willcox, K., Iaccarino, G., Optimization under turbulence model uncertainty for aerospace design, *Physics of Fluids*, Vol. 31, Issue 10, 105111, 2019.
- Frazier, P.I., Henderson, S.G., Waeber, R., Probabilistic Bisection Converges Almost As Quickly As Stochastic Approximation. *Mathematics of Operations Research*, 2019.
- Ghoreishi, S.F., Thomison, W.D. and Allaire, D.L., Sequential Information-Theoretic and Reification-Based Approach for Querying Multi-Information Sources, *Journal of Aerospace Information Systems*, 16(12), pp.575-587, 2019.
- Ghoreishi, S.F., Molkeri, A., Arróyave, R., Allaire, D., Srivastava, A., Efficient use of multiple information sources in material design, *Acta Materialia*, 180, pp.260-271, 2019.
- Ghoreishi, S.F., Friedman, S. and Allaire, D.L., Adaptive dimensionality reduction for fast sequential optimization with gaussian processes, *Journal of Mechanical Design*, 141(7), 2019.
- Ghoreishi, S.F. and Allaire, D., Multi-information source constrained Bayesian optimization. *Structural and Multidisciplinary Optimization*, 59(3), pp.977-991, 2019.

- Isaac, B. and Allaire, D., Expensive black-box optimization via a gold rush policy, American Society of Mechanical Engineers (ASME) Journal of Mechanical Design, 141(3):031401, 2019.
- Li, J., Bouhlef, M. A. and Martins, J. R. R. A. Data-based approach for fast airfoil analysis and optimization. Journal of Aircraft. 57: 581–596, February 2019. doi: 10.2514/1.J057129.
- Peherstorfer, B. & Marzouk, Y. A transport-based multifidelity preconditioner for Markov chain Monte Carlo. Advances in Computational Mathematics, 45:2321-2348, 2019.
- Peherstorfer, B. Multifidelity Monte Carlo estimation with adaptive low-fidelity models. SIAM/ASA Journal on Uncertainty Quantification, 7:579-603, 2019.
- Song, P., and Mignolet, M.P., Maximum Entropy-Based Uncertainty Modeling at the Elemental Level in Linear Structural and Thermal Problems, *Computational Mechanics*, Vol 64, No. 6, pp 1557–1566, 2019.

2018

- Baptista, R., Marzouk, Y., Willcox, K. & Peherstorfer, B. Optimal Approximations of Coupling in Multidisciplinary Models. AIAA Journal, 56:2412-2428, 2018.
- Chaudhuri, A., Lam, R. and Willcox, K. Multifidelity Uncertainty Propagation via Adaptive Surrogates in Coupled Multidisciplinary Systems. AIAA Journal, Vol. 56, No. 1, pp. 235-249, 2018, <https://dx.doi.org/10.2514/1.J055678>.
- Cook, L., Jarrett, J. and Willcox, K. Extending Horsetail Matching for Optimization Under Probabilistic, Interval and Mixed Uncertainties, AIAA Journal, Vol. 56, No. 2, pp. 849-861, 2018.
- Cook, L., Jarrett, J. and Willcox, K. Generalized information reuse for optimization under uncertainty with non-sample average estimators, International Journal for Numerical Methods in Engineering, Volume 115, Issue 12, pp. 1457-1476, September 2018.
- Frazier, P.I., Bayesian Optimization, INFORMS Tutorials, 2018. <https://arxiv.org/abs/1807.02811>
- Ghoreishi, S.F., Molkeri, A., Srivastava, A., Arroyave, R., and Allaire, D., Multi-information source fusion and optimization to realize ICME: application to dual phase materials, American Society of Mechanical Engineers (ASME) Journal of Mechanical Design, 140(11): 111409, 2018.
- Herbol, H.C., Hu, W., P.I. Frazier, Clancy, P., Poloczec, M. Efficient Search of Compositional Space for Hybrid Organic-Inorganic Perovskites via Bayesian Optimization. Computational Materials, 4, 2018.
- Hwang, J. T. and Martins, J. R. R. A. A computational architecture enabling modular coupling and differentiation of heterogeneous numerical models. International Journal for Numerical Methods in Engineering, 44:1–39, June 2018. doi: 10.1145/3182393.
- Jasa, J. P. and Hwang, J. T. and Martins, J. R. R. A. Open-source coupled aerostructural optimization using Python. Structural and Multidisciplinary Optimization. 57:1815–1827, April 2018. doi: 10.1007/s00158-018-1912-8.

- Peherstorfer, B., Kramer, B. & Willcox, K. Multifidelity preconditioning of the cross-entropy method for rare event simulation and failure probability estimation. *SIAM/ASA Journal on Uncertainty Quantification*, 6(2):737-761, 2018.
- Peherstorfer, B., Gunzburger, M. & Willcox, K. Convergence analysis of multifidelity Monte Carlo estimation. *Numerische Mathematik*, 139(3):683-707, 2018.
- Peherstorfer, B., Willcox, K. & Gunzburger, M. Survey of multifidelity methods in uncertainty propagation, inference, and optimization. *SIAM Review*, 60(3):550-591, 2018.
- Song, P., and Mignolet, M.P., Reduced Order Model-Based Uncertainty Modeling of Structures with Localized Response, *Probabilistic Engineering Mechanics*, Vol. 51, pp. 42-55, 2018.
- Tallorin, L., Wang, J., Kim, W.E., Sahu, S., Kosa, N.M., Yang, P., Thompson, M.C., Gilson, M.K., Frazier, P.I., Burkart, M.D., and Gianneschi N.C., Discovering *de novo* peptide substrates for enzymes using machine learning. *Nature Communications*, 2018.
- Yang, P., Iyer K., and Frazier, P.I., Mean Field Equilibria for Resource Competition in Spatial Settings. *Stochastic Systems*, 2018.
- Zimmermann, R., Peherstorfer, B. and Willcox, K. Geometric Subspace Updates with Applications to Online Adaptive Nonlinear Model Reduction, *SIAM Journal on Matrix Analysis and Applications*, Vol. 39, No. 1, pp. 234-261, 2018.

2017

- Ghoreishi, S.F., and Allaire, D., Adaptive uncertainty propagation for coupled multidisciplinary systems, *American Institute of Aeronautics and Astronautics (AIAA) Journal*, Vol. 55, No. 11, pp. 3940-3950, 2017.
- W. Han, P. Rajan, P.I. Frazier, and B.M. Jedynak. Probabilistic Group Testing under Sum Observations: A Parallelizable 2-Approximation for Entropy Loss. *IEEE Transactions on Information Theory*, vol 63, issue 2, pp 915–933, 2017.
- Peherstorfer, B., Kramer, B. & Willcox, K. Combining multiple surrogate models to accelerate failure probability estimation with expensive high-fidelity models. *Journal of Computational Physics*, 341:61-75, 2017.
- M. Poloczek and D. P. Williamson. An experimental evaluation of fast approximation algorithms for the maximum satisfiability problem. *ACM Journal of Experimental Algorithmics (JEA)* 22 (1), 1.6, 2017.

2016

- P.I. Frazier and J. Wang. Bayesian optimization for materials design. *Information Science for Materials Discovery and Design*, Springer Series in Materials Science. 225, pp. 45-75, 2016.
- Hwang, J. T. and Martins, J. R. R. A. A fast, robust interpolant for scattered multivariate data using regularized minimal-energy tensor-product splines. *ACM Transactions on Mathematical Software*, 2016.
- Peherstorfer, B., Willcox, K. & Gunzburger, M. Optimal model management for multifidelity Monte Carlo estimation. *SIAM Journal on Scientific Computing*, 38(5):A3163-A3194, 2016.

- Peherstorfer, B. & Willcox, K. Dynamic data-driven model reduction: Adapting reduced models from incomplete data. *Advanced Modeling and Simulation in Engineering Sciences*, 3(11), 2016.
- S.N. Pallone, P.I. Frazier, and S.G. Henderson. Coupled Bisection for Root Ordering. *Operations Research Letters*, 2016.
- J. Xie, P.I. Frazier, and S.E. Chick. Bayesian Optimization via Simulation with Pairwise Sampling and Correlated Prior Beliefs. *Operations Research*, 64(2), pp. 542-559, 2016.

2015

- S.J. Gershman, P.I. Frazier, D.M. Blei: Distance Dependent Infinite Latent Feature Models, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 37, no. 02, pp 334-345, 2015.
- I.O. Ryzhov, P.I. Frazier, and W.B. Powell: A New Optimal Stepsize for Approximate Dynamic Programming, *IEEE Transactions on Automatic Control*, vol. 60, no. 03, pp 743-758, 2015.
- B. Yang, C. Cardie, P.I. Frazier: A Hierarchical Distance-dependent Bayesian Model for Event Coreference Resolution, *Transactions of the Association for Computational Linguistics*, vol. 3, pp 517-528, 2015.

5.2 Journal papers in preparation or submitted

- Alsup, T. & Peherstorfer, B. Context-aware surrogate modeling for balancing approximation and sampling costs in multi-fidelity importance sampling and Bayesian inverse problems. arXiv:2010.11708, 2020. (*submitted*)
- Cashore, J.M. , Kumarga, L. and Frazier, P.I. Multi-Step Bayesian Optimization for One-Dimensional Feasibility Determination. (in revision for *Journal of Machine Learning Research*)
- Chaudhuri, A., Kramer, B., Norton, M., Royset, J.O. and Willcox, K., Certifiable Risk-Based Engineering Design Optimization. *AIAA Journal*, 2021, arXiv preprint arXiv:2101.05129.
- Du, X., He, P. and Martins, J. R. R. A. Rapid Airfoil Design Optimization via Neural Network-based Parameterization and Surrogate Modeling. *Aerospace Science and Technology*, 2020 (submitted).
- Kapteyn, M., Pretorius, J. and Willcox, K., A Probabilistic Graphical Model Foundation for Enabling Predictive Digital Twins at Scale. arXiv preprint arXiv:2012.05841, 2020. (*submitted*)
- J. Karandikar, A. Chaudhuri, K. Willcox, S. Smith, BORisk: Bayesian optimization imitating human risk preference, 2021. (in preparation)
- Rim, D., Peherstorfer, B. & Mandli, K.T. Manifold approximations via transported subspaces: Model reduction for transport-dominated problems. arXiv:1912.13024, 2019. (*submitted*)
- Qian, E., Farcas, I., and Willcox, K., Reduced operator inference for nonlinear partial differential equations. arXiv preprint arXiv:2102.00083, 2021. (*submitted*)

- Song, P., Wang, X.Q., and Mignolet, M.P., Maximum Entropy Uncertainty Modeling at the Finite Element Level for Heated Structures, *Mechanical Systems and Signal Processing*, Submitted.
- Song, P., Matney, A.K., Wang, X.Q., and Mignolet, M.P., Adaptive Reduced Order Models for Coupled Nonlinear Structural and Thermal Problems, *Computational Mechanics*, In Preparation.
- Toscano-Palmerin S. and Frazier, P.I., Bayesian Optimization with Expensive Integrands, <https://arxiv.org/abs/1803.08661> (in revision for SIAM Journal on Optimization)

5.3 Conference papers accepted or appearing during the reporting period

2020

- Du, X., He, P. and Martins, J. R. R. A. A B-Spline-based Generative Adversarial Network Model for Fast Interactive Airfoil Aerodynamic Optimization. AIAA SciTech Forum, January 2020. doi:10.2514/6.2020-2128.
- Drmac, Z. & Peherstorfer, B. Learning low-dimensional dynamical-system models from noisy frequency-response data with Loewner rational interpolation. Realization and Model Reduction of Dynamical Systems: A Festschrift in Honor of the 70th Birthday of Thanos Antoulas, Springer, 2020.
- Cortinovis, A., Kressner, D., Massei, S. & Peherstorfer, B. Quasi-optimal sampling to learn basis updates for online adaptive model reduction with adaptive empirical interpolation. In American Control Conference (ACC) 2020, IEEE, 2020.
- Chaudhuri, A., Peherstorfer, B. & Willcox, K. Multifidelity Cross-Entropy Estimation of Conditional Value-at-Risk for Risk-Averse Design Optimization. In AIAA Scitech 2020 Forum, AIAA, 2020.
- Khatamsaz, D. and Allaire, D., A Comparison of Reification and CoKriging for Sequential Multi-Information Source Fusion, AIAA SciTech Forum, 2020.
- Khatamsaz, D., Peddareddygar, L., Friedman, S., and Allaire, D., Efficient Multi-Information Source Multiobjective Bayesian Optimization, AIAA SciTech Forum, AIAA-2127-2020, Orlando, FL, 2020.
- Wang, X.Q., Song, P., and Mignolet, M.P., Applications Of Multifidelity Reduced Order Modeling To Single And Multiphysics Problems, *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2020)*, Orlando, Florida, Jan.6-10, 2020, AIAA Paper AIAA-2020-2131.
- Chaudhuri, A., Norton, M. and Kramer, B., Risk-based design optimization via probability of failure, conditional Value-at-Risk, and buffered probability of failure. In AIAA Scitech 2020 Forum (p. 2130), 2020.

2019

- Marques, A., Lam, R., Chaudhuri, A., Opgenoord, M., Willcox, K., A multifidelity method for locating aeroelastic flutter boundaries, 21st AIAA Non-deterministic Approaches Conference (AIAA Scitech), San Diego, CA, 2019.

- Chaudhuri, A., Marques, A., Lam, R., Willcox, K., Reusing information for multifidelity active learning in reliability-based design optimization, 21st AIAA Non-deterministic Approaches Conference (AIAA Scitech), San Diego, CA, 2019.
- Bartoli, N., Meliani, M., Morlier, J., Lefebvre, T., Bouhlel, M.A. and Martins, J. R. R. A. Multi-fidelity efficient global optimization: Methodology and application to airfoil shape design. In AIAA Aviation Forum, June 2019. doi:10.2514/6.2019-3236.
- Imani, M., Ghoreishi, S.F., Allaire, D. and Braga-Neto, U.M., MFBO-SSM: Multi-fidelity Bayesian optimization for fast inference in state-space models, In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 33, pp. 7858-7865), 2019.
- Song, P., Wang, X.Q., and Mignolet, M.P., Maximum Entropy Structural-Thermal Uncertainty Modeling at the Finite Element Level, *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2019)*, San Diego, California, Jan.7-11, 2019, AIAA Paper AIAA-2019-0443.
- Song, P., Wang, X.Q., and Mignolet, M.P., Nonlinear Reduced ROMs: Formulation and Applications, *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2019)*, San Diego, California, Jan.7-11, 2019, AIAA Paper AIAA-2019-1020.
- Astudillo, R., Frazier, P.I., Bayesian Optimization of Composite Functions, International Conference on Machine Learning (ICML), 2019.
- Wu, J., Frazier, P.I., Practical Two-Step Lookahead Bayesian Optimization, Neural Information Processing Systems (NeurIPS), 2019.
- Wu, J., Toscano, S., Wilson, A.G., Frazier, P.I., Practical Multi-fidelity Bayesian Optimization of Iterative Machine Learning Algorithms, Conference on Uncertainty in Artificial Intelligence (UAI), 2019.
- Yang, P., Iyer, K., Frazier, P.I., Information Design in Spatial Resource Competition, The 15th Conference on Web and Internet Economics (WINE), 2019.

2018

- Li, J., Bouhlel, M. A. and Martins, J. R. R. A. A Data-based Approach for Fast Airfoil Analysis and Optimization. 19th AIAA/ISSMO Multidisciplinary Design Optimization: Metamodeling and Approximation Methods, January 2018. doi: 10.2514/6.2018-1383.
- Chaudhuri, A., Jasa, J., Martins, J. R. R. A. and Willcox, K. Multifidelity Optimization Under Uncertainty for a Tailless Aircraft. 20th AIAA Non-deterministic Approaches Conference (AIAA Scitech), Kissimmee, FL, 2018. doi: 10.2514/6.2018-1658.
- Peherstorfer, B., Beran, P.S. & Willcox, K. Multifidelity Monte Carlo estimation for large-scale uncertainty propagation. In 2018 AIAA Non-Deterministic Approaches Conference, AIAA, 2018.
- Lam, R., Poloczek, M. Frazier, P. Willcox, K. Advances in Bayesian Optimization with Applications in Aerospace Engineering. In Proc. of the 2018 AIAA Non-Deterministic Approaches Conference, AIAA SciTech Forum, 2018.

- Marques, A., Lam, R. and Willcox, K. Contour location via entropy reduction leveraging multiple information sources. *Advances In Neural Information Processing Systems (NeurIPS)* 31, 2018.
- Ghoreishi, S.F. and Allaire, D. A fusion-based multi-information source optimization approach using knowledge gradient policies, *AIAA SciTech Forum*, AIAA-1159-2018, Kissimmee, FL, January, 2018.
- Ghoreishi, S.F., and Allaire, D. Gaussian process regression for Bayesian fusion of multi-fidelity information sources, *AIAA Aviation Forum*, AIAA-4176-2018, Atlanta, GA, June, 2018.
- Isaac, B., Friedman, S., and Allaire, D. Efficient approximation of coupling variable fixed point sets for decoupling multidisciplinary systems, *AIAA SciTech Forum*, AIAA-1908-2018, Kissimmee, FL, January, 2018.
- Song, P., and Mignolet, M.P., Maximum Entropy-Based Uncertainty Modeling at the Finite Element Level, *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2018)*, Kissimmee, Florida, Jan. 8-12, 2018, AIAA Paper AIAA-1657.
- Toscano-Palmerin S., and Frazier, P.I., Effort Allocation and Statistical Inference for 1-Dimensional Multistart Stochastic Gradient Descent, *Winter Simulation Conference (WSC)*, 2018.
- Chen, B., Frazier P.I., and Kempe D., Incentivizing Exploration with Heterogeneous Preferences *Conference on Learning Theory (COLT)*, 2018.
- Baptista, R. and Poloczek, M. Bayesian Optimization of Combinatorial Structures. In the *Proc. of the Thirty-fifth International Conference on Machine Learning (ICML)*, 2018.

2017

- Baptista, R., Marzouk, Y., Willcox, K. & Peherstorfer, B. Optimal Approximations of Coupling in Multidisciplinary Models. In *58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*, AIAA, 2017.
- Lam, R., and Willcox, K. Lookahead Bayesian Optimization with Inequality Constraints. In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 1888-1898, 2017.
- R. Morrison, R. Baptista, and Y. Marzouk. Beyond normality: Learning sparse probabilistic graphical models in the non-Gaussian setting. In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 2356-2366, 2017.
- S. Friedman, S.F. Ghoreishi, and D. Allaire. Quantifying the Impact of Different Model Discrepancy Formulations in Coupled Multidisciplinary Systems, *AIAA SciTech Forum*, AIAA-1950-2017, Grapevine, TX, January, 2017.
- W.D. Thomison, and D. Allaire. A Model Reification Approach to Fusing Information from Multifidelity Information Sources, *AIAA SciTech Forum*, AIAA-1949-2017, Grapevine, TX, January, 2017.

- Song, P., and Mignolet, M.P., Reduced Order Model-Based Uncertainty Modeling of Structures with Localized Response, *Proceedings of the 2nd International Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2017)*, Rhodes Island, Greece, 15–17 June 2017.
- Song, P., Wang, X.Q., Matney, A., Murthy, R., Mignolet, M.P., Nonlinear Geometric Thermoelastic Response of Structures with Uncertain Thermal and Structural Properties, *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2017)*, Dallas, Texas, Jan. 9-13, 2017, AIAA Paper AIAA 2017-0181.
- J. Wu, M. Poloczek, A. Wilson, and P.I. Frazier. Bayesian Optimization with Gradients. Neural Information Processing Systems (NeurIPS), 2017.
- M. Poloczek, J. Wang, and P.I. Frazier. Multi-Information Source Optimization. Neural Information Processing Systems (NeurIPS), 2017.
- S. Toscano-Palmerin, and P.I. Frazier. Stratified Bayesian Optimization. Proceedings of the 12th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC), 2017.
- N. Dong, D. Eckman, M. Poloczek, X. Zhao, and S. Henderson. Comparing the Finite-Time Performance of Simulation-Optimization Algorithms. In Proc. of Winter Simulation Conference (WSC), pp. 2206-2217, 2017.
- B. Chen, P.I. Frazier. Dueling Bandits with Weak Regret. International Conference on Machine Learning (ICML), 2017.
- R. Astudillo Marban and P.I. Frazier. Multi-Attribute Bayesian Optimization under Utility Uncertainty. NeurIPS Workshop on Bayesian Optimization (BayesOpt 2017), 2017.
- J. Wu and P.I. Frazier. Continuous-Fidelity Bayesian Optimization with Knowledge Gradient. NeurIPS Workshop on Bayesian Optimization (BayesOpt 2017), 2017.

2016

- Chaudhuri, A., and Willcox, K.E. Multifidelity uncertainty propagation for coupled multidisciplinary systems. 18th AIAA Non-Deterministic Approaches Conference, AIAA Science and Technology Forum and Exposition, San Diego, CA, January 2016.
- Lam, R.R., Willcox, K.E. and Wolpert, D.H., Bayesian optimization with a finite budget: An approximate dynamic programming approach. In Proceedings of the 30th International Conference on Neural Information Processing Systems (pp. 883-891), 2016.
- S.F. Ghoreishi and D. Allaire. Compositional uncertainty analysis via importance weighted Gibbs sampling for coupled multidisciplinary systems, AIAA SciTech Forum, AIAA-2016-1443, San Diego, CA, January, 2016.
- S. Friedman, and D. Allaire. Quantifying model discrepancy in coupled multi-physics systems. ASME 2016 International Design Engineering Technical Conferences, IDETC2016-59948, August, 2016.
- S.F. Ghoreishi, and D. Allaire, Compositional uncertainty analysis via importance weighted Gibbs sampling for coupled multidisciplinary systems, AIAA SciTech Forum, AIAA-2016-1443, San Diego, CA, January, 2016.

- P. Yang, K. Iyer, and P.I. Frazier. Mean Field Equilibria for Competitive Exploration in Resource Sharing Settings. WWW, 2016.
- J. Wu and P.I. Frazier. The Parallel Knowledge Gradient Method for Batch Bayesian Optimization, Neural Information Processing Systems (NeurIPS), 2016.
- T. Schnabel, T. Joachims, A. Swaminathan, and P.I. Frazier. Unbiased Concurrent Evaluation on a Budget. 2nd ACM International Conference on the Theory of Information Retrieval (ICTIR), 2016.
- M. Poloczek, and D. P. Williamson. An Experimental Evaluation of Fast Approximation Algorithms for the Maximum Satisfiability Problem. International Symposium on Experimental Algorithms (SEA), 2016.
- M. Poloczek, J. Wang, and P.I. Frazier. Warm Starting Bayesian Optimization. Winter Simulation Conference, 2016.
- W. Hu, and P.I. Frazier. Bayes-Optimal Effort Allocation in Crowdsourcing: Bounds and Index Policies. AISTATS 2016.
- B. Chen and P.I. Frazier. The Bayesian Linear Information Filtering Problem. IEEE International Conference on Tools with Artificial Intelligence (ICTAI), 2016.

2015

- S. Toscano-Palmerin and P.I. Frazier: Asymptotic Validity of the Bayes-Inspired Indifference Zone Procedure: the Non-Normal Known Variance Case, Winter Simulation Conference, 2015.
- D. Singhvi, S. Singhvi, P.I. Frazier, S.G. Henderson, E. O’Mahony, D.B. Shmoys and D.B. Woodard: Predicting Bike Usage for New York City’s Bike Sharing System, AAAI-15 Workshop on Computational Sustainability, 2015.
- P. Rajan, W. Han, R. Sznitman, P.I. Frazier, B.M. Jedynak: Bayesian Multiple Target Localization, International Conference on Machine Learning (ICML), 2015.

6 Presentations

2021

- Chaudhuri, A. A Generalized Multifidelity Framework for Active Learning Gaussian-Process-Based Reliability Analysis, SIAM CSE, 2021.
- Khatamsaz, D., A Comparison of Reification and CoKriging for Sequential Multi-Information Source Fusion, AIAA SciTech Forum, January 2021.
- Mignolet, M.P., and Soize, C., Non-Gaussian Vectors Modeling by Compressed Principal Component Analysis, *Presented at the 14th World Congress on Computational Mechanics*, Paris, France, in virtual, Jan. 11-15, 2021.
- Willcox, K. "Aerospace Design in the Age of Big Data and Big Compute." Invited Plenary Talk, AIAA SciTech Forum & Exhibition, January 2021.

2020

- Chaudhuri, A. Multifidelity Adaptive Experimental Design and Optimization Under Uncertainty, Facebook Adaptive Experimentation Workshop, NY, Feb 13, 2020.
- Chaudhuri, A. Risk-Based Design Optimization Via Probability of Failure, Conditional Value-at-Risk, and Buffered Probability of Failure, AIAA Scitech 2020, Orlando, FL, 2020.
- Peherstorfer, B. A biased introduction to projection-based model reduction. In Descriptors of Energy Landscapes Using Topological Data Analysis Seminar Series, online, 2020.
- Peherstorfer, B. Quasi-optimal sampling to learn basis updates for online adaptive model reduction with adaptive empirical interpolation. In American Control Conference (ACC) 2020, Denver, CO, 2020.
- Peherstorfer, B. Context-aware learning of surrogate models for multi-fidelity computations. In Computational Uncertainty Quantification: Mathematical Foundations, Methodology & Data, Vienna, Austria, 2020.
- Peherstorfer, B. Multifidelity Cross-Entropy Estimation of Conditional Value-at-Risk for Risk-Averse Design Optimization. In AIAA SciTech 2020, Orlando, FL, 2020.
- Khatamsaz, D., Efficient Multi-Information Source Multiobjective Bayesian Optimization, AIAA SciTech Forum, Orlando, FL, January 2020.
- Du, X., He, P. and Martins, J. R. R. A. A B-Spline-based Generative Adversarial Network Model for Fast Interactive Airfoil Aerodynamic Optimization. AIAA SciTech Forum, January 2020.
- Martins, J. R. R. A. Exploiting aircraft electrification via multidisciplinary design optimization. Aircraft Structural Design Conference, Royal Aeronautical Society (virtual event), Oct 2020. (Keynote presentation)
- Martins, J. R. R. A. Enabling large-scale multidisciplinary design optimization through the coupled-adjoint method. National Conference on Multidisciplinary Design, Analysis & Optimization, Trivandrum, India (virtual event), Oct 2020. (Keynote presentation)
- Martins, J. R. R. A. Multidisciplinary Design Optimization for the Next Generation of Aircraft. The 60th Israel Annual Conference on Aerospace Sciences, Tel-Aviv & Haifa, Israel, Mar 2020. (Plenary presentation)
- Willcox, K. "A technology roadmap towards Digital Thread." Invited talk, Panel on Multidisciplinary Design Optimization & Model-based Systems Engineering, AIAA Scitech Forum, Orlando, FL, January 2020
- Willcox, K. "Challenges and progress in learning physics-based reduced models for combustion processes." Invited plenary talk, Workshop on Exuberance of Machine Learning in Transport Phenomena, Dallas, TX, February 2020.
- Willcox, K. "Predictive data science: From physics-based models to scientific machine learning." Shell Lecture (invited), Rice University, February 2020.
- Willcox, K. "Predictive Digital Twins & Multifidelity Modeling." Invited talk, Lockheed Martin Aeronautics, Dallas, TX, February 2020.

- Willcox, K. "Predictive data science: From physics-based models to scientific machine learning." Invited talk, ICERM Workshop on the Mathematics of Model Reduction, Providence, RI, February 2020.
- Willcox, K. "Towards Predictive Data Science: From Scientific Machine Learning to Digital Twins." Keynote Talk, Women in Data Science (WiDS) Conference, Austin, TX, March 2020.
- Willcox, K. "Scientific Machine Learning: Where physics-based modeling meets data-driven learning." Invited Talk, Santa Fe Institute Colloquium, May 2020.
- Willcox, K. "Predictive digital twins: Where data-driven learning meets physics-based modeling." Invited Plenary Talk, Workshop on Learning for Dynamics and Control (L4DC), June 2020.
- Willcox, K. "Scientific Machine Learning: Where data-driven learning meets physics-based modeling." Keynote Talk, JuliaCon, July 2020.
- Willcox, K. "Toward predictive digital twins: From physics-based modeling to scientific machine learning." Keynote Talk, ASME Design Automation Conference, August 2020.
- Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, University of Pennsylvania, October 2020.
- Willcox, K. Invited Panelist, Mathematical Foundations Panel. Sandia National Laboratories Trusted AI Roundtable, October 2020.
- Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, Texas A&M University, October 2020.
- Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk at Workshop on Physics-guided AI to Accelerate Scientific Discovery, AAAI Fall Symposium, November 2020.
- Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." ECE Distinguished Lecture at George Washington University, December 2020.
- Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Workshop on Machine Learning for Engineering Modeling, Simulation, and Design. Neural Information Processing Systems (NeurIPS), December 2020.

2019

- Peherstorfer, B. Recovering (certified) reduced models from data with operator inference and time-domain Loewner. In European Numerical Mathematics and Advanced Applications Conference, Amsterdam, Netherlands, 2019.
- Peherstorfer, B. Multifidelity Uncertainty Quantification. In Multifidelity Modeling (MFM) Workshop, AIAA Aviation, Denver, CO, 2019.
- Peherstorfer, B. Data generation and time-delay corrections for learning reduced models with operator inference. In Physics Informed Machine Learning Workshop, Seattle, WA, 2019.

- Peherstorfer, B. Learning reduced dynamical-system models from data via operator inference and Loewner interpolation. In Oden Institute for Computational Engineering and Sciences (ICES), University of Texas at Austin, Austin, TX, 2019.
- Chaudhuri, A., Multifidelity methods in optimization under uncertainty: fusing models and reusing information, NASA Goddard Special Seminar, Greenbelt, Maryland, 2019.
- Chaudhuri, A., Information reuse for importance sampling in reliability-based design optimization, USNCCM, Austin, TX, 2019.
- Chaudhuri, A., How to Reuse Information from Optimization History for Efficient Reliability-Based Design Optimization, MIT Aerospace Computational Design Lab Seminar Series, Cambridge, MA, 2019.
- Chaudhuri, A., Information reuse for importance sampling in reliability-based design optimization, East Coast Optimization Meeting, Fairfax, Virginia, 2019.
- Chaudhuri, A., Adaptive multifidelity contour estimation for reliability-based design optimization, SIAM CSE Conference, Spokane, Washington, 2019.
- Marzouk, Y., Johns Hopkins University, USACM workshop on Uncertainty Quantification in Computational Solid and Structural Materials Modeling. Invited speaker. Baltimore, MD, January 2019.
- Marzouk, Y., ExxonMobil, Corporate Strategic Research. Clinton, NJ, January 2019.
- Marzouk, Y., SIAM Conference on Computational Science and Engineering (CSE19). Invited minisymposium. Spokane, WA, February 2019.
- Marzouk, Y., Oberwolfach workshop on Uncertainty Quantification. Oberwolfach, Germany, March 2019.
- Marzouk, Y., INRIA, Laboratoire Jean Kuntzmann. Grenoble, France, April 2019.
- Marzouk, Y., Schlumberger-Doll Research. Cambridge, MA, April 2019.
- Marzouk, Y., Auburn University, Department of Mathematics and Statistics, Colloquium. Auburn, AL, April 2019.
- Marzouk, Y., Worcester Polytechnic Institute, Department of Mathematical Sciences, Colloquium. Worcester, MA, April 2019.
- Marzouk, Y., MIT Laboratory for Information and Decision Systems (LIDS) seminar. Cambridge, MA, April 2019.
- Marzouk, Y., New England Statistics Symposium. Hartford, CT, May 2019.
- Marzouk, Y., Twelfth International Conference on Monte Carlo Methods and Applications (MCM 2019). Invited plenary speaker. Sydney, Australia, July 2019.
- Marzouk, Y., ExxonMobil Upstream Research Company. Houston, TX, October 2019.
- Marzouk, Y., RWTH-Aachen University, School for Simulation and Data Science seminar. Aachen, Germany, October 2019.

- Marzouk, Y., Universität Heidelberg, Department of Mathematics. Heidelberg, Germany, October 2019.
- Willcox, K. "Projection-based model reduction: Physics-based approaches to learn low-dimensional models." Invited Colloquium Talk, Department of Mathematics, University of Houston, February 2019.
- Willcox, K. "Projection-based model reduction: Formulations for Physics-based Machine Learning." Keynote Talk, LANL Workshop on Machine Learning for Computational Fluid and Solid Dynamics, February 2019.
- Willcox, K. "Projection-based model reduction: Formulations for Physics-based Machine Learning." Invited talk, Department of Mathematics, Southern Methodist University, March 2019.
- Willcox, K. "Projection-based model reduction: Formulations for Physics-based Machine Learning." Invited talk, Department of Mathematics, University of Texas at Dallas, March 2019.
- Willcox, K. "Data to Decisions: Computational Methods for the Next Generation of Engineering Systems." Keynote Talk, SIAM Central Valley Regional Student Conference, University of California, Merced, April 2019.
- Willcox, K. "Projection-based model reduction: Formulations for Physics-based Machine Learning." Charlemagne Distinguished Lecture, RWTH Aachen, April 2019.
- Willcox, K. "Data-driven reduced models, model adaptation, and Digital Twins." Invited talk, Lockheed Martin Aeronautics Internal Workshop on Digital Strategy, Fort Worth, TX, June 2019.
- Willcox, K. "Interdisciplinary Research and Education for a Computational Future." Invited talk, Aspen Symposium, Forum on Higher Education, Aspen, CO, June 2019.
- Willcox, K. "Predictive Data Science for Physical Systems: From Model Reduction to Scientific Machine Learning." Keynote Talk, New York Scientific Data Summit, New York, NY, June 2019.
- Willcox, K. "Predictive Data Science for Physical Systems: From Model Reduction to Scientific Machine Learning." Invited Lecture, International Congress on Industrial and Applied Mathematics (ICIAM), Valencia, Spain, July 2019.
- Willcox, K. "Predictive Data Science for Physical Systems: From Model Reduction to Scientific Machine Learning." Invited talk, ONERA Laboratories, Toulouse, France, July 2019.
- Willcox, K. "From Nonlinear Partial Differential Equations to Low-dimensional Models: Physics-based Model Reduction." Invited Plenary Talk, US National Congress on Computational Mechanics (USNCCM), Austin, TX, July 2019.
- Willcox, K. "Predictive data science for physical systems: From model reduction to scientific machine learning." Kalman Lecture, University of Potsdam, Germany, September 2019.
- Willcox, K. "Towards efficient multifidelity modeling for engineering design under uncertainty: From model reduction to scientific machine learning." Invited Keynote, European Numerical Mathematics and Advanced Applications Conference, Egmond aan Zee, The Netherlands.

- Willcox, K. "Predictive data science: From model reduction to scientific machine learning." Invited Keynote Talk, INFORMS Annual Meeting, Seattle, WA, October 2019.
- Willcox, K. "Predictive data science: From model reduction to scientific machine learning." Invited Keynote Talk, SC19, Denver, CO, November 2019.
- Willcox, K. "Multifidelity uncertainty quantification for optimization under uncertainty." Invited Plenary Lecture. Workshop on Uncertainty Quantification, The Australian National University, November 2019.
- Willcox, K. "Big Decisions need more than just Big Data." Invited Keynote Lecture. 23rd International Conference on Modelling and Simulation (MODSIM), Canberra, Australia, December 2019.
- Willcox, K. "Data-centric engineering: From physics-based models to scientific machine learning." Invited talk, International Workshop on Data-Centric Engineering, Cambridge, MA, December 2019.
- Allaire, D., Multifidelity Uncertainty Quantification for Technology Forecasting, ASME IDETC Workshop, Anaheim, CA, August 2019.
- Allaire, D., Prescriptive Analytics for Assess Management via Machine Learning, Petroliaam Nasional Berhad, Kuala Lumpur, Malaysia, July 2019.
- Allaire, D., What Next? Value-Optimal Decision Making for Engineering Analysis and Design, Singapore University of Technology and Design, January 2019.
- Sanghvi, M., Uncertainty Propagation via Probability Measure Optimized Importance Weights with Application to Parametric Materials Models, AIAA SciTech Forum, San Diego, CA, January 2019.
- Martins, J. R. R. A. CFD-based Aircraft Design Optimization. International Conference on Flow Dynamics, Sendai, Japan, Nov 2019. (Plenary presentation)
- Martins, J. R. R. A. Aerodynamic Design Optimization: Methods, Tools, and Applications. Aerodynamic Tools and Design Methods in Aircraft Design Conference, London, UK, Oct 2019. (Plenary presentation)
- Astudillo, R., Bayesian Optimization of Composite Functions, Winter Simulation Conference, National Harbor MD, Dec 2019
- Astudillo, R., Bayesian Optimization of Composite Functions With Application to Computationally Expensive Inverse Problems, Applied Inverse Problems Conference, Grenoble, France, July 2019
- Astudillo, R., Bayesian Optimization of Composite Functions, ICML, Long Beach CA, June 2019.
- Frazier, P.I., Grey-Box Bayesian Optimization for AutoML & More, 6th ICML Workshop on Automated Machine Learning (AutoML 2019), Long Beach CA, June 2019.
- Frazier, P.I., Bayesian Optimization, Two Sigma, New York City NY, June 2019.
- Frazier, P.I., Data Science Lessons from Uber, Pitney Bowes, Shelton CT, May 2019.

- Frazier, P.I., Grey-Box Bayesian Optimization, Industrial and Systems Engineering Department, Georgia Tech, Atlanta, GA, November 2019.
- Frazier, P.I., Grey-Box Bayesian Optimization, School of Computing, Informatics & Decision Systems Engineering, Arizona State University, Tempe AZ, November 2019.
- Frazier, P.I., Grey-Box Bayesian Optimization, Industrial Engineering and Operations Research Department, University of California, Berkeley CA, September 2019.
- Frazier, P.I., Bayesian Optimization for Materials Design, High Entropy Alloys Workshop, Arlington VA, Nov 2019.
- Frazier, P.I., A Tutorial on Partially Observable Markov Decision Processes (POMDPs), AFOSR Grant Review Meeting, Georgia Tech, Atlanta GA, Nov 2019
- Frazier, P.I., Accelerating Scientific Discovery through Interpretable Machine Learning and Intelligent Experimentation, Interpretable Learning in Physical Sciences Workshop, Institute for Pure and Applied Mathematics, UCLA, Los Angeles CA, Oct 2019.
- Frazier, P.I., Industry-related Career Paths in OR” 2019 INFORMS Doctoral Student Colloquium, INFORMS Annual Meeting, Seattle WA, Oct 2019
- Frazier, P.I., Working with Industry” 2019 INFORMS Doctoral Student Colloquium, INFORMS Annual Meeting, Seattle WA, Oct 2019
- Frazier, P.I., Bayesian Optimization for Peptide Design”, INFORMS Annual Meeting, Seattle WA, Oct 2019
- Frazier, P.I., Grey-box Bayesian Optimization” AFOSR Optimization and Discrete Mathematics Program Review, Arlington VA, Aug 2019.
- Frazier, P.I., An Asymptotically Optimal Index Policy For The Finite Horizon Restless Bandit” INFORMS Applied Probability Society Conference, Brisbane Australia, July 2019.
- Frazier, P.I., An Asymptotically Optimal Index Policy For The Finite Horizon Restless Bandit” INFORMS Computing Society Conference, University of Tennessee, Knoxville TN, Jan 2019.
- Frazier, P.I., Bayesian Optimization With Expensive Integrands” INFORMS Computing Society Conference, University of Tennessee, Knoxville TN, Jan 2019.

2018

- Peherstorfer, B. Data-Driven Multifidelity Methods for Monte Carlo Estimation. In Workshop on Big Data Meets Large-Scale Computing, Institute for Pure & Applied Mathematics (IPAM), Los Angeles, CA, 2018. (**invited presentation**)
- Peherstorfer, B. Multifidelity methods and context-aware model reduction for Monte Carlo estimation and beyond. In Seminar Numerische Mathematik, Technical University Berlin, Berlin, Germany, 2018.
- Peherstorfer, B. A Multifidelity Cross-Entropy Method for Rare Event Simulation. In SIAM Uncertainty Quantification 2018, Garden Grove, CA, 2018.

- Peherstorfer, B. Data-Driven Multifidelity Methods for Monte Carlo Estimation. In Model Reduction of Parametrized Systems (MoRePaS) IV, Nantes, France, 2018. (**plenary talk**)
- Peherstorfer, B. Multifidelity Monte Carlo estimation with adaptive low-fidelity models. In Reducing dimensions and cost for UQ in complex systems, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, 2018.
- Peherstorfer, B. Data-Driven Multifidelity Methods for Monte Carlo Estimation. In Engineering Physics Seminars and Colloquium, University of Wisconsin-Madison, Madison, USA, 2018.
- Peherstorfer, B. Multifidelity Monte Carlo estimation for large-scale uncertainty propagation. In 2018 AIAA Non-Deterministic Approaches Conference (AIAA SciTech), Kissimmee, USA, 2018.
- Song, P., and Mignolet, M.P., Maximum Entropy-Based Uncertainty Modeling at the Finite Element Level, *Presented at the 13th World Congress on Computational Mechanics, WCCM2018*, New York, New York, Jul. 22-27, 2018.
- Martins, J. R. R. A. Promise and Challenges of MDO for the Next Generation of Aircraft. AIAA Aviation MDO Keynote, Atlanta, GA, Jun 2018. (Keynote presentation)
- Li, J., Bouhlel, M., and Martins, J. R. R. A. A data-based approach for fast airfoil analysis and optimization. AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Kissimmee, FL, January 2018.
- Chaudhuri, A., Jasa, J., Martins, J. R. R. A. and Willcox, K. Multifidelity Optimization Under Uncertainty for a Tailless Aircraft. 20th AIAA Non-deterministic Approaches Conference (AIAA Scitech), Kissimmee, FL, 2018.
- M. A. Bouhlel, J. Li, and J. R. R. A. Martins. Michigan Institute for Computational Discovery & Engineering (MICDE) 2017 Annual Symposium Student Poster, April 18, 2018.
- Astudillo, R., A Utility Uncertainty Approach to Multiattribute Bayesian Optimization INFORMS Annual Meeting, Phoenix AZ, November 2018.
- Frazier, P., Bayesian Optimization, D.E. Shaw, New York City NY, March 2018.
- Frazier P., Bayesian Optimization for Problems with Exotic Structure, Cornell Center of Applied Mathematics Colloquium, March 2018
- Frazier P.I., Bayesian Optimization with Exotic Structure, SIAM Conference on Discrete Mathematics, Denver CO, May 2018.
- Frazier P.I., Bayesian Optimization in the Tech Sector, School of Industrial Engineering and Management Seminar Series, Oklahoma State University, Stillwater OK, August 2018
- Frazier P.I., Bayesian Optimization in the Tech Sector, Department of Industrial and Operations Engineering, University of Michigan, Ann Arbor MI, September 2018
- Frazier P.I., Bayesian Optimization in the Tech Sector, Management Sciences Guest Lecturer Seminar Series, University of Iowa, Iowa City IA, September 2018

- Frazier P.I., “Bayesian Optimization for Materials Design and Drug Discovery” Science at the Edge, Interdisciplinary Physics Seminar Series, Michigan State University, East Lansing MI, October 2018
- Frazier, P.I., Bayesian Optimization for Problems with Exotic Structure, Data and Decisions 2018, University of Arizona, Tucson AZ, November 2018
- Frazier, P., Incentivizing Exploration by Heterogeneous Users , INFORMS Annual Meeting, Phoenix AZ, November 2018
- Frazier. P., Bayesian Optimization (INFORMS Tutorial), INFORMS Annual Meeting, Phoenix AZ, November 2018
- Frazier, P., An Asymptotically Optimal Index Policy for the Finite Horizon Restless Bandit , INFORMS Annual Meeting, Phoenix AZ, November 2018
- Frazier, P. Bridging the Gap from Academic Research to Industry Impact (**Plenary talk**), Winter Simulation Conference, Gothenburg Sweden, December 2018.
- Messinger, P.R., Bitner, M.J., Frazier, P.I., Megahed, A., Wang, X., Machine Learning Meets Service Dominant Logic (Panel discussion) , 2018 Conference on Service Science (CSS2018), Phoenix AZ, November 2018
- Poloczek, M. Bayesian Optimization of Combinatorial Structures., Data and Decisions, Tucson, USA.
- Poloczek, M. Efficient Global Optimization of Expensive Functions with Applications in Engineering and Machine Learning., Systems and Industrial Engineering Seminar, UofA, Tucson, USA.
- Poloczek, M. Efficient Global Optimization of Expensive Functions in Data Science and Engineering., Data Science Institute, Tucson, USA.
- Poloczek, M. Bayesian Optimization with Applications in Aerospace Engineering., Aerospace and Mechanical Engineering Seminar, UofA, Tucson, USA.
- Poloczek, M. Novel Bayesian Optimization Algorithms for Expensive Functions., Facebook AI, Menlo Park, USA.
- Poloczek, M. Bayesian optimization of combinatorial structures., International Conference on Machine Learning (ICML), Stockholm, Sweden.
- Poloczek, M. Bayesian Optimization of Combinatorial Structures., International Symposium on Mathematical Programming (ISMP), Bordeaux, France.
- Poloczek, M. Bayesian Optimization of Combinatorial Structures with Application to Multi-component Systems., Air Force Research Lab, Dayton, USA.
- Poloczek, M. Cheaper Optimization of Expensive Functions., Uber AI Labs, San Francisco, USA.
- Poloczek, M. Optimal Sparsification of Couplings in Multi-Component Systems via Bayesian Optimization., UA Center for Risk and Reliability, Tucson, USA.

- Poloczek, M. Fast Search for Novel Materials enabled by Transfer Learning., Materials Research Society (MRS) 2018 Spring Meeting & Exhibit, Phoenix, USA.
- Poloczek, M. Multi-Information Source Optimization., INFORMS Optimization Society Conference, Denver, USA.
- Poloczek, M. Multi-Information Source Optimization., U2 can UQ Symposium on Uncertainty Quantification, Tucson, USA.
- Poloczek, M. Bayesian optimization of expensive functions., University of Pittsburgh, Pittsburgh, USA.
- Toscano-Palmerin, S. Effort Allocation and Statistical Inference for 1-Dimensional Multistart Stochastic Gradient Descent, Winter Simulation Conference, Gothenburg Sweden, Dec 2018
- Toscano-Palmerin S., Effort Allocation and Statistical Inference for Multistart Stochastic Gradient Descent, INFORMS Annual Meeting, Phoenix AZ, November 2018
- Toscano-Palmerin S., Bayesian Optimization with Expensive Integrands , INFORMS Annual Meeting, Phoenix AZ, November 2018
- Toscano-Palmerin S., Bayesian Optimization with Expensive Integrands, 23rd International Symposium on Mathematical Programming (ISMP), Bordeaux France, June 2018
- Yang, P., Mean Field Equilibria for Resource Competition in Spatial Settings INFORMS Annual Meeting, Phoenix AZ, November 2018
- Chaudhuri, A. Multifidelity Robust Optimization with Information Reuse. WCCM, New York, NY, July 22-27 2018.
- Chaudhuri, A. Multifidelity Robust Optimization. SIAM UQ Conference, Garden Grove, CA, Apr 16-19, 2018.
- Chaudhuri, A. Multifidelity Optimization Under Uncertainty. 15th Copper Mountain Conference on Iterative Methods. Copper Mountain, CO, Mar 25-30, 2018.
- Chaudhuri, A., Jasa, J., Martins, J.R.R.A., and Willcox, K. Multifidelity Optimization Under Uncertainty for a Tailless Aircraft. 20th AIAA Non-deterministic Approaches Conference (AIAA Scitech), Kissimmee, FL, 2018.
- Cook, L. Generalized Information Reuse for Optimization Under Uncertainty with non-Sample Average Estimators. SIAM UQ Conference, Garden Grove, CA, Apr 16-19 2018.
- Feng, C., and Marzouk, Y. Robust decisions in the presence of unobserved heterogeneity. SIAM Conference on Uncertainty Quantification, Garden Grove, CA, April 2018
- Feng, C., and Marzouk, Y. A Bayesian Framework for Robust Decisions in the Presence of Unobserved Heterogeneity. SAMSI Model Uncertainty: Mathematical and Statistical (MUMS) Workshop, Duke University, August 2018
- Willcox, K. Data to Decisions: Computational methods for the next generation of aerospace systems. Future CFD Technologies Workshop, Orlando, FL, January 2018.

- Willcox, K. Data to Decisions: Computational methods for the next generation of engineering systems. Engineering Product Development Research Seminar Series, Singapore University of Technology and Design, February 2018.
- Willcox, K. Data to Decisions: Computational methods for the next generation of engineering systems. Institute of High Performance Computing A*STAR, Singapore, March 2018.
- Willcox, K. Data-driven operator inference for learning physics-based low-dimensional models. Engineering Systems Design Distinguished Speaker Seminar, Singapore University of Technology and Design, April 2018.
- Willcox, K. Data-driven operator inference for learning physics-based low-dimensional models. Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen, Germany, April 2018.
- Willcox, K. Data to Decisions: Computational methods for the next generation of aerospace systems. Temasek Laboratories, Singapore, May 2018.
- Willcox, K. Data-driven operator inference for learning physics-based low-dimensional models. Hong Kong University, Hong Kong, May 2018.
- Willcox, K. Data to Decisions: Towards the next generation of engineering systems. Design Innovation Workshop, University of Auckland, New Zealand, July 2018.
- Willcox, K. Learning low-dimensional models: Nonlinear model reduction via lifting transformations and proper orthogonal decomposition.
- Willcox, K. Learning low-dimensional models: Nonlinear model reduction via lifting transformations and proper orthogonal decomposition. Workshop on HPC and Data Science for Scientific Discovery, Institute for Pure and Applied Mathematics, October 2018.
- Willcox, K. Learning low-dimensional models: Nonlinear model reduction via lifting transformations and proper orthogonal decomposition. Department of Civil Engineering, Johns Hopkins University, November 2018.
- Willcox, K. Multifidelity approaches for design, uncertainty quantification, and stability boundary location. Institute of High Performance Computing A*STAR, Singapore, November 2018.
- Willcox, K. Lift & Learn: From nonlinear PDEs to low-dimensional polynomial approximations. Lawrence Livermore National Laboratories, December 2018.
- Willcox, K. Lift & Learn: From nonlinear PDEs to low-dimensional polynomial approximations. Sandia National Laboratories, December 2018.
- Marzouk, Y. University of Wisconsin, Systems Information Learning Optimization (SILO) Seminar. Madison, WI. February 2018.
- Marzouk, Y. RIKEN International Workshop on Uncertainty Quantification. Kobe, Japan. February 2018.
- Marzouk, Y. SFB 1294 Spring School on Data Assimilation. Göhren-Lebbin, Germany. March 2018.

- Marzouk, Y. Cambridge University, Isaac Newton Institute for Mathematical Sciences. Workshop on Uncertainty Quantification for Inverse Problems in Complex Systems. Cambridge, England. April 2018.
- Marzouk, Y. SAMSI Workshop on Probabilistic Numerics. London, England. April 2018.
- Marzouk, Y. Notre Dame University. Center for Informatics and Computational Science. South Bend, IN. April 2018.
- Marzouk, Y. Institute for Mathematical Sciences, program on Bayesian Computation for High-Dimensional Statistical Models. Keynote speaker. National University of Singapore. August 2018.
- Marzouk, Y. Duke University, Department of Civil and Environmental Engineering. Durham, NC. October 2018.
- Marzouk, Y. Finnish Meteorological Institute. Helsinki, Finland. October 2018.
- Marzouk, Y. University of Michigan, Michigan Institute for Computational Discovery and Engineering. Ann Arbor, MI. December 2018.

2017

- R. Baptista, Y. Marzouk, B. Peherstorfer, and K. Willcox. Optimal Approximations of Coupling in Multidisciplinary Models, AIAA Scitech Forum, Grapevine, Texas, January 2017.
- R. Baptista, Y. Marzouk, B. Peherstorfer, and K. Willcox. Optimal Approximations of Coupling in Multidisciplinary Models, SIAM Conference on Computational Science and Engineering, Atlanta, GA, March 2017.
- R. Baptista. Review of Uncertainty Quantification and Optimal Approximations of Coupling in Multidisciplinary Models, NASA Glenn Research Center, Cleveland, Ohio, April 2017.
- C. Feng, and Y. Marzouk. A hierarchical Bayesian framework for representing model inadequacy, SIAM Conference on Computational Science & Engineering. Atlanta, GA, March 2017.
- Y. Marzouk. Uncertainty quantification tools and challenges: exploring parameters, models, and data, ANSYS, 2017.
- Y. Marzouk. Bayesian modeling and Bayesian computation, ARL, 2017.
- R. Morrison, R. Baptista, and Y. Marzouk. Learning sparse probabilistic graphical models in the non-Gaussian setting, SIAM Conference on Computational Science & Engineering. Atlanta, GA, March 2017.
- R. Morrison. Towards reliable predictions: Bridging the gap between physics-based and data-driven models, CS Department Seminar, CU Boulder, Boulder, CO, April 2017.
- R. Morrison. Beyond normality: Learning sparse probabilistic graphical models in the non-Gaussian setting, Star-Talks Seminar, Institute for Computational Mathematics and Engineering (ICME), Stanford, Palo Alto, CA, May 2017.

- R. Morrison. Beyond normality: Learning sparse probabilistic graphical models in the non-Gaussian setting, Workshop on Computational Uncertainty Quantification, Banff International Research Station, Banff, Canada, October 2017.
- K. Willcox. Multifidelity Monte Carlo Methods for Uncertainty Quantification. In SIAM Computational Science and Engineering 2017, Atlanta, USA, February 2017.
- K. Willcox. Data to Decisions: Multifidelity and Surrogate Modeling for Next-Generation Engineering Systems. IAM-PIMS Distinguished Colloquium Series, University of British Columbia, March 2017.
- K. Willcox. Data to Decisions via Multifidelity Modeling and Adaptive Reduced Models. Semi-plenary lecture, 19th International Conference on Finite Elements in Flow Problems, Rome, Italy, April 2017.
- K. Willcox. Data to Decisions via Adaptive Reduced Models and Multifidelity Uncertainty Quantification. Keynote talk, British Applied Mathematics Colloquium, University of Surrey, April 2017.
- K. Willcox. Data to Decisions via Adaptive Reduced Models and Multifidelity Uncertainty Quantification. University of Southampton, April 2017.
- K. Willcox. Multifidelity and Surrogate Modeling for Next-Generation Engineering Systems. 2017 MICDE Symposium, Michigan Institute for Computational Discovery & Engineering, April 2017.
- K. Willcox. Data to Decisions via Adaptive Reduced Models and Multifidelity Uncertainty Quantification. CMDA Distinguished Lecture Series, Virginia Tech, April 2017.
- K. Willcox. Data to Decisions: Multifidelity and Surrogate Modeling for Next-Generation Engineering Systems. Dr. Joseph E. Flaherty Lecture Series, Rensselaer Polytechnic Institute, May 2017.
- K. Willcox. Data to Decisions via Adaptive Reduced Models and Multifidelity Uncertainty Quantification. Center for Applied Mathematics Colloquium, Cornell University, May 2017.
- K. Willcox. Data to Decisions via Adaptive Reduced Models and Multifidelity Modeling. In MATRIX Workshop on Inverse Problems, Melbourne, Australia, June 2017.
- K. Willcox. Data-Driven Operator Inference for Non-Intrusive Projection-based Model Reduction Workshop on Mathematical Foundations of Data Assimilation and Inverse Problems, Foundations of Computational Mathematics, Barcelona, Spain, July 2017.
- K. Willcox. Data to Decisions: Multifidelity and Surrogate Modeling for Next-Generation Engineering Systems. Aerospace Engineering Seminar, University of Michigan, September 2017.
- K. Willcox. Managing Multiple Information Sources of Multi-Physics Systems, AvTechSymposium Dayton, OH, October 2017.
- K. Willcox. Computational Methods for the Next Generation of Aerospace Systems. GALCIT Colloquium, Caltech, October 2017.

- K. Willcox. Multi-fidelity Methods for Design, Optimization and Uncertainty Quantification, Embraer MDO Community of Practice, November 2017.
- A. Chaudhuri. Multifidelity Uncertainty Propagation in Coupled Multidisciplinary Systems. SIAM Computational Science and Engineering 2017, Atlanta, GA, Feb 27- Mar 3, 2017.
- Peherstorfer, B. Multifidelity methods for rare event simulation. In European Numerical Mathematics and Advanced Applications (ENUMATH), Bergen, Norway, 2017.
- Peherstorfer, B. Online adaptive discrete empirical interpolation for nonlinear model reduction. In European Numerical Mathematics and Advanced Applications (ENUMATH), Bergen, Norway, 2017.
- Peherstorfer, B. Multifidelity methods for uncertainty propagation and rare event simulation. In QUIET 2017 - Quantification of Uncertainty: Improving Efficiency and Technology SISSA, Trieste, Italy, 2017.
- Peherstorfer, B. Multifidelity Monte Carlo Methods for Rare Event Simulation. In MATRIX Workshop on Inverse Problems, Melbourne, Australia, 2017.
- Peherstorfer, B. Multifidelity Methods for Uncertainty Propagation and Rare Event Simulation. In Workshop on Data-Driven Modeling and Uncertainty Quantification (UQPM), Austin, USA, 2017.
- Peherstorfer, B. Multifidelity Monte Carlo Methods with Optimally-Adapted Surrogate Models. In SIAM Computational Science and Engineering 2017, Atlanta, USA, 2017.
- Peherstorfer, B. Optimal sampling in multifidelity Monte Carlo estimation for efficient uncertainty propagation. In SILO Seminar Wisconsin Institute for Discovery, Madison, USA, 2017.
- W.D. Thomison, and D. Allaire. A Model Reification Approach to Fusing Information from Multifidelity Information Sources, SIAM Conference on Computational Science and Engineering, Atlanta, GA 2017.
- S. Friedman, and D. Allaire. Quantifying the Impact of Different Model Discrepancy Formulations in Coupled Multidisciplinary Systems, AIAA SciTech Forum, Grapevine, TX 2017.
- D. Allaire, W.D. Thomison, and S.F. Ghoreishi. A Model Reification Approach to Fusing Information from Multifidelity Information Sources, Texas A&M University Data Driven Design of Energy Materials (D3EM) Seminar Series, College Station, TX 2017.
- Song, P., Wang, X.Q., Matney, A.K., Murthy, R., and Mignolet, M.P., Modeling and Identification of Multi-Physics Uncertainties in the Response of Heated Structures, *Presented at the SIAM Conference on Computational Science and Engineering (CSE17)*, Atlanta, GA, Feb. 27-Mar. 3, 2017.
- Martins, J. R. R. A. The Promise and Challenges of MDO for the Next Generation of Aircraft. Workshop on MDO for Industrial Applications in Aeronautics, Braunschweig, Germany, Oct 2017. (Keynote presentation)
- Martins, J. R. R. A. Aircraft Design via Numerical Optimization Are We There Yet?. EU-ROGEN Conference, Madrid, Spain, Sep 2017. (Keynote presentation)

- Martins, J. R. R. A. Aircraft Design via Numerical Optimization: A Multidisciplinary Approach. MOPTA Conference, Bethlehem, PA, Aug 2017. (Plenary presentation)
- Bartoli, N., Lefebvre, T., Bons, N., Martins, J. R. R. A. and Morlier, J. An adaptive optimization strategy based on mixture of experts for wing aerodynamic design optimization. 18th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Denver, CO, June 2017.
- P. Frazier. Bayesian Optimization in the Tech Sector and Beyond. IBM Research Accelerated Discovery Forum Distinguished Speaker Series, Accelerated Discovery Lab, IBM Research Almaden, San Jose CA, January 2017.
- P. Frazier. Bayesian Optimization with Gradients. SIAM Computational Science and Engineering Conference, Atlanta GA, March 2017.
- P. Frazier. Bayesian Optimization with Gradients. Applied Probability Society Conference, Evanston IL, July 2017.
- P. Frazier. Using Simulation to Improve Statistical Power in Switchback Experiments at Uber. Applied Probability Society Conference, Evanston IL, July 2017.
- P. Frazier, A.G. Wilson. Bayesian Optimization with Gradients. Cornell AI Seminar, Ithaca NY, November 2017.
- P. Frazier. An Introduction to Exploration vs. Exploitation: Reinforcement Learning, Multi-Armed Bandits, and Active Learning. American Express, New York NY, September 2017.
- P. Frazier, A.G. Wilson. Bayesian Optimization with Gradients. Neural Information Processing Systems (NIPS) Conference, Los Angeles CA, December 2017.
- P. Frazier. Knowledge-Gradient Methods for Bayesian Optimization. NIPS Workshop on Bayesian Optimization (BayesOpt 2017), Los Angeles CA, December 2017.
- P. Frazier. Simulation and Direct Experimentation in the Tech Sector. 2018 INFORMS Simulation Society Workshop, Durham UK, July 2017.
- M. Poloczek. Multi-Information Source Optimization. NIPS, Long Beach, USA.
- M. Poloczek. New methods for Bayesian optimization of expensive functions. University of Arizona, Tucson, USA.
- M. Poloczek. Bayesian Optimization with Gradients. INFORMS Annual Meeting, Houston, USA.
- M. Poloczek. New methods for Bayesian optimization of expensive functions. University of Arizona, Tucson, USA.
- M. Poloczek. Bayesian Optimization with Gradients. INFORMS Annual Meeting, Houston, USA.
- M. Poloczek. Multi Information Source Optimization. The University of Warwick, Coventry, United Kingdom.

- M. Poloczek. Multi Information Source Optimization. Johannes Gutenberg Universität Mainz, Mainz, Germany.
- M. Poloczek. Scalable Algorithms for Classic and Emerging Problems. Queen Mary University, London, United Kingdom.
- M. Poloczek. Scalable Algorithms for Classic and Emerging Problems. University of Hamburg, Hamburg, Germany.
- M. Poloczek. Multi Information Source Optimization. University of Arizona, Tucson, USA.
- M. Poloczek. Multi Information Source Optimization and Warm Starts. INFORMS Computing Society Conference, Austin, USA.
- J. Wu. Reducing Cost of Bayesian Optimization for Expensive to Evaluate Functions. SIAM Computational Science and Engineering Conference, Atlanta GA, March 2017.
- J. Wu. The Parallel Knowledge Gradient Method for Batch Bayesian Optimization. SIAM Computational Science and Engineering Conference, Atlanta GA, March 2017.

2016

- K. Willcox. Data to decisions in aerospace systems: Reduced-order modeling and multi-fidelity methods. Presentation to Airbus Group, October 2016.
- K. Willcox. Multifidelity and Surrogate Modeling for Data to Decisions in Engineering Systems. Applied Mathematics Seminar Series, University of Auckland, May 2016.
- K. Willcox. Multifidelity Methods for Design and Uncertainty Quantification. Plenary talk, ANZIAM Conference, Canberra, Australia, February 2016.
- Y. Marzouk. Focused Bayesian optimal experimental design. International Conference on Design of Experiments.(Invited lecture.) Memphis, TN, May 2016.
- Y. Marzouk. Optimal Bayesian experimental design: formulations and computational strategies. Los Alamos National Laboratory, workshop on “Data science and optimal learning for materials discovery and design.” (Invited lecture.) Los Alamos, NM, May 2016.
- Y. Marzouk. Sequential nonlinear Bayesian optimal experimental design via approximate dynamic programming. 2016 Joint Statistical Meetings (invited session). Chicago, IL, July 2016.
- Y. Marzouk. Optimal Bayesian experimental design: some advances and reflections. University of Texas-Austin. August 2016.
- A. Chaudhuri. Multifidelity Uncertainty Propagation in Coupled Multidisciplinary Systems, 18th AIAA Non-deterministic Approaches Conference (AIAA Scitech), San Diego, CA, January 2016.
- A. Chaudhuri. Uncertainty Propagation in Coupled Multi-Physics Systems. In Workshop on Data to Decisions in Aerospace Engineering, Auckland, New Zealand, 2016.
- A. Chaudhuri. Stochastic optimization and machine learning: cross-validation for cross-entropy method, Optimizing the Optimizers Workshop at Neural Information Processing Systems (NIPS), Barcelona, Spain, December 2016.

- Peherstorfer, B. Optimal sampling in multifidelity Monte Carlo estimation for efficient uncertainty propagation. In Applied and Computational Mathematics Seminar Department of Mathematics, University of Wisconsin-Madison, Madison, USA, 2016.
- Peherstorfer, B. Safe and Efficient Data-Driven Model Reduction for Critical Engineering Applications. In Next Generation Mobility Modeling and Simulation, Novi, USA, 2016.
- Peherstorfer, B. Multifidelity Methods for Uncertainty Quantification. In Workshop on Data to Decisions in Aerospace Engineering, Auckland, New Zealand, 2016.
- Peherstorfer, B. Multifidelity Methods for Uncertainty Quantification. In SIAM Uncertainty Quantification 2016, Lausanne, Switzerland, 2016.
- Peherstorfer, B. Multifidelity Monte Carlo estimation with multiple surrogate models. In Copper Mountain conference on iterative methods, Copper Mountain, USA, 2016.
- D. Allaire. A Compressed Sensing Approach to Uncertainty Quantification for Approximately Additive Functions, ASME 2016 Computers and Information in Engineering Conference, Charlotte, NC, August 2016.
- D. Allaire. Compositional Uncertainty Quantification for Coupled Multi-Physics Systems, SIAM Conference on Uncertainty Quantification, Lausanne, Switzerland, April 2016.
- D. Allaire. Offline/Online Data-Driven Approaches to Engineering Analysis, National University of Singapore, Department of Mechanical Engineering Seminar Series, Singapore, May 2016.
- S.F. Ghoreishi. Compositional Uncertainty Analysis via Importance Weighted Gibbs Sampling for Coupled Multidisciplinary Systems, AIAA SciTech Forum, San Diego, CA, January 2016.
- Song, P., Matney, A., Murthy, R., Wang, X.Q., and Mignolet, M.P., Probabilistic Modeling of Thermal Properties of Hot Structures and its Propagation to the Nonlinear Geometric Structural Response, *Presented at the Probabilistic Mechanics and Reliability Conference PMC 2016*, Nashville, Tennessee, May 23-25, 2016.
- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp Departmental Seminar, Sauder School of Business, University of British Columbia, Vancouver BC, January 2016.
- P. Frazier. Incentivizing Exploration Departmental Seminar, Operations Research Center, MIT, Boston MA, February 2016.
- P. Frazier. Stochastic Optimization in the Tech Sector: Yelp and Uber Plenary Talk, INFORMS Optimization Society Conference 2016, Princeton University, March 2016.
- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp Departmental Seminar, Department of Industrial Engineering and Operations Research, University of California, Berkeley CA, March 2016.
- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp IEOR-DRO Seminar, Department Industrial Engineering and Operations Research and the Decision Risk and Operations Division of the Columbia Business School, Columbia University, New York NY, April 2016.

- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp Departmental Seminar, Department of Mathematics, Portland State University, Portland OR, April 2016.
- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp Departmental Seminar, Department of Industrial Engineering and Management Sciences, Northwestern University, Evanston IL, May 2016.
- P. Frazier. Coding for Researchers Department of Industrial Engineering and Management Sciences, Northwestern University, Evanston IL, May 2016.
- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp Departmental Seminar, Booth School of Business, University of Chicago, Chicago IL, May 2016.
- P. Frazier. A Unified Mathematical and Algorithmic Framework for Managing Multiple Information Sources of Multi-Physics Systems, AFOSR Computational Math Program Review, Arlington VA, August, 2016.
- P. Frazier. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp Plenary Talk, The 12th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing, Stanford University, Palo Alto CA, August 2016.
- P. Frazier. Using Simulation To Improve Statistical Power In Switchback Experiments At Uber INFORMS Annual Meeting, Nashville TN, November 2016.
- S. N. Pallone. Bayes-optimal Entropy Minimization For Active Learning In Conjoint Analysis. INFORMS Annual Meeting, Nashville TN, November 2016.
- M. Poloczek. Bayesian Optimization of Expensive Functions with Multiple Information Sources and Warm Starts. Goethe University, Frankfurt am Main, Germany.
- M. Poloczek. Bayesian Optimization with Multiple Information Sources and Warm Starts. Massachusetts Institute of Technology, Cambridge, USA.
- M. Poloczek. Multi-Information Source Optimization and Warm Starting Bayesian Optimization. Modeling and Optimization: Theory and Applications, Bethlehem, USA.
- M. Poloczek. Multi-Information Source Optimization with General Model Discrepancies. European Conference on Operational Research, Poznań, Poland.
- M. Poloczek. Multi-Information Source Optimization with General Model Discrepancies. INFORMS International Meeting 2016, Hawaii, USA.
- M. Poloczek. Multi-information Source Optimization With Applications. INFORMS Annual Meeting, Nashville TN, November 2016.
- S. Toscano-Palmerin. Learning In Multi-stage Rollouts. INFORMS Annual Meeting, Nashville TN, November 2016.
- J. Wang. Multifidelity Optimization Exploiting Correlation Across Information Sources. INFORMS Optimization Society Conference 2016, March, 2016.

- J. Wang. Multi-Information Source Optimization with General Model Discrepancies. SIAM UQ 2016, April 2016.
- J. Wu. Parallel Knowledge Gradient For Global Optimization Of Expensive Functions. INFORMS Annual Meeting, Nashville TN, November 2016.
- J. Wu. The Parallel Knowledge Gradient Method For Batch Bayesian Optimization. NIPS 2016, Barcelona Spain, December 2016.

2015

- Willcox, K. Multifidelity and Adaptive Optimization Methods. Phoenix Integration User Conference, Los Angeles, CA, April 2015.
- Willcox, K. Data-driven model reduction to support decision under uncertainty. Keynote talk, 3rd International Workshop on Reduced Basis, POD and PGD Model Reduction Techniques, Cachan, France, November 2015.
- Willcox, K. Reducing, Learning, and Adapting Models: Data-Driven Model Reduction. ESD Distinguished Speaker Seminar Series, Singapore University of Technology and Design, October 2015.
- Willcox, K. Multifidelity Methods for Design, Optimization, and Uncertainty Quantification. Keynote talk, EUROGEN 2015: 11th International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications to Industrial and Societal Problems, Glasgow, United Kingdom, September 2015.
- Willcox, K. Data-driven model reduction to support decision under uncertainty. Keynote talk, 26th Biennial Numerical Analysis Conference, Glasgow, United Kingdom, June 2015.
- Willcox, K. Multifidelity modeling: Exploiting structure in high-dimensional problems. Boeing Distinguished Lecture Series, University of Washington, Seattle, WA, June 2015.
- Willcox, K. Reducing, Learning, and Adapting Models: Data-Driven Model Reduction. Santa Fe Institute, March 2015.
- Willcox, K. Data-Driven Model Reduction to Support Decision Making in Complex Systems. Invited minisymposium talk, SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 2015.
- Marzouk, Y. Harvard University, Department of Statistics Colloquium. Cambridge, MA. November 2015.
- Marzouk, Y. Boston University, Department of Mathematics and Statistics, Statistics and Probability seminar. Boston, MA. November 2015.
- Marzouk, Y. Institut Henri Poincaré. Paris, France. November 2015.
- Marzouk, Y. University of Maryland, Department of Computer Science, Numerical Analysis seminar. College Park, MD. October 2015.
- Marzouk, Y. Centro de Investigación en Matemáticas (CIMAT). Probability and Statistics colloquium. Guanajuato, Mexico. October 2015.

- Marzouk, Y. Virginia Tech, Department of Mathematics colloquium. Blacksburg, VA. September 2015.
- Marzouk, Y. Workshop on Big Data and Predictive Computational Modeling, TU-Munich. (Invited plenary.) Munich, Germany, May 2015.
- Marzouk, Y. University of California at Santa Barbara. Center for Control, Dynamical Systems, and Computation. Santa Barbara, CA. March 2015.
- Marzouk, Y. King Abdullah University of Science and Technology (KAUST). Applied Mathematics and Computational Science. Thuwal, Saudi Arabia. January 2015.
- Allaire, D. An Offline/Online Compositional Approach to Uncertainty Quantification for Coupled Multidisciplinary Systems. Invited numerical analysis seminar, Texas A&M University Mathematics Department, College Station, TX, October 2015.
- Allaire, D. Robustness, Prevention, and Resilience: Design Under Uncertainty for Complex Engineered Systems, Complex Systems Digital Campus, October 2015.
- Allaire, D. A Scalable Compositional Approach to Uncertainty Quantification for the Optimization Under Uncertainty of Multi-Physics Systems. Invited mini symposium talk, SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 2015.
- Mignolet, M.P., Modèles Réduits Couplés Thermique-Structure Nonlinéaire: Analyse Déterministe et Considération d'Incertitudes, Université Paris-Est Marne-la-Vallée, October 2015.
- Martins, J. R. R. A. High-Fidelity Multidisciplinary Design Optimization for the Next Generation of Aircraft, Congress on Numerical Methods in Engineering, Lisbon, Portugal, July 2015.
- Martins, J. R. R. A. A parallel computational framework for the simulation and optimization of coupled systems, Boeing MDAO Meeting, January 2015.
- Toscano-Palmerin, S. Asymptotic Validity of the Bayes-Inspired Indifference Zone Procedure: the Non-Normal Known Variance Case. Conference presentation of accepted paper, Winter Simulation Conference, Huntington Beach, CA, December 2015.
- Cashore J.M. Multi-step Bayesian Optimization For One-dimensional Feasibility Determination Invited conference talk, INFORMS Annual Meeting, Philadelphia, PA, November 2015.
- Frazier, P.I. A Tutorial on Bayesian Optimization. Invited seminar, Quora, Mountain View, CA, November 2015.
- Frazier, P.I. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp. Invited seminar, Optimization Seminar, Department of Operations Research and Financial Engineering, Princeton University, Princeton NJ, November 2015.
- Toscano-Palmerin, S. Asymptotic Validity of the Bayes-inspired Indifference Zone Procedure Invited conference talk, INFORMS Annual Meeting, Philadelphia, PA, November 2015.
- Fei, Y. Optimal Learning for Novel Materials Discovery. Poster, CUNY ASRC Active and Adaptive Materials Symposium, New York, October 2015.

- Frazier, P.I. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp. Invited conference talk, INFORMS Simulation Society Workshop, Purdue University, West Lafayette IN, July 2015.
- Frazier, P.I. Bayesian Multiple Target Localization. Conference presentation of accepted paper, International Conference on Machine Learning (ICML), Lille France, July 2015.
- Toscano-Palmerin, S. Derivative-Free Optimization of Expensive Noisy Functions using Stratified Bayesian Optimization Invited conference talk, Modeling and Optimization: Theory and Application (MOPTA), Bethlehem, PA, July 2015.
- Toscano-Palmerin, S. Stratified Bayesian Optimization Invited conference talk, International Symposium on Mathematical Programming, Pittsburgh, PA, July 2015.
- Toscano-Palmerin, S. Stratified Bayesian Optimization Invited conference talk, INFORMS Applied Probability Society Conference, Istanbul Turkey, July 2015.
- Wang, J. Parallel Bayesian Global Optimization, with Application to Metrics Optimization at Yelp Invited conference talk, International Symposium on Mathematical Programming, Pittsburgh, PA, July 2015.
- Toscano-Palmerin, S. Asymptotic Validity of the Bayes-Inspired Indifference Zone Procedure. Invited conference talk, 2015 CORS/INFORMS International Conference, Montreal, June 2015.
- P.I. Frazier, Parallel Bayesian Policies for Multiple Comparisons with a Known Standard Invited conference talk, 2015 CORS/INFORMS International Conference, Montreal, June 2015.
- Frazier, P.I. Cornell ORIE: Engaged with the Private Sector, Cornell Club, New York City, May 2015.
- Frazier, P.I., Thoughts on Informatics in Materials Science, Invited workshop talk, Information-Driven Approach to Materials Discovery and Design, LDRD-DR Review, Los Alamos National Lab, NM, April 2015.
- Frazier, P.I. Optimal Learning for Molecular Discovery. Invited seminar, Sante Fe Institute, Sante Fe NM, April 2015.
- Wang, J. Parallel Bayesian Global Optimization, with Application to Metrics Optimization at Yelp Invited conference talk, SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 2015.
- Frazier, P.I. Bayesian Global Optimization of Expensive Functions: Exploiting Noise with Low-Dimensional Structure Invited conference talk, SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 2015.
- Frazier, P.I. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp. Invited seminar, Google Distinguished Lecture Series, Carnegie Mellon University Machine Learning Department, Pittsburgh PA, February 2015.
- Frazier, P.I. Parallel Bayesian Global Optimization of Expensive Functions, for Metrics Optimization at Yelp. Invited seminar, Operations Research and Industrial Engineering, University of Texas, Austin TX, February 2015.

- Frazier, P.I. Things I've Done and Things I'd Like to Do. Invited seminar, Uber, San Francisco CA, January 2015.
- Frazier, P.I. Optimal Learning for Scientific Discovery Invited conference talk, INFORMS Computing Society Conference, Richmond, VA, January 2015.
- Frazier, P.I. Information Filtering for arXiv.org: Bandits, Exploration vs. Exploitation, and the Cold Start Problem Invited conference talk, INFORMS Computing Society Conference, Richmond, VA, January 2015.
- Session on Optimization via Simulation: Ranking and Selection, and Multiple Comparisons, 2015 CORS/INFORMS International Conference, Montreal, June 2015.
- Session on Adaptive Sampling and Selection in Simulation, Medicine and Machine Learning, INFORMS Annual Meeting, Philadelphia, PA, November 2015.
- Session on Sampling and Learning Methods in Stochastic Optimization, INFORMS Annual Meeting, Philadelphia, PA, November 2015.
- Session on Selection and Uncertainty Quantification in Simulation Optimization, Winter Simulation Conference, Huntington Beach, CA, December 2015.

7 Transitions and exchange

Transitions via software, datasets and testbed problems

- OpenMDAO: MURI methods form the foundations of NASA's OpenMDAO toolset, which is used by many groups around the world (<http://openmdao.org>)
- Webfoil: An online database of airfoil shapes and multi-source data, with capability for rapid design optimization (<http://webfoil.engin.umich.edu>)
- Surrogate Modeling Toolbox (SMT): An open-source Python package now being used by NASA, ONERA, and SupAero (<https://smt.readthedocs.io/en/latest/>)
- OpenAeroStruct: A wing MDO tool and scalable benchmark MDO problem used by many research groups across the world (<https://mdolab.github.io/OpenAeroStruct>)
- MURI PIs authored a highly cited survey paper on multifidelity methods [1].
- MURI multifidelity methods were transitioned to practitioners at Boeing, ExxonMobil, Uber, Facebook, Lawrence Livermore National Laboratory, AFRL, and NASA Goddard.
- Bayesian optimization algorithms, including knowledge gradient for multi-information source optimization and BayesOpt for composite functions, were implemented in Facebook's BoTorch software package.
- Batch multi-information source Bayesian optimization software (github.com/RichardCouperthwaite/BB0-Reification)
- MIT Uncertainty Quantification Library (<http://muq.mit.edu>)
- Transport maps (including graph learning) (<http://transportmaps.mit.edu>)

- Multifidelity Monte Carlo method (<https://github.com/pehersto/mfmc>)
- Multifidelity global sensitivity analysis (mfGSA) package being used by NASA Goddard for UQ of the James Webb space telescope (github.com/elizqian/mfgsa)

Personnel transitions

- Five MURI students/postdocs became tenure-track faculty: Hwang (UCSD), Kramer (UCSD), Morrison (UC Boulder), Peherstorfer (NYU), Poloczek (U Arizona).
- MIT postdoc Sergio Amaral (supervisor Willcox) hired by Millennium Management.
- TAMU student Seyede Fatemeh Ghoreishi (advisor Allaire) hired as a Postdoctoral Associate at the University of Maryland.
- TAMU student Benson Isaac (advisor Allaire) hired by Boeing.
- TAMU student William Dillon Thomison (advisor Allaire) hired by Lockheed Martin Skunk Works.
- Cornell PhD student Jialei Wang (2016, Frazier’s group) hired by IBM.
- Cornell PhD student Stephen Pallone (2017, Frazier’s group) hired by Uber.
- Cornell PhD student Weici Hu (2017, Frazier’s group) hired by Google.
- Cornell PhD student Jian Wu (2017, Frazier’s group) hired by TwoSigma.
- Cornell Postdoc Matthias Poloczek (from Frazier’s group) was hired into a tenure-track position in 2017 in the Department of Systems & Industrial Engineering at University of Arizona.
- Matthias Poloczek then went on leave from the University of Arizona in October 2018 to lead the Bayesian optimization team at Uber AI Labs in San Francisco.
- Cornell PhD student Saul Toscano (2019, Frazier’s group) hired by TwoSigma.

Transitions through workshops, conferences and summer schools

- The MURI team played a leadership role in the organization and delivery of the AIAA Workshop on Multifidelity Modeling in Support of Design and Uncertainty Quantification. The workshop was held in conjunction with the AIAA Aviation conference in June 2019. The workshop had 39 attendees, mostly from government and industry. The workshop objectives were: (1) Dissemination of recent methods developments to the MDO practitioner community. (2) Discussion of challenges and opportunities to identify new collaborations and new research directions. Former MURI researcher Matthias Poloczek gave a tutorial on surrogate modeling and machine learning. MURI co-PI Benjamin Peherstorfer gave a tutorial multifidelity uncertainty quantification.
- Y. Marzouk was a lecturer at the 2019 Computational Physics School for Fusion Research (summer school), MIT PSFC, 26–31 August 2019, Cambridge, MA.
- Y. Marzouk was a lecturer at the MASCOT-NUM Research School on Uncertainty in Scientific Computing (summer school), 23–27 September 2019, Fréjus, France.

Transitions through collaborations and personnel exchange

- J. Martins: MAUD/OpenMDAO transitioned to AFRL.
- J. Martins: OpenAeroStruct low-fidelity aerostructural optimization code and wing design test problem transitioned to AFRL, SFI, MIT, and TAMU.
- J. Martins: X-56A data exchange with AFRL (ultimately not enough data)
- Transfer of structural-thermal reduced order modeling testbed problem from ASU to MIT, August 2015.
- Collaboration with Prof. Christian Soize (Université Paris-Est Marne-la-Vallée). Regular visits of U-PEM by Marc Mignolet and visit of ASU by Christian Soize through the period 2015-2020 to work on the Compressed Principal Component Analysis (CPCA) modeling approach.
- Collaboration with Prof. Yabin Liao (Penn State Erie) on the application of the MaxEnt uncertainty modeling at the elemental level for structural-thermal problems [43, 44] to structures with piezoelectric elements.
- Y. Marzouk visited B. Peherstorfer at University of Wisconsin-Madison to give a seminar presentation at the Wisconsin Institute for Discovery and to work on a collaboration that resulted in a submitted journal manuscript (2018).
- Y. Marzouk visited the Michigan Institute for Computational Discovery and Engineering at the University of Michigan, delivered a seminar there, and interacted with J. Martins and his group during the visit (2018).
- P. Frazier: Exchange of technical expertise and data with Yelp. (2016)
- P. Frazier visited American Express in September 2017, gave a tutorial on Bayesian optimization, reinforcement learning, and active learning methods, and gave advice on applying these methods within their business.
- TwoSigma (<https://www.twosigma.com>) is using Cornell-MOE (<https://github.com/wujian16/Cornell-MOE/tree/master/examples>), which is an open-source Bayesian optimization codebase developed at Cornell. Cornell-MOE is based on MOE, an open source codebase developed at Yelp by Frazier's former PhD students Scott Clark and Jialei Wang using AFOSR-supported research from their dissertations. Cornell-MOE adds algorithms to MOE that were developed with support from this MURI. TwoSigma hired three of Frazier's students (Jian Wu, Saul Toscano, and Bangrui Chen), and Frazier visited to give a tutorial talk in 2019.
- ExxonMobil has been extremely interested in the work that the MURI has been doing. Damian Burch, a research scientist there, hired one of Frazier's PhD students as an intern, Raul Astudillo Marban, and has been discussing additional collaborations based around the ideas in the MURI.
- P. Frazier is engaged with SigOpt, a Bayesian Optimization startup company founded by Frazier's former PhD student Scott Clark. Frazier has visited their offices in San Francisco a number of times during the grant period, is in regular contact through email, and researchers at the company have read a number of the publications resulting from this MURI.

- Facebook implemented a number of the Frazier group's Bayesian optimization methods, including our multi-information source optimization method, into their publicly available Bayesian optimization code, BoTorch.
- P. Frazier has an ongoing relationship with Uber and has discussed research on Bayesian optimization developed as a part of this MURI with a number of personnel inside the company. Frazier works with Uber as a Staff Data Scientist while taking a partial leave from teaching at Cornell.
- K. Willcox: Visited Boeing May 2016, ongoing discussions about multidisciplinary design tool needs.
- K. Willcox and Youssef Marzouk: Briefed Airbus engineering leadership team on MURI research, October 2016.
- K. Willcox attended AVTech Symposium in Dayton in October 2017. She presented MURI work and had multiple discussions with AFRL and industry attendees.
- K. Willcox presented MURI work to the Embraer MDO Community of Practice in November 2017.
- K. Willcox has ongoing discussions with Lockheed Martin Aeronautics about transition of the multifidelity and reduced order modeling methods to their conceptual design flows. This resulted in a funded research project that started Fall 2020.
- Y. Marzouk gave an invited seminar to ANSYS in December 2016.
- MIT student R. Baptista visited NASA Glenn Research Center in April 2017.
- MIT research scientist A. Chaudhuri visited J. R. R. A. Martins group at University of Michigan in October 2017 to work on a collaboration that resulted in a conference paper.
- MIT research scientist A. Chaudhuri visited NASA Goddard Space Flight Center, Greenbelt, Maryland in 2019 and gave a seminar on multifidelity methods.
- MIT research scientist A. Chaudhuri is collaborating with Oak Ridge National Laboratory on Bayesian optimization methods and stability boundary identification through active learning methods for advanced manufacturing.
- MIT postdoc L. Cook visited AFRL at Wright-Patterson to present work on multifidelity methods and exchange ideas for future work.
- MIT postdoc L. Cook visited the Centre for Turbulence Research at Stanford University to discuss methods for design under turbulence-based uncertainty, and has been collaborating since.
- K. Willcox, P. Frazier, Y. Marzouk, D. Allaire, and students and postdocs from Cornell and MIT met while attending the SIAM Conference on Computational Science and Engineering in Salt Lake City, March 2015.
- P. Frazier visited SFI, April 2015.
- P. Frazier, students and postdoc collaborated with Christina Harsch (AFRL) involving periodic conference calls and email exchanges.

- Benjamin Smarslok and Diane Villanueva (AFRL) visited Youssef Marzouk and students/postdocs at MIT, September 2015.

Other

- MURI PIs authored a highly cited survey paper on multifidelity methods [1].
- Frazier leveraged research in efficient resource allocation to play significant role in Cornell’s fall reopening; designed the targeted asymptomatic COVID-19 screening strategy that is a key part of the reopening.
- K. Willcox was elected Fellow of SIAM (2018).
- K. Willcox was elected Fellow of AIAA (2019).
- J. Martins was elected Fellow of AIAA (2020).
- M. Mignolet received the European Association of Structural Dynamics (EASD) Senior Research Prize in the area of Computational Structural Dynamics (2020).
- M. Mignolet was elected Fellow of the ASCE Engineering Mechanics Institute (2019).
- M. Mignolet was elected Fulton Faculty Exemplar, ASU Fulton Schools of Engineering (2017).

8 Supported Personnel

- **MIT:** Postdoctoral Associates: Anirban Chaudhuri, Boris Kramer, Alexandre Marques, Rebecca Morrison, Laurence Cook, Shahab Ilbeigi. Students: Renee Swischuk, Ricardo Santos-Baptista, Chi Feng, Benjamin Zhang.
- **TAMU:** Students: Samuel Friedman, Arjun Singh, Meet Sanghvi, Danial Khatamsaz, Seyede Fatemeh Ghoreishi, William Thomison, Benson Isaac.
- **UMich:** Postdocs: John Hwang, Mohamed A. Bouhlel, Xiaosong Du. Research investigator: Charles A. Mader. Students: John Jasa, Eirikur Jonsson.
- **Cornell:** Postdoctoral Associate: Matthias Poloczec. Students: Tom Fei, Saul Toscano-Palmerin, Jialei Wang, Jian Wu, Yunxiang Zhang, John Massey Cashore, Pu Yang, Raul Astudillo, Aman Jain.
- **ASU:** Research Scientist: X.Q. Wang. Postdoctoral Fellows: Yuting Wang, Raghavendra Murthy. Students: Pengchao Song.
- **NYU:** Postdoctoral Associates: Donsub Rim. Students: Terrence Alsup, Nihar Sawant.

References

- [1] Peherstorfer, B., Willcox, K., and Gunzburger, M., “Survey of multifidelity methods in uncertainty propagation, inference, and optimization,” *Siam Review*, Vol. 60, No. 3, 2018, pp. 550–591.

- [2] Lam, R., Willcox, K., and Wolpert, D. H., “Bayesian Optimization with a Finite Budget: An Approximate Dynamic Programming Approach,” *Advances in Neural Information Processing Systems 29*, edited by D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, Curran Associates, Inc., 2016, pp. 883–891.
- [3] Wu, J. and Frazier, P., “Practical Two-Step Lookahead Bayesian Optimization,” *Advances in Neural Information Processing Systems*, 2019, pp. 9813–9823.
- [4] Cashore, J., Kumarga, L., and Frazier, P., “Multi-Step Bayesian Optimization for One-Dimensional Feasibility Determination,” in revision for *Journal of Machine Learning Research*, arXiv:1607.03195.
- [5] Pallone, S. N., Frazier, P. I., and Henderson, S. G., “Coupled bisection for root ordering,” *Operations Research Letters*, Vol. 44, No. 2, 2016, pp. 165–169.
- [6] Chen, B. and Frazier, P. I., “The Bayesian linear information filtering problem,” *2016 IEEE 28th International Conference on Tools with Artificial Intelligence (ICTAI)*, IEEE, 2016, pp. 270–277.
- [7] Zhao, X., *Exploration vs. Exploitation In The Information Filtering Problem And Its Application In arXiv.org*, Ph.D. thesis, 2015.
- [8] Rajan, P., Han, W., Sznitman, R., Frazier, P., and Jedynak, B., “Bayesian multiple target localization,” *International conference on machine learning*, PMLR, 2015, pp. 1945–1953.
- [9] Han, W., Rajan, P., Frazier, P. I., and Jedynak, B. M., “Probabilistic group testing under sum observations: A parallelizable 2-approximation for entropy loss,” *arXiv preprint arXiv:1407.4446*, 2014.
- [10] Poloczek, M., Wang, J., and Frazier, P., “Multi-Information Source Optimization,” *Advances in Neural Information Processing Systems 30*, Curran Associates, Inc., 2017, pp. 4291–4301.
- [11] Wu, J., Toscano-Palmerin, S., Frazier, P. I., and Wilson, A. G., “Practical multi-fidelity Bayesian optimization for hyperparameter tuning,” *35th Conference on Uncertainty in Artificial Intelligence, UAI 2019*, 2019.
- [12] Astudillo, R. and Frazier, P. I., “Bayesian Optimization of Composite Functions,” *ICML*, 2019.
- [13] Toscano-Palmerin, S. and Frazier, P. I., “Stratified bayesian optimization,” *International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing*, Springer, 2016, pp. 145–166.
- [14] Toscano-Palmerin, S. and Frazier, P. I., “Bayesian optimization with expensive integrands,” *arXiv preprint arXiv:1803.08661*, 2018.
- [15] Wu, J., Poloczek, M., Wilson, A. G., and Frazier, P., “Bayesian optimization with gradients,” *Advances in Neural Information Processing Systems*, 2017, pp. 5267–5278.
- [16] Astudillo, R. and Frazier, P., “Multi-attribute bayesian optimization under utility uncertainty,” *Proceedings of the NIPS Workshop on Bayesian Optimization*, 2017.
- [17] Astudillo, R. and Frazier, P. I., “Bayesian Optimization with Uncertain Preferences over Attributes,” *Proceedings of the 23rd International Conference on Artificial Intelligence and Statistics*, AISTATS, 2020.

- [18] Poloczek, M., Wang, J., and Frazier, P. I., “Warm Starting Bayesian Optimization,” *2016 Winter Simulation Conference*, 2016.
- [19] Wu, J. and Frazier, P., “The Parallel Knowledge Gradient Method for Batch Bayesian Optimization,” *Advances in Neural Information Processing Systems*, 2016.
- [20] Toscano-Palmerin, S. and Frazier, P., “Effort Allocation and Statistical Inference for 1-Dimensional Multistart Stochastic Gradient Descent,” *Proceedings of the 2018 Winter Simulation Conference*, Winter Simulation Conference, 2018.
- [21] Peherstorfer, B., Willcox, K., and Gunzburger, M., “Optimal model management for multifidelity Monte Carlo estimation,” *SIAM Journal on Scientific Computing*, Vol. 38, No. 5, 2016, pp. A3163–A3194.
- [22] Peherstorfer, B., Beran, P., and Willcox, K., “Multifidelity Monte Carlo estimation for large-scale uncertainty propagation,” *2018 AIAA Non-Deterministic Approaches Conference*, AIAA, 2018.
- [23] Peherstorfer, B. and Marzouk, Y., “A transport-based multifidelity preconditioner for Markov chain Monte Carlo,” *Advances in Computational Mathematics*, Vol. 45, 2019, pp. 2321–2348.
- [24] Chaudhuri, A., Marques, A. N., and Willcox, K. E., “mfEGRA: Multifidelity Efficient Global Reliability Analysis for Failure Boundary Location,” *Structural and Multidisciplinary Optimization*, 2021.
- [25] Chaudhuri, A., Jasa, J., Martins, J. R., and Willcox, K. E., “Multifidelity optimization under uncertainty for a tailless aircraft,” *2018 AIAA Non-Deterministic Approaches Conference*, 2018, p. 1658.
- [26] Jasa, J. P., Hwang, J. T., and Martins, J. R., “Open-source coupled aerostructural optimization using Python,” *Structural and Multidisciplinary Optimization*, Vol. 57, No. 4, 2018, pp. 1815–1827.
- [27] Chaudhuri, A., Kramer, B., and Willcox, K. E., “Information Reuse for Importance Sampling in Reliability-Based Design Optimization,” *Reliability Engineering & System Safety*, Vol. 201, 2020, pp. 106853.
- [28] Yu, Y., Sisco, J. C., Rosen, S., Madhav, A., and Anderson, W. E., “Spontaneous longitudinal combustion instability in a continuously-variable resonance combustor,” *Journal of Propulsion and Power*, Vol. 28, No. 5, 2012, pp. 876–887.
- [29] Chaudhuri, A., Kramer, B., Norton, M., Royset, J. O., and Willcox, K., “Certifiable Risk-Based Engineering Design Optimization,” *arXiv preprint arXiv:2101.05129*.
- [30] Lam, R. R., Zahm, O., Marzouk, Y. M., and Willcox, K. E., “Multifidelity dimension reduction via active subspaces,” *SIAM Journal on Scientific Computing*, Vol. 42, No. 2, 2020, pp. A929–A956.
- [31] Soize, C., “A nonparametric model of random uncertainties for reduced matrix models in structural dynamics,” *Probabilistic Engineering Mechanics*, Vol. 15, 2000, pp. 27–294.
- [32] Durand, J.-F., Soize, C., and Gagliardini, L., “Structural-acoustic modeling of automotive vehicles in presence of uncertainties and experimental identification and validation,” *Journal of the Acoustical Society of America*, Vol. 124, 2008, pp. 1513–1525.

- [33] Mignolet, M. P. and Soize, C., “Stochastic reduced order models for uncertain geometrically nonlinear dynamical systems,” *Computer Methods in Applied Mechanics and Engineering*, Vol. 197, 2008, pp. 3951–3963.
- [34] Richter, L. and Mignolet, M. P., “Stochastic modeling of uncertain mass characteristics in rigid body dynamics,” *Mechanical Systems and Signal Processing*, Vol. 87, 2017, pp. 43–53.
- [35] Murthy, R., Mignolet, M. P., and El-Shafei, A., “Nonparametric stochastic modeling of structural uncertainty in rotordynamic systems: part I - formulation,” *Journal of Engineering for Gas Turbines and Power*, Vol. 132, 2010.
- [36] Murthy, R., Tomei, J., Wang, X. Q., Mignolet, M. P., and El-Shafei, A., “Nonparametric stochastic modeling of structural uncertainty in rotordynamics: unbalance and balancing aspects,” *Journal of Engineering for Gas Turbines and Power*, Vol. 197, 2008, pp. 3951–3963.
- [37] Soize, C., *Stochastic Models of Uncertainties in Computational Mechanics*, American Society of Civil Engineers (ASCE), 2012.
- [38] Soize, C., *Uncertainty Quantification: An Accelerated Course in Advanced Applications in Computational Engineering*, Springer, 2017.
- [39] Song, P. and Mignolet, M. P., “Reduced order model-based uncertainty modeling of structures with localized response,” *Probabilistic Engineering Mechanics*, Vol. 51, 2018, pp. 42–55.
- [40] Perez, R., Wang, X. Q., and Mignolet, M. P., “Nonlinear reduced order models for thermoelastodynamic response of isotropic and FGM panels,” *AIAA Journal*, Vol. 49, 2011, pp. 630–641.
- [41] Song, P., Wang, X. Q., Murthy, R., Matney, A. K., and Mignolet, M. P., “Nonlinear geometric thermoelastic response of structures with uncertain thermal and structural properties,” *AIAA Journal*, Vol. 58, 2020, pp. 3639–3652.
- [42] Song, P. and Mignolet, M. P., “Maximum entropy-based uncertainty modeling at the elemental level in linear structural and thermal problems,” *Computational Mechanics*, Vol. 64, 2019, pp. 1557–1566.
- [43] Song, P., Wang, X. Q., and Mignolet, M. P., “Maximum entropy uncertainty modeling at the finite element level for heated structures,” *Mechanical Systems and Signal Processing*, Vol. Submitted.
- [44] Song, P., Wang, X. Q., and Mignolet, M. P., “Maximum entropy structural-thermal uncertainty modeling at the finite element level,” *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2019)*, Vol. San Diego, California, Jan.7-11, 2019, pp. AIAA Paper AIAA–2019–0443.
- [45] Wang, X. Q., Liao, Y., and Mignolet, M. P., “Uncertainty analysis of piezoelectric vibration energy harvesters using a finite element level-based maximum entropy approach,” *ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems Part B: Mechanical Engineering*, Vol. 7, 2021, pp. 010906.
- [46] Mignolet, M. P. and Soize, C., “Compressed principal component analysis of non-gaussian vectors,” *SIAM/ASA Journal on Uncertainty Quantification*, Vol. To appear, 2021.

- [47] Song, P., Wang, X. Q., and Mignolet, M. P., “Nonlinear reduced ROMs: formulation and applications,” *Proceedings of the AIAA Science and Technology Forum and Exposition (SciTech2019)*, Vol. San Diego, California, Jan.7-11, 2019, pp. AIAA Paper AIAA–2019–1020.
- [48] Ng, L. W. and Willcox, K. E., “Multifidelity approaches for optimization under uncertainty,” *International Journal for Numerical Methods in Engineering*, Vol. 100, 2014, pp. 746–772.
- [49] Song, P., Wang, X. Q., and Mignolet, M. P., “Applications of multifidelity reduced order modeling to single and multiphysics nonlinear structural problems,” *Applications in Engineering Science*, Vol. 5, 2021, pp. 100035.
- [50] Peherstorfer, B., Kramer, B., and Willcox, K., “Combining multiple surrogate models to accelerate failure probability estimation with expensive high-fidelity models,” *Journal of Computational Physics*, Vol. 341, 2017, pp. 61–75.
- [51] Peherstorfer, B., “Multifidelity Monte Carlo estimation with adaptive low-fidelity models,” *SIAM/ASA Journal on Uncertainty Quantification*, Vol. 7, 2019, pp. 579–603.
- [52] Peherstorfer, B. and Willcox, K., “Dynamic data-driven model reduction: Adapting reduced models from incomplete data,” *Advanced Modeling and Simulation in Engineering Sciences*, Vol. 3, No. 11, 2016.
- [53] Chaudhuri, A., Lam, R., and Willcox, K., “Multifidelity uncertainty propagation via adaptive surrogates in coupled multidisciplinary systems,” *AIAA Journal*, Vol. 56, No. 1, 2018, pp. 235–249.
- [54] Baptista, R., Marzouk, Y., Willcox, K., and Peherstorfer, B., “Optimal approximations of coupling in multidisciplinary models,” *AIAA journal*, Vol. 56, No. 6, 2018, pp. 2412–2428.
- [55] Marques, A. N., Opgenoord, M. M., Lam, R. R., Chaudhuri, A., and Willcox, K. E., “Multifidelity method for locating aeroelastic flutter boundaries,” *AIAA Journal*, Vol. 58, No. 4, 2020, pp. 1772–1784.
- [56] Marques, A., Lam, R., and Willcox, K., “Contour location via entropy reduction leveraging multiple information sources,” *Advances in Neural Information Processing Systems 31*, edited by S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, Curran Associates, Inc., 2018, pp. 5222–5232.